Substance Name: Medium-chain chlorinated paraffins (MCCP)[1]

EC Number: -

CAS Number: -

MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR IDENTIFICATION OF

MEDIUM-CHAIN CHLORINATED PARAFFINS (MCCP)[1] AS SUBSTANCES OF VERY HIGH CONCERN BECAUSE OF THEIR PBT[2] (ARTICLE 57D), vPvB[3] (ARTICLE 57E) PROPERTIES

Adopted on 15 June 2021

[1] Medium-chain chlorinated paraffins [UVCB substances consisting of more than or equal to 80% linear chloroalkanes with carbon chain lengths within the range from C_{14} to C_{17}]
[2] PBT means persistent, bioaccumulative and toxic
[3] vPvB means very persistent and very bioaccumulative

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DEFINITIONS

It is important to note that in this report the terminology ‘congener’ is used. Individual constituents sharing the same empirical formula are congeners of each other. The wording ‘congeners’ or ‘congener group’ refers to a group of constituents sharing the same empirical formula irrespective of the position of the chlorine substituents on the carbon chain (e.g. the $C_{15}Cl_7$ congener group).

ABBREVIATIONS / ACRONYMS

APCI	Atmospheric-pressure chemical ionisation
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BCF_k	kinetic bioconcentration factor
BCF_{kgL}	Lipid normalised, growth corrected kinetic bioconcentration factor
BMF	Biomagnification factor
BMF_{kgL}	Lipid normalised, growth corrected kinetic biomagnification factor
BOD	Biological oxygen demand
BSAF	Biota-sediment accumulation factor
CP	Chlorinated paraffins
Cl wt.	Chlorine content by weight
CLP	Classification, labelling and packaging
CoRAP	Community rolling action plan
DOC	Dissolved organic carbon
DT_{50}	Time to reach 50% disappearance/dissipation
DT_{90}	Time to reach 90% disappearance/dissipation
dw	Dry weight
EC_{50}	Half maximal effective concentration
ECD	Electron capture detector
ECHA	European Chemicals Agency
ECNI	Electron capture negative ionisation
ED	Endocrine disrupters
EFSA	European Food Safety Agency
eMSCA	Evaluating Member State Competent Authority
EALs	Environmentally adapted lubricants
ESR	Existing Substances Regulation
FID	Flame ionisation detector
GC	Gas chromatography
GCxGC	Two dimensional gas chromatography

GLP	Good laboratory practise
HRMS	High-resolution mass spectrometry
k_1	Uptake rate constant
k_2	Overall depuration rate constant
k_{2g}	Growth corrected depuration rate constant
kM	Rate constant for metabolism
Kaw	Air-water partition coefficient
Koa	Octanol-air partition coefficient
Koc	Organic carbon-water partition coefficient
Kow or P	Octanol-water partition coefficient
LCCP	Long-chain chlorinated paraffins
LOD	Limit of detection
LOQ	Limit of quantification
LRMS	Low-resolution mass spectrometry
LRTP	Long-range transport potential
LSC	Liquid scintillation counting
lw	Lipid weight
MCCP	Medium-chain chlorinated paraffins
M-factors	Multiplication factors
MS	Mass spectrometry
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
POPs	Persistent organic pollutants
QSAR	Quantitative structure activity relationships
QToF	Quantitative Time-of-Flight
RCR	Risk characterisation ratio
REACH	Registration, Evaluation and Authorisation of Chemicals
RMOA	Risk management option analysis
SCCP	Short-chain chlorinated paraffins
SD	Standard deviation
SMILES	Simplified Molecular Input Line Entry System

SVHC	Substance of very high concern
TG	Test guideline
ThOD	Theoretical oxygen Demand
TOF	Time-of-flight
TMF	Trophic magnification factor
UVCB	Substances of unknown or variable composition, complex reaction products or biological materials
vPvB	Very Persistent very Bioaccumulative
WoE	Weight-of-evidence
ww	Wet weight

IDENTIFICATION OF SUBSTANCES OF VERY HIGH CONCERN ON THE BASIS OF THE CRITERIA SET OUT IN REACH ARTICLE 57

Substance Name: Medium-chain chlorinated paraffins (MCCP)[4]

EC Number: -

CAS number: -

- The substances are identified as persistent, bioaccumulative and toxic (PBT) according to Article 57 (d) of Regulation (EC) No 1907/2006 (REACH).
- The substances are identified as very persistent and very bioaccumulative (vPvB) according to Article 57 (e) of Regulation (EC) No 1907/2006 (REACH).

Summary of how the substances meet the criteria set out in Article 57 of the REACH Regulation

A weight-of-evidence determination according to the provisions of Annex XIII of REACH is used in order to conclude on the PBT/vPvB properties of MCCP at the level of the investigated congener groups ($C_{14\text{-}17}Cl_{1\text{-}(14\text{-}17)}$). All information (such as the results of standard tests, monitoring and modelling, information from the application of a trend analysis with respect to persistence among the MCCP congener groups of different carbon chain lengths and different levels of chlorination and (Q)SAR results) was considered together in a weight-of-evidence approach. All studies used have been assessed as reliable (with or without restrictions), relevant and adequate for the assessment, unless otherwise stated and specified in this document.

Persistence

The assessment and the conclusions on persistence are based on the following information:

- An OECD TG 308 study performed on C_{14} chlorinated n-alkane, 50% Cl. wt. indicates that the total water-sediment DT_{50} values for the $C_{14}Cl_{3\text{-}14}$ congener groups of MCCP (equivalent to 35.32–72.98% Cl wt.) are greater than 120 days at 12°C (under aerobic conditions). The fact that there was no significant measurable degradation over 120 days suggests that it is unlikely that ≥50% mineralisation or primary degradation would occur over a subsequent 60-day period. Therefore, based on this study, it can be reasonably assumed that the $C_{14}Cl_{3\text{-}14}$ groups of congeners are very persistent in sediment (degradation half-lives >180 days). The outcome of this higher tier study is given a high weight as it provides information directly comparable with the P and vP criteria set out in Annex XIII, points 1.1.1 (d) and 1.2.1 (b) of the REACH Regulation;
- Based on modelling data, almost all of the congener groups of MCCP ($C_{14\text{-}17}$ congener groups with three or more chlorine substituents at the carbon chain) are predicted to be not readily biodegradable and hence potentially persistent. No experimental degradation data for specific C_{15}, C_{16} or C_{17} chloroalkane substances and their congener groups is available while they are expected to be less water soluble and more adsorptive than the C_{14} substances. Based on the predicted and observed trends in physico-chemical properties of structures of the different MCCP congeners, which are in line with the general scientific knowledge on the expected partitioning behaviour and environmental

[4] Medium-chain chlorinated paraffins [UVCB substances consisting of more than or equal to 80% linear chloroalkanes with carbon chain lengths within the range from C_{14} to C_{17}]

fate of hydrophobic aliphatic chloroalkanes, it can be reasonably estimated that the C_{15-17} congeners with the same or higher chlorine contents than the congeners of C_{14} chlorinated n-alkane, 50% Cl. wt. (which contains $C_{14}Cl_{3-14}$ congeners that all are P/vP) will be equally or more adsorptive to sediment, have lower water solubilities and partition stronger to octanol. They therefore will at least be equally if not more persistent in sediments;

- Several ready biodegradation screening studies under conditions of enhanced bioavailability have been performed with commercial MCCP product types. Based on the results of the screening tests, it seems that the overall level of degradation appears to decline with increasing levels of chlorination and that the substances tested contain potentially persistent congeners. However, these screening studies are not considered appropriate for assessing and concluding on the persistence properties of UVCB substances such as MCCP and their constituents, as without further supplementary information enabling the possibility for the dossier submitter to verify the claims made with regard to the composition of the test substance, i.e. the identity of the individual congener groups and their concentration in the substance as well as on the degree of degradation of the individual congener groups in a test, it is not possible to draw conclusions on the persistence of the constituents of MCCP. Therefore the outcomes of the screening tests for MCCP have been assigned low weight in the WoE;
- Hydrolysis of MCCP is expected to be negligible in the environment. Photodegradation in air for MCCP congeners is unlikely to be a significant degradation pathway in the environment (estimated atmospheric half-lives in the range of 0.6–7.1 days for some of the MCCP congener groups). As a conclusion, abiotic degradation of MCCP and MCCP congeners is not considered to be a significant degradation pathway in the environment;
- Monitoring data support findings from experimental and predicted data on biodegradation and abiotic degradation of MCCP congeners and MCCP. The available monitoring data, particularly from sediment core studies, suggest some dechlorination of chlorinated paraffins with high chlorine contents in sediment over time, but they also suggest that degradation in the environment may be slow and provide indirect evidence that MCCP with chlorine contents of ~ 55% by weight can persist in sediments for more than a decade. The detection and/or quantification of MCCP in marine sediments from the Arctic, in locations far away from point sources, point towards persistence of MCCP in marine sediments under aerobic conditions.

As an overall conclusion, based on the above information used in a weight-of-evidence-approach, it is concluded that the $C_{14}Cl_{3–14}$ congener groups of MCCP (equivalent to 35.32–72.98% Cl wt.) meet the ‘persistence’ criterion (P) and the ‘very persistent’ criterion (vP) in accordance with Annex XIII, points 1.1.1 and 1.2.1, of the REACH Regulation on the basis of their persistent and very persistent (P/vP) properties in sediment (degradation half-lives > 180 days).

Based on the predicted and observed trends in physico-chemical properties it further can be reasonably estimated that also the C_{15-17} congener groups of MCCP with the same or higher chlorine contents than the congeners present in C_{14} chlorinated n-alkane, 50% Cl. wt. (which contains $C_{14}Cl_{3-14}$ congener groups that all are P/vP) will at least be equally if not more persistent in sediment than the congeners of C_{14} chlorinated n-alkane, 50% Cl. wt. Consequently, it is concluded that also the $C_{15}Cl_{3-15}$, $C_{16}Cl_{3-16}$ and $C_{17}Cl_{3-17}$ congener groups of MCCP meet the ‘persistence’ (P) and ‘very persistent’ (vP) criteria of REACH Annex XIII (degradation half-life in sediment > 180 days).

Finally, since MCCP always will contain congener groups with P/vP properties at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet both the ‘persistence’ (P) and ‘very persistent’ (vP) criteria of REACH Annex XIII (degradation half-life in sediment > 180 days).

Monitoring data on MCCP support the above conclusions as they point towards persistence of MCCP in sediments.

<u>Bioaccumulation</u>

The assessment and conclusions on bioaccumulation are based on the following information. The results of the studies having been given a high weight in the WoE[5] are considered to provide sufficient evidence to conclude the congener groups present in the MCCP test material used in these studies as B and/or vB. The results of the other experimental studies and the QSAR predictions are used as supplementary supporting information to conclude in the WoE approach applied.

- An OECD TG 305 study (dietary exposure) performed on C_{14} chlorinated n-alkane, 50% Cl. wt. indicates a high bioaccumulation potential with lipid-normalised kinetic fish BCF values > 5000 for $C_{14}Cl_{5-11}$ (based on the less conservative scenario with $k_g=0$, see further information in Table 40). This study is given a high weight and its results are used to conclude that the $C_{14}Cl_{5-11}$ congener groups have B/vB properties;
- An OECD TG 305 study (aqueous exposure) performed on C_{14} chlorinated n-alkane, 45% Cl wt. (which contains $C_{14}Cl_{3-6}$ congener groups) indicates a high bioaccumulation potential with a lipid-normalised and growth-corrected kinetic fish BCF value of ca. 11 530 L/kg. This study is given a high weight and its results are used to conclude that the $C_{14}Cl_{3-6}$ congener groups have B/vB properties;
- An OECD TG 305 study (aqueous exposure) performed on C_{15} chlorinated n-alkane, 51% Cl wt. (which contains $C_{15}Cl_{5-8}$ congener groups) indicates a bioaccumulation potential with a growth-corrected kinetic fish aquatic BCF of around 1 833 – 2 072 L/kg. The growth corrected depuration half-lives are between 28 to 36 days. The results of this study are used as part of the weight-of-evidence to conclude that the $C_{15}Cl_{5-8}$ congener groups have B and/or vB properties;
- Toxicokinetic data on mammals using radiolabelled MCCP indicate that absorption following oral exposure is significant. MCCP have been demonstrated to have relatively long elimination or depuration half-lives in fish and mammals (growth corrected depuration half-lives in the range of 29–80 days in rainbow trout and half-life up to 8 weeks in abdominal fat of rats). These long elimination half-lives mean that significant concentrations of the substance may remain within an organism for several months, possibly years, after cessation of emission. Based on the outcome of dietary accumulation studies equivalent to OECD TG 305, experimental depuration rate constants for MCCP congeners were used in order to predict BCF values based on the work by Brooke and Crookes, which 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 as growth-corrected depuration rate constants between 0.009–0.024 day^{-1} were found for $C_{14}H_{26}Cl_4$, $C_{14}H_{25}Cl_5$, $C_{14}H_{24}Cl_6$, $C_{14}H_{23.3}Cl_{6.7}$ (with $C_{14}Cl_{5-8}$), $C_{16}H_{31}Cl_3$ (with $C_{16}Cl_{2-5}$) and $C_{16}H_{21}Cl_{13}$ (with $C_{16}Cl_{12-15}$) congener groups. The results of these studies are used as part of the weight-of-evidence to conclude that the $C_{14}Cl_{4-8}$ and $C_{16}Cl_{2-5}$ congener groups have B/vB properties. For the remaining groups of congeners ($C_{16}H_{21}Cl_{13}$ with $C_{16}Cl_{12-15}$ as chlorination range) present in the tested substances, it is not possible to conclude on their potential for bioaccumulation since insufficient data is available;
- A bioaccumulation study (aqueous and dietary exposure) on *Daphnia magna* indicates a high bioaccumulation potential with lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45; which contains $C_{14}Cl_{4-9}$, $C_{15}Cl_{3-9}$, $C_{16}Cl_{2-8}$ and $C_{17}Cl_{2-9}$ congener groups (including congeners found in Daphnia upon exposure even if not detected in the original substance tested)). The outcome of this study is used as part of the weight-of-

[5] Details on the weight (or confidence level) given to the experimental studies/data and to the QSAR predictions used in the weight-of-evidence approach are provided in 'Annex X – Experimental and modelling data used as part of a weight-of-evidence (WoE) approach in order to conclude on the bioaccumulation potential of the congener groups of MCCP.

evidence to conclude that the $C_{14}Cl_{4-9}$, $C_{15}Cl_{3-9}$, $C_{16}Cl_{2-8}$ and $C_{17}Cl_{5-9}$ congener groups have B and/or vB properties. For the remaining groups of congeners ($C_{17}Cl_{2-4}$) present in the test substance, it is not possible to conclude on their potential for bioaccumulation since insufficient data is available;

- A bioaccumulation study (aqueous and dietary exposure) on *Mytilus edulis* indicates a high bioaccumulation potential with lipid-normalised BAF value of 7 031 L/kg (steady-state value) and 7 204 L/kg (statistically determined) with confidence limits of 4 694–9 723 L/kg for $C_{16}H_{30.7}Cl_{3.3}$ (34.1% Cl wt.; which contains $C_{16}Cl_{2-5}$). The results of this study are used as part of the weight-of-evidence to conclude that the $C_{16}Cl_{2-5}$ congener groups have B/vB properties;
- As part of an earthworm toxicity study, uptake of C_{15} chlorinated n-alkane, 51% Cl wt. by earthworms (*Eisenia fetida*) from soil was measured. Based on this study, earthworm-soil accumulation factors (BAFs) of 2.4 for adults and 2.3 for juveniles were determined for C_{15} chlorinated n-alkane, 51% Cl wt. (which contains C_{15} Cl_{5-8} congener groups). The outcome of this study suggests that these group of congeners have bioaccumulative (B) properties in earthworms. The results of this study are used as part of the weight-of-evidence to conclude that the C_{15} Cl_{5-8} congener groups have B and/or vB properties;
- A biomagnification study indicates a high bioaccumulation potential with lipid normalised BMFs >1 in the muscles and livers of a snake-frog predator-prey relationship for the congener groups $C_{14}Cl_{3-11}$, $C_{15}Cl_{3-11}$, $C_{16}Cl_{3-10}$ and $C_{17}Cl_{5-10}$. The results of this study are used as part of the weight-of-evidence to conclude that the $C_{14}Cl_{3-11}$, $C_{15}Cl_{3-9}$, $C_{16}Cl_{3-8}$ and $C_{17}Cl_{5-8}$ congener groups have B and/or vB properties. For other group of congeners ($C_{15}Cl_{10-11}$, $C_{16}Cl_{9-10}$ and $C_{17}Cl_{9-10}$), it is not possible to conclude on their potential for bioaccumulation since insufficient data is available;
- Modelling data are used as supporting information to the experimental data in the bioaccumulation assessment. The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_{2-11}$, $C_{15}Cl_{3-10}$ and $C_{16}Cl_{5-10}$ congener groups which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and/or log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential. Furthermore, all groups of congeners of MCCP meet the screening criterion set out in the PBT Guidance (REACH Chapter R.11; ECHA, 2017b) for aquatic organisms as being potentially 'bioaccumulative' (B) and/or 'very bioaccumulative' (vB) with a range of log Kow > 4.5.
- The available (limited) field bioaccumulation studies for MCCP are equivocal: trophic magnification factors below and above 1 have been derived.
- Monitoring data support findings from experimental and predicted data on bioaccumulation of MCCP congeners and MCCP. MCCP have been detected in human blood and milk samples which indicates that MCCP are absorbed to some extent in humans. Detection of MCCP in umbilical cord blood and placenta indicates that MCCP can be transferred to the foetus. Furthermore, monitoring data demonstrate widespread contamination of wildlife by MCCP at all trophic levels (including predatory species). MCCP have also been detected in samples from remote regions, including the Arctic. These data provide supporting evidence that MCCP are taken up by organisms in the environment.

Based on the weight of evidence of the data available, it can be concluded that the $C_{14}Cl_{3–11}$ congener groups of MCCP (equivalent to 35.3–67.6% Cl wt.) have B/vB properties, $C_{15}Cl_{3–9}$ congener groups of MCCP (equivalent to 33.8–61.15% Cl wt.) have B and/or vB properties, $C_{16}Cl_{2–9}$ congener groups of MCCP (equivalent to 24.1–59.55% Cl wt.) have B and/or vB properties and $C_{17}Cl_{5–9}$ congener groups of MCCP (equivalent to 43–58% Cl wt.) have B properties in accordance with REACH Annex XIII. For other congener groups of MCCP, it is not possible to conclude on their potential for bioaccumulation due to the lack of appropriate data.

Based on the information available, as MCCP contain congener groups with B and/or vB properties at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet the 'bioaccumulation' criterion (B) and the 'very bioaccumulative' criterion (vB) in accordance with Annex XIII, points 1.1.2 and 1.2.2, of the REACH Regulation.

Monitoring data on MCCP support the above conclusion as they point towards bioaccumulation of MCCP in biota.

Toxicity

Only limited experimental information is available on the aquatic toxicity of individual MCCP congeners. The majority of the ecotoxicity data is available for the commercial C_{14-17}, 52% Cl wt. substance.

48h EC_{50} results from acute *Daphnia magna* studies fall in the range < 6.5 – 2200 µg/L. The most reliable result is 48h EC_{50} 5.9 µg/L for the C_{14-17}, 52% Cl wt. substance. According to the PBT guidance (REACH Chapter R.11, ECHA, 2017b), a short-term aquatic toxicity result in fish, daphnia, or algae with EC_{50} or LC_{50} < 0.01 mg/L (≈ 10 µg/L) is sufficient to meet the T criterion. Based on this guidance, the T criterion is met.

For the chronic toxicity of MCCP to *Daphnia magna*, 21d NOEC (reproduction) values range from ~ 4 - 15.6 µg/L. The most reliable result is 21d NOEC 8.7 µg/L for the C_{14-17}, 52% Cl wt. substance which meets the toxicity criterion (T) in accordance with Annex XIII, point 1.1.3 (a), of the REACH Regulation.

For a UVCB substance like MCCP, observed toxicity may represent toxicity of one or more of its constituents. As the testing material of the acute and chronic toxicity studies available for MCCP contained several groups of congeners of MCCP and no testing and analysis was performed at the level of the congener groups, it is not possible to identify whether the congener groups present in the tested substance contributed differently to the observed toxicity.

However, the congener groups expected to be present in the test material for both these tests are C_{14} congener groups having 4, 5, 6 and 7 chlorine atoms; C_{15-16} congener groups having 5, 6, 7 and 8 chlorine atoms and C_{17} congener groups having 6, 7, 8 and 9 chlorine atoms. These same congener groups have been detected in *Daphnia magna* in a bioaccumulation test reported in Section 3.4.2.3 Other supporting data. This indicates that these congener groups are bioavailable to *Daphnia magna* and taken up by this organism. Since these congener groups are structurally very similar (they differ only in carbon chain length and number of chlorine substituents), they can be expected to exert toxic effects by the same mode(s) of action. It is therefore reasonable to assume that all congener groups present in the C_{14-17}, 52% Cl wt. test substance contributed equivalently to the observed toxicity.

It is therefore concluded that MCCP and all the following congener groups of MCCP meet the toxicity criterion (T) in accordance with Annex XIII, point 1.1.3 (a), of the REACH Regulation: C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; C_{15} congeners having 5, 6, 7 and 8 chlorine atoms; C_{16} congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms.

Conclusion on the P, B and T properties

On the basis of all the evidence available, it is concluded that the $C_{14}Cl_{3–11}$ congener groups of MCCP (equivalent to 35.3–67.6% Cl wt.) have PBT and/or vPvB properties, $C_{15}Cl_{3–8}$ congener groups of MCCP (equivalent to 33.8–58.2% Cl wt.) have PBT and/or vPvB properties, $C_{16}Cl_{3–8}$ congener groups of MCCP (equivalent to 32.3–56.6% Cl wt.) have PBT and/or vPvB properties and $C_{17}Cl_{6–9}$ congener groups of MCCP (equivalent to 47.65–58% Cl wt.) have PBT properties in accordance with Annex XIII of the REACH Regulation (see Table 1).

Based on the information available, as MCCP contain congener groups with PBT and/or vPvB properties (see Table 1) at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet the

criteria for a PBT and/or vPvB substance in accordance with Annex XIII of the REACH Regulation, and thereby they fulfil the criteria set out in REACH Articles 57(d) and/or (e).

(Note - some of the PBT and/or vPvB congener groups of MCCP listed in Table 1 have been identified in other substances than MCCP, thus suggesting that these substances also could be considered to meet the REACH Annex XIII criteria for a PBT and/or vPvB substance if these congener groups are present in a concentration ≥ 0.1 % (w/w)).

Table 1: Congener groups of MCCP concluded as PBT and/or vPvB in accordance with the criteria set out in Annex XIII of the REACH Regulation

Number chlorine atoms and Carbon chain length	Cl_1	Cl_2	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}
C_{14}	-	-	vPvB	vPvB PBT	vPvB PBT	vPvB PBT	vPvB PBT	vPvB	vPvB	vPvB	vPvB	-	-	-			
C_{15}	-	-	vPvB	vPvB	vPvB PBT	PBT	PBT	PBT	-	-	-	-	-	-	-		
C_{16}	-	-	vPvB	vPvB	vPvB PBT	PBT	PBT	PBT	-	-	-	-	-	-	-	-	
C_{17}	-	-	-	-	-	PBT	PBT	PBT	PBT	-	-	-	-	-	-	-	-

Note: Symbol '-' means that not enough information is available to conclude whether the congener group has PBT and/or vPvB properties. Grey cells means congener groups not considered in the PBT/vPvB assessment.

Summary of other considerations

Based on their physical-chemical properties, some congeners of MCCP are predicted to have long-range environmental transport (estimated atmospheric half-lives in the range of 0.6–7.1 days for different MCCP congeners). Indeed, MCCP have similar physical-chemical properties to legacy persistent organic pollutants (POPs).

Monitoring data tend to confirm this prediction as it has been found that MCCP with C_{14-15} and Cl_{4-9} were found in biota from the Arctic and in air from the Antarctic. MCCP have been detected in various media in the Arctic, including in air from Svalbard, in marine sediments from the Barents Sea and the Norwegian Sea, in terrestrial, avian and marine biota samples from the Norwegian Arctic, including in top predators such as Polar Bears. MCCP were also found in air samples from the Antarctic and from the Tibetan Plateau at high altitude.

The presence of MCCP at sites remote from known point sources such as the Arctic and Antarctic therefore indicates long-range environmental transport.

Furthermore, monitoring data indicate that concentrations of MCCP have increased in biota, in sediment and in air (from the Arctic, the Tibetan Plateau and the Antarctic) during the last decades. In addition, in the Antarctic air, an increasing trend was observed in the ratio of MCCP to SCCP suggesting that the use of MCCP as substitute to SCCP had increased. Due to the PBT/vPvB properties of MCCP, the increasing trend of the concentrations of MCCP in the environment gives reason for concern.

Registration dossiers submitted for the substances? Yes

Justification

This report provides justification for identifying medium-chain chlorinated paraffins (MCCP) - as UVCB[6] substances that contain congeners that are considered to be persistent, bioaccumulative and toxic and/or very persistent and very bioaccumulative (PBT/vPvB) in accordance with the criteria set out in Annex XIII of the REACH Regulation. It is therefore targeted to environmental endpoints. With regard to human health hazards only a short summary is provided, supplemented by information on toxicokinetics, which is relevant for the bioaccumulation assessment.

The United Kingdom Competent Authority (UK CA) was the rapporteur for MCCP 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 transitional 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 MCCP in leather fat liquors was agreed at the 15th Risk Reduction Strategy meeting, and this was communicated to ECHA in the transitional Annex XV 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 by UK CA 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. More recently, UK CA finalised the substance evaluation for MCCP under REACH (EA, 2019).

This report is based on the substance evaluation report (EA, 2019) prepared by UK CA in December 2019. Following the finalisation of the substance evaluation, additional literature search has been performed for the purpose of drafting this report. In particular, a literature search of new information published after December 2019 was performed. In addition, the long-range transport potential (LRTP) section was further developed at the request of the European Commission.

MCCP are UVCB substances which contain linear chloroalkanes with carbon chain lengths predominantly in the range of C_{14-17} with chlorination levels that can differ depending on the application. MCCP therefore contain thousands of congeners and it is neither feasible nor justifiable to experimentally determine key properties for every constituent separately. The assessment approach has therefore been based on test substances that provide a representative structural match for a significant number of congeners, described by carbon chain length and degree of chlorination.

In addition to the medium-chain chlorinated paraffins described above, two other groups of chlorinated paraffins are made commercially. These are known as short-chain (typically C_{10-13}) and long-chain (typically $\geq C_{18}$ or C_{20-30}). The short-chain chlorinated paraffins (SCCP) are on the Candidate List due to their PBT properties and are also listed as persistent organic pollutants (POPs) under the United Nations' Stockholm Convention on POPs. The assessment provided in this report is only concerned with the medium-chain chlorinated paraffins, but some information on the other types is included where it is considered useful and relevant for the PBT/vPvB assessment of MCCP.

[6] Substances of unknown or variable composition, complex reaction products or biological materials.

1. Identity of the substances and physical and chemical properties

MCCP are UVCB substances. MCCP contain linear chloroalkanes with carbon chain lengths predominantly within the range of C_{14-17} with chlorination levels that can differ depending on the application. The number of congeners in MCCP is large.

1.1 Name and other identifiers of the substances

This SVHC identification addresses the group of substances which composition corresponds to the following description:

UVCB substances consisting of more than or equal to 80% linear chloroalkanes with carbon chain lengths within the range from C_{14} to C_{17}.

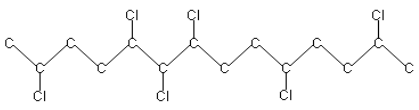
Data on the substance identity of the MCCP registered under the EC entry with EC number 287-477-0 (Alkanes, C14-17, chloro) is presented in Table 2.

Table 2: Substance identity for Alkanes, C14-17, chloro

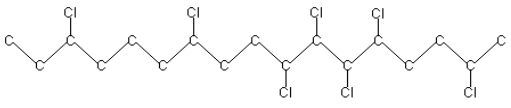
EC number:	287-477-0
EC name:	Alkanes, C_{14-17}, chloro
CAS number (in the EC inventory):	85535-85-9
CAS name:	Chloroalkanes, C14-17
Index number in Annex VI of the CLP Regulation	602-095-00-X
Molecular formula:	Approximately within the range $C_xH_{(2x - y+2)}Cl_y$, where x = 14 - 17 and y = 1 – 17
Molecular weight range:	300 - 800 g/mol (approximately)
Synonyms:	Medium-chain chlorinated paraffins (MCCP); Chlorinated paraffins, C_{14-17}; Alkanes C14-C17, chloro; Chloroalkanes C14-17; Chlorinated paraffin liquid; Chloroparaffin

Structural formula:

Example structures (hydrogen atoms removed for simplicity) include:



$C_{14}H_{24}Cl_6$



$C_{17}H_{29}Cl_7$

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. Table 3 includes a non-exhaustive list of identifiers describing substances covered by the MCCP entry. Table 4 includes a list of identifiers that may have been used to describe substances containing medium-chain chlorinated paraffins (also this list may not necessarily be exhaustive).

Table 3: Non-exhaustive list of substances covered by the MCCP entry

Substance	CAS number	EC number
Alkanes, C_{14-17}, chloro	85535-85-9	287-477-0
Di-, tri- and tetrachlorotetradecane	-	-
Alkanes, C_{14-16}, chloro	1372804-76-6	-
Tetradecane, chloro derivs.	198840-65-2	-

Table 4: Non-exhaustive list of other CAS numbers that may have been associated with medium-chain chlorinated paraffins

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_{10-21}, 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_{16-27}, chloro	84776-07-8	283-931-7
Alkanes, C_{16-35}, chloro	85049-26-9	285-195-2
Paraffin oils, chloro	85422-92-0	287-196-3
Paraffins (petroleum), normal $C_{>10}$, chloro	97553-43-0	307-202-0

MCCP have so far essentially been registered under REACH using the EC number 287-477-0 and CAS number 85535-85-9 (based on ECHA's public dissemination database (consulted on 14 September 2020)). One exception is an MCCP registered using the substance name Alkanes, C_{14}, chloro (or di-, tri- and tetrachlorotetradecane).

It is important to note that all relevant information for the P, B and T assessment has been considered from the above mentioned registered substances.

1.2 Composition of the substance

Name: Medium-chain chlorinated paraffins (MCCP)

Description: They are UVCB substances containing linear chloroalkane constituents predominantly within the range of C_{14-17} (governed by the feedstock) (EA, 2019). The commercially supplied products consist of different carbon chain lengths (reflecting the carbon chain length distribution in the parent hydrocarbon feedstocks used), and have different degrees of chlorination (EC, 2005). The position of the chlorination and the chlorination level varies within the constituents, and so MCCP contain many thousands of constituents[7]. Constituents outside of the C_{14-17} range may also be present in the composition at lower concentration levels. However, the constituents within the C_{14-17} range are expected to represent at least 80% of the composition.

According to the UK Environment Agency (EA, 2009), it is possible that chlorinated paraffins with carbon chain lengths of C_{18} and above may be present in other types of chlorinated paraffins than long-chain chlorinated paraffins (LCCP), such as the MCCP. In addition, the registered substances (Alkanes, C_{14-17}, chloro) may contain unintentional constituents having alkyl chains shorter than C_{14}. This means that constituents having C_{10-13} chlorinated alkyl chains corresponding to constituents of alkanes, C_{10-13}, chloro (short-chain chlorinated paraffins or SCCP, CAS no. 85535-84-8) may as well be present in Alkanes, C_{14-17}, chloro.

It is important to note that in this report the terminology 'congener' is used. Individual constituents sharing the same empirical formula are congeners of each other. The wording 'congeners' or 'congener group' refers to a group of constituents sharing the same empirical formula irrespective of the position of the chlorine substituents on the carbon chain (e.g. the $C_{15}Cl_7$ congener group).

Substance type: UVCB

The ECHA dissemination portal (checked in September 2020) lists 10 active Registrants and 3 inactive Registrants for the substance Alkanes, C_{14-17}, chloro.

Typical concentration and concentration range of congeners of MCCP is confidential information.

All constituents in commercial chlorinated paraffins are likely to be related to those present in the hydrocarbon feedstock, in which the major non-linear hydrocarbon fraction is a small proportion of aromatic constituents (generally less than 100 mg/kg). The content of branched hydrocarbon constituents of the feedstock is less than 1 - 2% (EC 2005).

According to EC (2005), various substances can be added to commercial chlorinated paraffins to improve their thermal or light stability.

The percentage chlorine content of the commercially available product types varies according to the applications they are used for. Table 5 indicates the molecular formulae of possible congeners of different MCCP product types (EA, 2019). Table 5 shows the theoretical % weight chlorine content of several compounds that can be considered as medium-chain chlorinated paraffins. The amount of chlorine present in the commercial products is usually expressed as a percentage by weight (% Cl wt.) corresponding to an average value. Wherever possible in this report, the actual carbon chain length (or range of chain length) and the degree of chlorination (% Cl wt.) will be given following the theoretical % weight chlorine content of congeners as reported in 'Annex I – Theoritical % weight chlorine content of congeners of MCCP'.

Table 5: Theoretical chlorine content of congeners in MCCP

Chlorine content, % w/w	Congener formula							
	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}
<40	$C_{10}H_{21}Cl_1$ &	$C_{11}H_{23}Cl_1$ &	$C_{12}H_{25}Cl_1$	$C_{13}H_{27}Cl_1$	$C_{14}H_{29}Cl_1$	$C_{15}H_{31}Cl_1$	$C_{16}H_{33}Cl_1$	$C_{17}H_{35}Cl_1$

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

Chlorine content, % w / w	Congener formula							
	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}
	$C_{10}H_{20}Cl_2$	$C_{11}H_{22}Cl_2$	to $C_{12}H_{27}Cl_3$	to $C_{13}H_{25}Cl_3$	to $C_{14}H_{27}Cl_3$	to $C_{15}H_{29}Cl_3$	to $C_{16}H_{30}Cl_4$	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 congener groups that are structurally analogous to SCCP.

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 chlorine content refers to the average degree of chlorination for the substance itself. Where a chlorinated paraffin includes more than one carbon chain length, the chlorine content of the congeners having the same carbon number has been found to be close to the chlorine content of the substance itself (Yuan *et al.*, 2017a). The commercially available MCCP generally include more than one carbon chain length with the presence of significant amounts of at least C_{14} chloroalkanes (EA, 2019).

For an MCCP with a given chlorine content, the number of chlorine atoms varies within the congeners. This is the result of the manufacturing process where the positional selectivity of the chlorination reaction on the hydrocarbon chain is low. The presence of congeners with varying degree of chlorination is observed in the composition of MCCP. This is also the case for short-chain chlorinated paraffins. A Gaussian distribution has been considered to describe the composition of chlorinated congeners with a given carbon number (Yuan *et al.*, 2017a). The distribution is expected to be centred within the congeners having a chlorine content just above and below the degree of chlorination of the substance.

By way of example, for an MCCP consisting of C_{14} chlorinated alkanes with a degree of chlorination of 45% by weight, the distribution of congeners is in principle centred in-between the tetrachlorotetradecanes ($C_{14}H_{26}Cl_4$; chlorine content: 42.3% by weight) and the pentachlorotetradecanes ($C_{14}H_{25}Cl_5$; chlorine content: 47.9% by weight). As it can be seen from chemical analyses of commercial chlorinated paraffins in the literature, the distribution of the congener groups per carbon number involves more than two different chlorine contents. Although varying from one composition to another, the distribution is spread over congener groups with at least four different chlorine contents (Bogdal *et al.*, 2015; Yuan *et al.*, 2020; Chen *et al.*, 2011). The composition of an MCCP consisting of C_{14} chlorinated alkanes with a degree of chlorination of 45% can thus be expected to include congener groups with chlorine numbers from at least 3 to 6. For MCCP containing more than one carbon chain length, the same reasoning can be applied for each carbon number, given the close matching between the degree of chlorination at the substance and at the carbon number level.

Despite the challenges in determining the precise composition of chlorinated paraffins, specifications of the chlorine content for a commercial product can thus still be used to identify the different groups of congeners that are expected to be present in its composition. For the

PBT/vPvB assessment of constituents of MCCP, the above methodology has been used in order to determine the groups of congeners present in the testing materials when this information was not available.

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

The details of the registrations for short-chain chlorinated paraffins (SCCP) and long-chain chlorinated paraffins (LCCP) can be found in Table 6 and Table 7.

Table 6: Structurally related substance (SCCP) identity (ECHA, 2008 and ECHA's dissemination site accessed in February 2021)

EC number:	287-476-5
EC name:	Alkanes, C_{10-13}, chloro
CAS number (in the EC inventory):	85535-84-8
CAS number:	85535-84-8
CAS name:	Alkanes, C_{10-13}, chloro
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
Molecular weight range:	320 - 500 g/mol (approximately)
Synonyms:	Short-chain chlorinated paraffins (SCCP); Chlorinated paraffins, C_{10-13}; Alkanes, chlorinated; Alkanes (C_{10-13}), chloro-(50-70%); Alkanes (C_{10-12}), chloro-(60%); Chlorinated alkanes; Chloroalkanes; Chlorocarbons; Polychlorinated alkanes

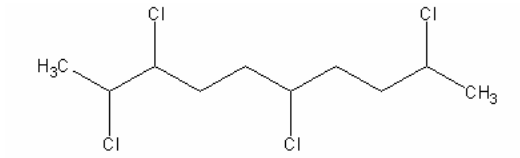
Note: The abbreviation SCCP will be used for the substance throughout this report.

Substance type: UVCB

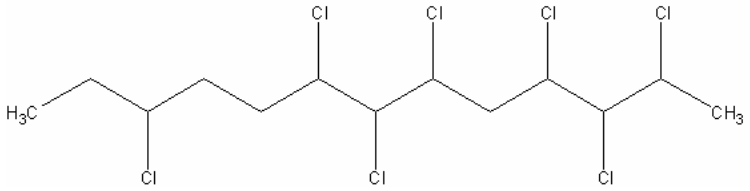
SCCP are no longer registered in the EU.

Structurally related substance (SCCP) formula:

Example structures (hydrogen atoms removed for simplicity) include:



$C_{10}H_{18}Cl_4$



$C_{13}H_{21}Cl_7$

Table 7: Structurally related substance (LCCP) identity (EA, 2009 and ECHA's dissemination site accessed in February 2021)

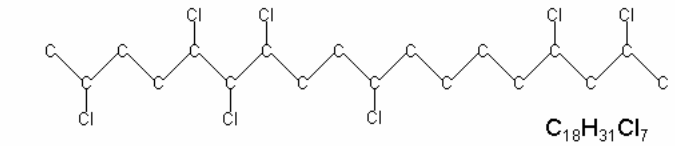
EC number:	264-150-0
EC name:	Paraffin waxes and Hydrocarbon waxes, chloro
CAS number (in the EC inventory):	63449-39-8
CAS number:	63449-39-8
CAS name:	Paraffin waxes, chloro
Index number in Annex VI of the CLP Regulation	-
Molecular formula:	-
Molecular weight range:	420 - 1355 g/mol (approximately)
Synonyms:	Long-chain chlorinated paraffins (LCCP); Alkanes, C_{18-30}, chloro; Chlorinated paraffins, C_{18-30}; Chlorinated paraffins waxes; Hydrocarbon waxes, chlorinated; Chloroparaffin; Paraffin waxes and hydrocarbon waxes, chloro

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

Substance type: UVCB

Structurally related substance (LCCP) formula:

Example structures (hydrogen atoms removed for simplicity) include:



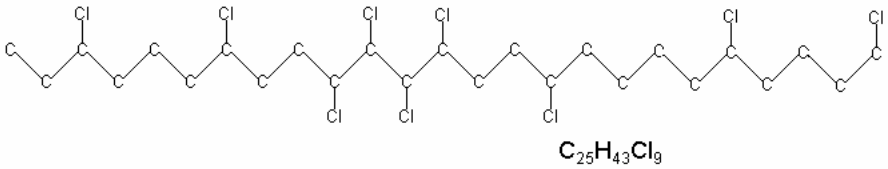


Table 8 contains CAS numbers that may have been used to describe chlorinated paraffins that contain chlorinated alkanes with carbon chain lengths $<C_{14}$ and $>C_{17}$. This list is not necessarily exhaustive. No REACH registrations had been made for any of the CAS numbers in Table 8 when ECHA's public dissemination database was checked on 15 September 2020.

Table 8: Other CAS numbers associated with short- and long-chain chloroparaffins

Substance	CAS number	EC number
Alkanes, C_{12-13}, chloro	71011-12-6	-
Chloroalkanes, C_{18-28}	85535-86-0	287-478-6
Alkanes, C_{18-20}, chloro	106232-85-3	-
Alkanes, C_{22-40}, chloro	106232-86-4	-
C_{10-12} chloroalkanes	108171-26-2	-
Chloroalkanes, C_{22-26}	108171-27-3	-
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	-

1.4 Physicochemical properties

Only physico-chemical properties that are relevant for the PBT/vPvB assessment were considered for these substances. This information is reported in Table 9.

MCCP consist of thousands of congeners and the chain length and chlorination degree of the molecules influence most of the chemical properties. Therefore, for most of the properties exists not one "true" value but rather a range of values (Glüge *et al.*, 2018).

Table 9: Overview of physicochemical properties

Property	Value	Reference / source of information / remarks
Physical state at 20°C and 101.3 kPa	*Liquid*	*EC, 2005*
Melting / freezing point	*The pour point of C_{14-17} chlorinated paraffins vary between -50 °C and +25 °C*	*BUA, 1992 (as cited in EC, 2005)* *Euro Chlor, 1999 (as cited in EC, 2005)*
Boiling point	*MCCP begin to decompose at around 200 °C before boiling*	*EC, 2005*
Vapour pressure	*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.* *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*	*EC, 2005* *Campbell and McConnell, 1980* *BUA, 1992 (as cited in EC, 2005 and UK 2020)*
Density	*1.10 g/cm^3 at 25°C for C_{14-17} chlorinated n-alkane 40% Cl wt.* *1.16 g/cm^3 at 25°C for C_{14-17} chlorinated n-alkane 45% wt. Cl wt.* *1.25 g/cm^3 at 25°C for C_{14-17} chlorinated n-alkane 52% wt. Cl wt.* *1.36 g/cm^3 at 25°C for C_{14-17} chlorinated n-alkane 58% wt. Cl wt.*	*Kirk-Othmer, 1993 (as cited in EC, 2005)*
Water solubility	*0.0061 mg/L at 20 °C for C_{14} chlorinated n-alkane 50% Cl wt.* *0.005 - 0.027 mg/L at 20 °C for C_{15} chlorinated n-alkane 51% Cl wt.* *0.01 mg/L in freshwater and 0.004 mg/L in seawater at 16-*	*Unpublished, 2019a; non-GLP OECD Test Guideline (TG) 105. Analytical method: APCI-ToF-HRMS.* *Madeley, et al., 1983; non-standard method. Analytical method: thin-layer chromatography and radioactivity measurements. Key study used in EC (2005)* *Campbell and McConnell, 1980; method unknown. Analytical method: radioactivity measurements*

Property	Value	Reference / source of information / remarks
	20 °C for C_{16} chlorinated n-alkane 52% Cl wt.	*The water solubility of 0.027 mg/L is considered to be a realistic upper limit for MCCP.*
Organic carbon normalised adsorption coefficient (log K_{OC})	*A K_{OC} value of 588,844 L/kg (or log K_{OC} of 5.77) was derived based on a log Kow of 7.* *In sediments:* *K_{OC} = 103,846 L/kg for the $C_{16}H_{30.7}Cl_{3.3}$ 35% wt. Cl and* *K_{OC} = 175,333 L/kg for $C_{16}H_{20.6}Cl_{13.4}$ 69% wt. Cl, based on ^{14}C measurements*	*EC, 2005* *Fisk et al., 1998a* *The estimated Koc value of 588,844 L/kg (or log K_{OC} of 5.77) is used in EC, 2005.*
Partition coefficient n-octanol / water (log Kow)	*6.58 ± 0.09 for C_{14} chlorinated n-alkane 50% Cl wt.* *7.2 (4.7-8.3) for C_{16} chlorinated n-alkane 35% Cl wt.* *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.* *6.2-8.25 for $C_{14}Cl_{1-14}$* *6.63 – 8.76 for $C_{15}Cl_{1-15}$* *7.07 - 9.28 for $C_{16}Cl_{1-16}$* *7.33 - 9.8 $C_{17}Cl_{1-17}$.*	*Unpublished, 2019b; non-GLP OECD TG 123 (slow stir). Analytical method: APCI-ToF-HRMS. Very little variability in Kow was observed between differently chlorinated constituent groups* *Fisk, 1998b; cited in EC (2005). Analytical method: high performance liquid chromatography (HPLC)* *Renberg et al. (1980); non-GLP non-guideline study. Analytical method: reversed-phase high performance thin layer chromatography (RP-HPTLC)* *Predicted log Kow with log P methods of ACD Percepta, ACD/Labs release 2019.2.1, Advanced Chemistry Development, Inc., 2019*
Partition coefficient octanol / air (log Koa)	*5.96 to 16.08* *C_{14-17} chlorinated n-alkane 30 - 70% Cl wt.*	*Gawor and Wania, 2013* *Log Koa was calculated as log Kow* (selected model) - log Kaw (selected model); log Kow* adjusted to dry octanol* *model for log Kow = ACD Labs Classic log P model; model for log Kaw, see below.*
Partition coefficient Air / water (log Kaw)	*-7.66 to 1.13* *C_{14-17} chlorinated n-alkane 30 - 70% Cl wt.*	*Gawor and Wania, 2013* *Combination of ACD/ Absolved (ADME Suite v. 5.0) with Abraham's LFER (linear free energy relationship) equation.*

The variable composition of MCCP and the analytical challenges make it difficult to assess the accuracy/precision and relevance of physico-chemical endpoints without detailed information about the test item identity/composition and analytical methods.

2. Harmonised classification and labelling

Alkanes, C_{14-17}, chloro are covered by Index number 602-095-00-X in part 3 of Annex VI to the CLP Regulation as follows:

Table 10: Classification according to Annex VI, Table 3.1 (list of harmonised classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008

Index No	International Chemical Identification	EC No	CAS No	Classification		Labelling			Spec. Conc. Limits, M-factors	Notes
				Hazard Class and Category Code(s)	Hazard statement code(s)	Pictogram, Signal Word Code(s)	Hazard statement code(s)	Suppl. Hazard statement code(s)		
602-095-00-X	Alkanes, C_{14-17}, chloro; chlorinated paraffins, C_{14-17}	287-477-0	85535-85-9	Lact. Aquatic Acute 1 Aquatic Chronic 1	H362 H400 H410	GHS09 Wng	H362 H410	EUH066	-	-

According to the harmonised classification for Alkanes, C_{14-17}, chloro, MCCP are very toxic to aquatic life (with long lasting effects), they may cause harm to breast-fed children and after repeated exposure they may cause skin dryness or cracking.

No multiplication factors (M-factors) for mixtures are given in the harmonised classification of MCCP under the CLP Regulation. However, it is worth noting that the self-classification as reported by notifiers includes an M-factor of 100 and 10 for acute and chronic aquatic hazards, respectively. The self-classification for physical or human health hazards is not considered in this report. In the substance evaluation report for MCCP (EA, 2019), UK noted that the harmonised classification could be updated with this information.

3. Environmental fate properties

3.1 Degradation

3.1.1 Abiotic degradation

3.1.1.1 Hydrolysis

EC (2005) concluded that MCCP are not expected to hydrolyse significantly.

3.1.1.2 Oxidation

No information is available on potential oxidation of MCCP.

3.1.1.3 Phototransformation/photolysis

3.1.1.3.1 Phototransformation in air

No data are included in the registration dossiers (based on ECHA's dissemination site accessed in February 2021) on phototransformation of MCCP in air. EC (2005) reports that second order rate constants (kOH) for reaction with atmospheric hydroxyl radicals of 8.0-14.4.10^{-12} cm^3 molecule^{-1} s^{-1} have been calculated for medium-chain chlorinated paraffins with chlorine contents between 40% Cl wt. and 56% Cl wt. using the method of Atkinson.

Atmospheric half-lives for MCCP estimated by AOPWIN (v.1.92) (EPI Suite™) have been reported to be approximately 0.6 – 6 days (log –0.2 – 0.8 days; C_{14}-$_{17}$ 30 - 70% Cl wt.; Gawor and Wania, 2013) and 1.7 days (40.2 h) for $C_{14}H_{24}Cl_6$ (52.6% Cl wt.) and 2.1 days (49.2 h) for $C_{17}H_{29}Cl_7$ (51.6% Cl wt.) by UK (2021). It should be noted that there are no measured data with which to directly compare the current estimates. Since there are no similar analogue to the chlorinated C_{14-17} structures within the training set of AOPWIN, 1-chlorohexane being the nearest analogue, there is considerable uncertainty in the reliability of these predictions (UK, 2021).

In the UK Substance Evaluation (EA, 2019) estimated atmospheric half-life between 1 - 2 days was reported. However, it should be noted that MCCP with >65% Cl wt. has estimated half-lives in air which are longer than 2 days. The longest half-life was predicted for C_{14} n-alkane, 70% Cl wt. which has a predicted half-life in air of 6.75 days (EA, 2019).

Gawor and Wania (2013) used 12 058 congeners in their study and they concluded that atmospheric half-lives of chlorinated paraffins increase with the degree of chlorination but is less affected by the chain length.

Environment Canada (2008) concluded that the atmospheric half-lives for vapour phase MCCP ranged from 2.7 to 7.1 days, with the longest half-lives for MCCP with the highest chlorine contents and also with the shorter chain lengths.

UK (2021) explains that AOPWIN calculates atmospheric half-life based on estimated values for the second order rate constant for reaction with atmospheric hydroxyl radicals. These predictions estimate the rate of reaction of the C-H bond in the substance. The rate constant is influenced by the number of C-H bonds and their relative position in the chemical structure. Therefore, for a given chain length, increasing the chlorination level decreases the rate constant for reaction with atmospheric hydroxyl radicals as fewer C-H bonds exist for reaction with the hydroxyl radicals. For example, a C_{14} chain length with higher levels than 52.6% Cl wt. will have an atmospheric half-life longer than 49.2 h. For a given chlorination level, increasing the chain length will increase the rate constant as more C- H bonds are available for reaction. This can also be seen in the longer half-lives for the POPs listing of SCCP, where estimated atmospheric half-lives ranged between 47 and 175 h (Wegmann *et al.*, 2007 as cited in UK, 2021).

Howard *et al.* (1975) reported that medium-chain chlorinated paraffins with chlorine contents of 45% wt. Cl and 52% wt. Cl were not decomposed when exposed to high energy light (13% of energy in the 220-280 nm range) in petroleum ether. They concluded that direct photolysis of medium-chain chlorinated paraffins is unlikely to be a significant degradation pathway in the environment.

3.1.1.3.2 Phototransformation in water

No data are included in the registration dossiers on phototransformation of MCCP in water (based on ECHA's dissemination site accessed in February 2021). Koh and Thiemann (2001) investigated the degradation of chloroparaffins in water after irradiation with UV light for 300 minutes. The reported half-life in water was 9.6 h and 12.8 h for a C_{17-24} n-alkane, 35% Cl wt. and a C_{12-18} n-alkane, 52% Cl wt., respectively. The relevance of photodegradation for degradation in the environment is likely to be low in most natural waters due to depth, turbidity, quenching agents, etc. According to the PBT guidance (REACH Chapter R.11; ECHA, 2017b), due to the large variation in the light available in different environmental compartments, the use of photolysis data is not generally recognised for persistence assessment.

3.1.1.3.3 Phototransformation in soil

No data are included in the registration information on ECHA's dissemination site (accessed in February 2021) on phototransformation of MCCP in soil.

3.1.2 Biodegradation

3.1.2.1 Biodegradation in water

3.1.2.1.1 Estimated data

BIOWIN 2 (non-linear probability model), BIOWIN 3 (ultimate biodegradation model) and BIOWIN 6 (MITI nonlinear model) of the BIOWIN v4.10 program (EPI Suite 4.1) predictions for biodegradation have been carried out for the following hypothetical groups of MCCP congeners $C_{14}Cl_{1-14}$, $C_{15}Cl_{1-15}$, $C_{16}Cl_{1-16}$ and $C_{17}Cl_{1-17}$ and their constituents (i.e. structural isomers) (see 'Annex II – Modelling of log Kow and biodegradation and generation of representative structures for MCCP' for the enumeration of structures for MCCP). The results of these calculations are given in Table 55 of Annex II and it is specified in the table how many structures per congener group have been used in the predictions.

The predictions have been compared against the screening criteria for persistence in accordance with the PBT guidance (Chapter R.11, ECHA, 2017b) as follows; BIOWIN 2 <0.5 and BIOWIN 3 <2.25, or BIOWIN 6 <0.5 and BIOWIN 3 <2.25: potentially persistent (P) or very persistent (vP). BIOWIN 2 <0.5 and BIOWIN 3 between 2.25 and 2.75, or BIOWIN 6 <0.5 and BIOWIN 3 between 2.25 and 2.75: potentially persistent or very persistent, more information needed. Congener groups, for which the screening criteria are met for at least one of its considered constituents, are concluded as screening 'potentially persistent or very persistent', or 'potentially persistent or very persistent and more information is needed'.

The following congener groups were found to not screen as persistent or very persistent; $C_{14}Cl_1$, $C_{15}Cl_1$ and $C_{16}Cl_1$. The congener groups $C_{14}Cl_2$, $C_{15}Cl_2$, $C_{16}Cl_2$, $C_{17}Cl_1$ and $C_{17}Cl_2$ screen as potentially persistent or very persistent and more information is needed. MCCP congener groups $C_{14}Cl_{3-14}$, $C_{15}Cl_{3-15}$, $C_{16}Cl_{3-16}$ and $C_{17}Cl_{3-17}$ screen as potentially persistent or very persistent (P/vP). This means that all MCCP congeners with three chlorine atoms or more are potentially persistent or very persistent according to the BIOWIN predictions. See Table 11 for a summary of the predictions for MCCP. It is important to note that the predicted values for different structural isomers of some of the congener groups differed slightly (see Table 55 of Annex II), which is an effect of the positioning of the chlorine atom resulting in slightly different fragments being used in the BIOWIN calculations.

When considering the predictions, it is important to note that not all of the MCCP congeners fall within the applicability domain of the BIOWIN models 2, 3 and 6 and this may affect the reliability of the predictions. The maximum occurrence of the aliphatic chlorine fragment (-Cl-) in the training set of the BIOWIN 3, BIOWIN 2 and BIOWIN 6 models are three, six and twelve respectively. This means that congener groups with more than three chlorine atoms substituted on the hydrocarbon chain have more instances of the aliphatic chlorine fragment than the maximum for all the training set compounds in the BIOWIN 3 model. Hence these congener groups can be considered to be outside of the applicability domain of this model. The Biowin 6 model can yield predictions for structures with up to 12 chlorine atoms that are in domain, hence this model can be considered the preferred one as compared to BIOWIN 2 for the MCCP congeners. When combining the models, only the predictions for congener groups with one to three chlorine atoms can be considered fully reliable and most of the MCCP congeners are outside of the applicability domains of the models, which may affect the accuracy of the predictions. However, the reliable predictions for $C_{14}Cl_3$, $C_{15}Cl_3$, $C_{16}Cl_3$ and $C_{17}Cl_3$ are already below the thresholds of the guidance, i.e, they fulfil the conditions for screening as potentially persistent or very persistent. The BIOWIN models are fragment-based models that assume additivity of fragments no matter what their type and number. This means that in the calculations the negative coefficient for the aliphatic chlorine fragment,will be subtracted for each addition of chlorine in the input structure, meaning that an increase of chlorine atoms will successively lead to lower predictions. The molecular weight (MW) also influences the calculation, with increasing MW leading to successively lower values. This could lead to an underestimation of the predicted rate of biodegradation for the congeners of higher degrees of chlorination. Even so, the trend is clear, indicating that MCCP congener groups with three chlorine atoms or more are not readily biodegradable and hence screen as potentially persistent or very persistent. The BIOWIN predictions are consistent with the experimental data for $C_{14}Cl_{3\text{-}14}$ showing that these congeners as very persistent.

Table 11: Summary of BIOWIN predictions for MCCP

Carbon chain length	Number chlorine atoms	BIOWIN Predictions			Screening outcome based on predictions
		BIOWIN 2	BIOWIN 3	BIOWIN 6	
C_{14}	1	0.4239 - 0.823	2.81 - 3.11	0.4572	Does not screen as P/vP
	2	0.0661 - 0.309	2.56 - 2.89	0.0883 - 0.1986	Potentially P/vP, more information needed*
	3 - 14	< 0.5	≤ 2.31**	< 0.5	Potentially P/vP
C_{15}	1	0.3762 - 0.7921	2.78-3.08	0.4633	Does not screen as P/vP
	2	0.0548	2.53	0.0113 - 0.0284	Potentially P/vP, more information needed
	3 - 15	< 0.5	≤ 2.28**	< 0.5	Potentially P/vP
C_{16}	1	0.3307 - 0.7574	2.75 - 3.05	0.4694	Does not screen as P/vP
	2	0.0453 - 0.2309	2.5 - 2.8	0.0013	Potentially P/vP, more information needed
	3 - 16	< 0.5	≤ 2.55**	< 0.5	Potentially P/vP
C_{17}	1	0.2882 - 0.719	2.72 - 3.02	0.4755 - 0.6987	Potentially P/vP, more information needed
	2	0.0375 - 0.1987	2.47- 2.77	0.0944 - 0.2106	Potentially P/vP, more information needed
	3 - 17	< 0.5	< 2.25	< 0.5	Potentially P/vP

* Potentially persistent or very persistent, more information needed due to the BIOWIN 3 predictions being between 2.25 and 2.75 according to PBT guidance, Chapter R.11 (ECHA, 2017b).
**The range for the $C_{14}Cl_3$ congener is 2.01- 2.31 (number of input structures 6), for $C_{15}Cl_3$ it is 1.98- 2.28 (number of input structures 6) and for $C_{16}Cl_3$ it is 1.95 - 2.55 (number of input structures 6) and since there are predictions which are < 2.25, these groups of congeners have been concluded to fulfil the screening criteria for P/vP.

3.1.2.1.2 Screening tests

EC (2005) does not describe any standard ready or inherent biodegradation tests or simulation studies. Based on non-standard test data from biological oxygen demand (BOD) studies (Madeley and Birtley, 1980), MCCP are not expected to be readily or inherently biodegradable within the criteria and thresholds applicable for standard screening tests. EC (2005) reports evidence that some microorganisms may be capable of degrading MCCP in the environment in acclimated or co-metabolic systems, but it was not possible to estimate a realistic environmental half-life.

Since EC (2005) was published, a series of modified or enhanced standard screening studies (OECD TG 301D and 302A) were performed at 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 in the test systems and/or by increasing the incubation period beyond 28 days. All available data are summarised below.

1) Test Substance - C_{14} chlorinated n-alkane, 45% Cl wt. (Unpublished 2010a)

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 $C_{14}H_{25.4}Cl_{4.6}$ (congeners having 3, 4, 5 and 6 chlorine atoms at least are expected to be present in this substance (equivalent to 35.3–52.6% Cl wt.) based on a Gaussian distribution, as considered by the dossier submitter). 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 wastewater 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 ultra-sonification 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 12.

Table 12: Results of the closed bottle test study (OECD TG 301D) with a C_{14} chlorinated n-alkane, 45% Cl wt. (average value; Unpublished, 2010a)

Time (days)	Mean dissolved oxygen concentration (mg/L)				Percentage degradation (%)	
	Control	Control with PAAP	Chlorinated paraffin with PAAP	Positive control (sodium acetate)	Chlorinated paraffin (based on O_2 consumption)	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)

A GLP-certified enhanced OECD TG 301D study was performed using a commercial 45.6% Cl wt. MCCP product (average value; a Gaussian distribution has been considered by the dossier sumbitter to describe the composition of the chlorinated congeners as follows: C_{14-15} congeners having 3,4,5 and 6 chlorine atoms at least are expected to be present in this substance and C_{16-17} congeners having 4,5,6 and 7 chlorine atoms at least are expected to be present in this substance (equivalent to 33.8–53.15% Cl wt.); Unpublished, 2010b). The inoculum was prepared from pre-conditioned secondary activated sludge from a sewage treatment plant treating predominantly domestic wastewater. 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 ultra-sonification 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 13.

Table 13: Results of the closed bottle test study (OECD TG 301D) with a C_{14-17} chlorinated n-alkane, 45.6% Cl wt. (average value; Unpublished, 2010b)

Time (days)	Mean dissolved oxygen concentration (mg/L)				Percentage degradation (%)	
	Control	Control with PAAP	Chlorinated paraffin with PAAP	Positive control (sodium acetate)	Chlorinated paraffin (based on O_2 consumption)	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%	-

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 consumption began 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. In other studies (Unpublished, 2010a, 2010c and 2010d) a similar lag phase was observed where the degradation started slowly at 7 days or 14 days. It is worth noting that no data are available using river water as the inoculum, although the degradation rate would be expected to be slower, as observed for C_{14} chlorinated n-alkane, 45.5% Cl wt. (Unpublished, 2010e).

3) Test Substance - Commercial C_{14-17}, 63.2% Cl wt.(Unpublished, 2010c)

[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).

A GLP-certified OECD TG 301D study was performed using a commercial 63.2% Cl wt. MCCP product (average value; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{14-15} constituents having 8, 9, 10 and 11 chlorine atoms at least are expected, C_{16} constituents having 9, 10, 11 and 12 chlorine atoms at least are expected and C_{17} constituents having 10, 11, 12 and 13 chlorine atoms at least are expected to be present in this substance (equivalent to 58.2–67.6% Cl wt.; 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 with this study are the same as with (Unpublished, 2010b). The ThOD of the test substance was calculated to be 1.05 mg O_2/mg. The results are summarised in Table 14.

Table 14: Results of the closed bottle test study (OECD TG 301D) with a C_{14-17} chlorinated n-alkane, 63.2% Cl wt. (average value; Unpublished, 2010c)

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 (based on O_2 consumption)	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. From the results presented in Table 14, a mean biodegradation level of only 5% to 14% had occurred by days 21 to 60, respectively, for this substance having a higher chlorination level compared to other test materials as reported in Section '3.1.2.1.2 Screening tests'.

4) Test Substance - Commercial C_{14-17}, 51.7% Cl wt. (Unpublished, 2010d)

A GLP-certified enhanced OECD TG 301D study was performed using a commercial 51.7% Cl wt. MCCP product (average value; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{14} congeners having 4,5,6 and 7 chlorine atoms at least are expected to be present in this substance; C_{15-16} congeners having 5,6,7 and 8 chlorine atoms at least are expected to be present and C_{17} congeners having 6,7,8 and 9 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–58.2% Cl wt.); 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 are identical. The ThOD for the test substance was 1.5 mg O_2/mg. The results of the test are summarised in Table 15.

Table 15: Results of the closed bottle test study (OECD TG 301D) with a C_{14-17} chlorinated n-alkane, 51.7% Cl wt. (average value; Unpublished, 2010d)

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 (based on O_2 consumption)	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 level 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)

Unpublished (2010e) reports the non-GLP assessment of biodegradability of chlorinated tetradecane (C_{14}) using enhanced ready biodegradability 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. A Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: for C_{14} chlorinated n-alkane, 41.3% Cl wt. (average value), congeners having 2, 3, 4 and 5 chlorine atoms at least are expected to be present in this substance (equivalent to 26.6–47.9% Cl wt.). For C_{14} chlorinated n-alkane, 45.5% Cl wt. (average value), congeners having 3, 4, 5 and 6 chlorine atoms at least are expected to be present in this substance (equivalent to 35.3–52.6% Cl wt.). For C_{14} chlorinated n-alkane, 50% Cl wt. (average value), congeners having 4, 5, 6 and 7 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–56.5% Cl wt.). For C_{14} chlorinated n-alkanes, 55% Cl wt., congeners having 5, 6, 7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 47.9–59.9% Cl wt.). For C_{14} chlorinated n-alkanes, 60.2% Cl wt. (average value), congeners having 7, 8, 9 and 10 chlorine atoms at least are expected to be present in this substance (equivalent to 56.5–65.4% Cl wt.). 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 wastewater. 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 16. No explanation is provided as to why the Sturm test results have been omitted.

Table 16: Results of the closed bottle test study (OECD TG 301D) with C_{14} chlorinated n-alkane, 41.3, 45.5, 50, 55 and 60.2% Cl wt. (average values) using activated sludge or river water inocula (Unpublished, 2010e)

Substance	Inoculum	Percentage degradation (%) on day (based on O_2 consumption)						
		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 degradation of C_{14} congeners with chlorine contents of 41.3% Cl wt. exceeds the 60% pass level by day 28. The rate of biodegradation of C_{14} congeners 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. It is noted 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.

The OECD "Guidelines for the Testing of Chemicals, Revised Introduction to the OECD Guidelines for Testing of Chemicals, Section 3 Part I: Principles and Strategies Related to the Testing of Degradation of Organic Chemicals" (OECD, 2006) indicates that ready biodegradability tests are intended for pure substances and are generally not applicable for complex compositions containing different types of congeners, like UVCB. For an UVCB substance, observed biodegradation may indeed represent the biodegradation of only some of its constituents. Similarly, the PBT guidance (REACH Chapter R.11, ECHA, 2017b), indicates that if the test item composition does not consist of similar structures or is not well characterised, it may still contain a certain amount of congeners that are persistent although the amount of easily degradable congeners is high enough to lead to an overall degradation percentage sufficient to meet the criteria for ready biodegradation. The results of the OECD TG 301D for the C_{14} chlorinated n-alkane, 55.0% Cl wt. and the C_{14} chlorinated n-alkane, 60.2% Cl wt. substances indicate that these substances are potentially persistent based on this screening study. It is worth noting that C_{14} chlorinated n-alkane, 55.0% Cl wt. contains C_{14} congeners having 5, 6, 7 and 8 chlorine atoms that are considered as potentially persistent. Furthermore, C_{14} chlorinated n-alkane, 41.3% Cl wt., C_{14} chlorinated n-alkane, 45.5% Cl wt. and C_{14} chlorinated n-alkane, 50% Cl wt. contain one or more congeners (at a relevant concentration ≥0.1% (w/w)) with a similar number of chlorine atoms per molecule than for C_{14} chlorinated n-alkane, 55.0% Cl wt. As a conclusion, these substances (C_{14} chlorinated n-alkane, 41.3% Cl wt., C_{14} chlorinated n-alkane, 45.5% Cl wt. and C_{14} chlorinated n-alkane, 50% Cl wt.) cannot be rated as biodegradable as they always will contain some of the congeners that screen potentially persistent.

As already mentioned before, it cannot be excluded that the lack of degradation observed for C_{14} chlorinated n-alkane, 55.0% Cl wt. and the C_{14} chlorinated n-alkane, 60.2% Cl wt. substances is due to toxicity to microorganisms. However, it is worth noting that a 24h NOEC of 800 mg/L was found for a C_{14-17}, 41% Cl wt. (average value; with C_{14} congeners having 2, 3, 4 and 5 chlorine atoms; C_{15-17} congeners having 3, 4, 5 and 6 chlorine atoms (equivalent to 26.6–50.8% Cl wt.)) substance using anaerobic bacteria from a domestic waste water treatment plant (EC, 2005) which indicated a lack of toxicity to microorganisms. In addition, the toxicity of a C_{14-17}, 52% wt. Cl chlorinated paraffin (average value; C_{14} congeners having 4, 5, 6 and 7 chlorine atoms at least are expected to be present in this substance; C_{15-16} congeners having 5, 6, 7 and 8 chlorine atoms at least are expected and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–58.2% Cl wt.)) has been tested in a 3-hour respiration inhibition test (unpublished study; EC, 2005). No effect on respiration was seen up to the highest concentration tested (2,000 mg/L) (Hoechst AG; as reported in BUA, 1992; EC, 2005). Based on these studies, it is unlikely that the testing materials used in this study (Unpublished, 2010e) are toxic to the microorganisms, even if specific information on toxicity for the above mentioned degradation study is missing.

6) Biodegradation assessment using a Sequencing Batch Reactor (Unpublished, 2010f)

Three C_{14} chlorinated n-alkanes (chlorine contents of 41.3% Cl wt., 50.0% Cl wt. and 60.2% Cl wt.) have been assessed for biodegradability in sequencing batch reactors (Unpublished, 2010f). A Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: for C_{14} chlorinated n-alkane, 41.3% Cl wt. (average value), constituents having 2, 3, 4 and 5 chlorine atoms at least are expected to be present in this substance (equivalent to 26.6–47.9% Cl wt.). For C_{14} chlorinated n-alkane, 50% Cl wt. (average value), constituents having 4, 5, 6 and 7 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–56.5% Cl wt.). For C_{14} chlorinated n-alkanes, 60.2% Cl wt. (average value), constituents having 7, 8, 9 and 10 chlorine atoms at least are expected to be present in this substance (equivalent to 56.5–65.4% Cl wt.). 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), these studies are comparable to inherent biodegradation OECD TG 302A (Inherent Biodegradability: Modified SCAS Test) studies. Data generated from studies performed to this guideline cannot be used on their own to reach conclusion on persistence by demonstrating inherent biodegradability because the test conditions are too favourable to the selection and/or adaptation of micro-organisms (REACH Guidance R.7b and R.11 (ECHA, 2017a and b)). Regarding inherent biodegradation tests, results of a Zahn-Wellens test (OECD TG 302B) or MITI II test (OECD TG 302C) only may be used to assess if the substance would not fulfil the criteria for P.

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 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 MCCP.

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 MCCP 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 17.

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, 50.0% 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 17: Summary of the results of biodegradation tests using sequencing batch reactors (Unpublished, 2010f)

Day	C_{14}, 41.3% Cl wt.		C_{14}, 50.0% Cl wt.		C_{14}, 60.2% 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)

A GLP-certified enhanced OECD TG 301D study was performed using C_{15} chlorinated n-alkane, 51% Cl wt. (average; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{15} congeners having 5,6,7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 46.2–58.2% Cl wt.); Unpublished, 2014a). The inoculum was prepared from secondary activated sludge from a sewage treatment plant treating predominantly domestic wastewater. 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 18.

Table 18: Results of the closed bottle test study (OECD TG 301D) with C_{15} chlorinated n-alkane, 51% Cl wt. (average value) using activated sludge as inoculum (Unpublished, 2014a)

Time (days)	Percentage degradation (%)	
	Chlorinated paraffin (based	Positive control (sodium

	on O_2 consumption)	acetate)
14	17	87
21	23	-
28	43	-
42	50	-
60	63	-

The degradation of the test substance did not exceed the 60% pass level by day 28 but was 63 % by day 60.

8) *Test Substance - C_{15} chlorinated n-alkane, 51% Cl wt. (Unpublished, 2014b)*

A GLP-certified enhanced OECD TG 301D study was performed using C_{15} chlorinated n-alkane, 51% Cl wt. (average; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{15} congeners having 5,6,7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 46.2–58.2% 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 19.

Table 19: Results of the closed bottle test study (OECD TG 301D) with C_{15} chlorinated n-alkane, 51% Cl wt. (average value) using river water as inoculum (Unpublished, 2014b)

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 level by day 60.

9) Test Substance - C_{14} chlorinated n-alkane, 50% Cl wt. (Unpublished 2018a)

A GLP-certified enhanced OECD TG 301D study was performed using C_{14} chlorinated n-alkane, 50.07% Cl wt. (average value, a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners (present at a relevant concentration ≥0.1% (w/w)) as follows: C_{14} congeners having 4, 5, 6 and 7 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–56.5% Cl wt.); Unpublished, 2018a). The composition of chlorinated congeners was determined by isomer-specific analyses as follows: C_{14} congeners having 4 to 12 chlorine atoms were present in this substance (equivalent to 42.3–69.6% Cl wt.); however, the proportion of each congener group in the testing material was not reported (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 wastewater. 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, isomer-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 ionisation time-of-flight mass spectrometry (APCI-TOF-MS) for quantification of C_{14} congeners using a range of C_{14} mixtures (40%, 45%, 50%, 55%, 60%, 65% Cl wt.). No extraction efficiencies or method development details were reported. The results are summarised in Table 20.

Table 20: Results of the closed bottle test study (OECD TG 301D) with C_{14} chlorinated n-alkane, 50% Cl wt. substance (average value) (Unpublished, 2018a)

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 regard 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, it was not possible to verify these statements. No data have been presented in the study report that would allow to confirm the claims with regard to removal of the substance and partitioning between dissolved fraction and

particles. Also, 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 results based on oxygen consumption are therefore considered to be the most reliable.

10) Test Item - C_{14} chlorinated n-alkane, 55% Cl wt. (Unpublished 2018b)

A GLP-certified OECD TG 301D study was performed using C_{14} chlorinated n-alkane, 55.34% Cl wt. (average value, a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners (present at a relevant concentration ≥0.1% (w/w)) as follows: C_{14} congeners having 5, 6, 7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 47.9–59.9% Cl wt.); Unpublished, 2018b). The composition of chlorinated congeners was determined by isomer-specific analyses as follows: C_{14} congeners having 4 to 12 chlorine atoms were present in this substance (equivalent to 42.3–69.6% Cl wt.); however, the proportion of each congener group in the testing material was not reported (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 21.

Table 21: Results of the closed bottle test study (OECD TG 301D) with C_{14} chlorinated n-alkane, 55% Cl wt. substance (average value) (Unpublished, 2018b)

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 15% at 60 days and 22% at 120 days).

The final report presents the following data with regard 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 results based on oxygen consumption are considered to be the most reliable.

11) Test Substance - C_{14} chlorinated n-alkane, 60% Cl wt. (Unpublished 2018c)

A GLP-certified OECD TG 301D study was performed using C_{14} chlorinated n-alkane, 60.14% Cl wt. (average value, a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners (present at a relevant concentration ≥0.1% (w/w)) as follows: C_{14} congeners having 7,8,9 and 10 chlorine atoms at least are expected to be present in this substance (equivalent to 56.5–65.4% Cl wt.); Unpublished, 2018c). The composition of chlorinated congeners was determined by isomer-specific analyses as follows: C_{14} congeners having 4 to 12 chlorine atoms were present in this substance (equivalent to 42.3–69.6% Cl wt.); however, the proportion of each congener group in the testing material was not reported (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 22.

Table 22: Results of the closed bottle test study (OECD TG 301D) with C_{14} chlorinated n-alkane, 60% Cl wt. substance (average value) (Unpublished, 2018c)

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 and by day 60, 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 regard 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 results based on oxygen consumption are considered to be the most reliable.

12) Test Substance - C_{15} chlorinated n-alkane, 51% Cl wt. (Unpublished 2018d)

A GLP-certified OECD TG 301D study was performed using C_{15} chlorinated n-alkane, 51.12% Cl wt. (average value; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners (present at a relevant concentration ≥0.1% (w/w)) as follows: C_{15} congeners having 5, 6, 7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 46.2–58.2% Cl wt.); Unpublished, 2018d). The composition of chlorinated congeners was determined by isomer-specific analyses as follows: C_{15} congeners having 4 to 12 chlorine atoms were present in this substance (equivalent to

40.6–68.05% Cl wt.); however, the proportion of each congener group in the testing material was not reported (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 23.

Table 23: Results of the closed bottle test study (OECD TG 301D) with C_{15} chlorinated n-alkane, 51% Cl wt. substance (average value) (Unpublished, 2018d)

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 was observed 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, no conclusion can be drawn concerning inherent biodegradability.

The final report presents the following data with regard 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 results based on oxygen consumption are considered to be the most reliable.

Discussion on the screening tests

Comparison of data from different studies that use the same test substance should be undertaken with caution, due to variable sources of inocula, test setups and applied modifications/deviations from the test guidelines and methods of calculation.

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 (Chapter R.11; ECHA, 2017b and Chapter R.7b; ECHA, 2017a). 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 approximately two orders of

magnitude higher than the water solubility limit (≤0.027 mg/L) (Chapter R.7b, p. 209; ECHA, 2017a).

- 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 R.7.9—3 of Chapter R.7b of the REACH Guidance; ECHA, 2017a); this is also permitted by 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 for all congeners present at ≥0.1% (w/w) 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, 2017b).

- 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 R.7.9—3 of Chapter R.7b of the REACH Guidance (p. 273); ECHA, 2017a). Most of the studies for MCCP 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.

- The PBT guidance (Chapter R.11; ECHA, 2017b) and the REACH guidance Chapter R.7b (ECHA, 2017a) recommend that for enhanced screening tests, the test duration is not extended beyond 60 days in order to avoid the deterioration of the test system. For some studies (Unpublished, 2018a; Unpublished, 2018b; Unpublished, 2018c; Unpublished, 2018d), the test was extended up to 120 days.

- According to the REACH guidance Chapter R.7b (ECHA, 2017a) on pages 214–215, 'the prolongation of the test duration should only be considered if some initial, slow but steady, biodegradation was observed but did not reach a plateau by the end of the ready biodegradability test, i.e. after 28 days. However, a late acceleration of biodegradation is likely to reflect an adaptation of the microorganisms and in that case the prolongation of the test duration should not be regarded as adequate for the P/vP assessment'. Furthermore, this guidance also mentions on page 214 that 'the purpose of those enhancements should only be to compensate the poor bioavailability to the degrading microorganisms of poorly soluble and/or adsorptive substances, but should not be used to induce additional adaptation of the inoculum'. Considering that for UVCB substances such as MCCP, the ultimate degradation kinetics reflect the degradation of the whole test substance and the constituents/congener groups of MCCP may differ in their bioavailability, it may be difficult to demonstrate whether the guidance pre-conditions for using the extended test period are fulfilled (such as: 'some initial, slow but steady, biodegradation'), in particular when the primary degradation of the constituents/congener groups of MCCP is not measured.

Taking account of these considerations, the overall results of the various screening tests are presented in Table 24[9]. All listed studies are considered to be in technical terms reliable with restrictions, however not necessarily relevant and adequate for the assessment and determination of the P-properties of MCCP and in particular of its different chloroalkane constituents (see 2nd paragraph below for details).

[9] Studies that more closely resemble inherent biodegradability assessments have not been included (i.e. Unpublished, 2010f).

Table 24: 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)
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	Suspension using PAAP		Fail	Pass	Unpublished

Substance tested	Inoculum	Administration method	Pass/fail (*)		Reference
			Modified	Modified & Enhanced	
	sludge River water	Unspecified solubilising agent	Fail	Fail	(2014a) 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)

(*) 'Modified' means use of solubiliser. 'Enhanced' means extended timescale. In this assessment following pass level criteria have been applied: under the 'modified' condition 60% degradation within 28 days and under the 'modified & enhanced" condition 60% degradation within 60 days.
It is worth noting that there are certain reservations for using the 60 days results, considering the difficulty to demonstrate whether the REACH guidance Chapter R.7b (see pages 214–215; ECHA, 2017a) pre-conditions for using the extended test period are fulfilled for UVCB substances such as MCCP.

Based on the results of the screening tests, it seems that the overall level of degradation appears to decline with increasing levels of chlorination (only average chlorination levels are reported in Table 24). This observed trend is however associated with some uncertainty as it cannot definitively ruled out that the lack of degradation observed for substances having higher chlorination levels might be due to toxicity to microorganisms. However, it is worth noting that a 24h NOEC of 800 mg/L was found for a C_{14-17}, 41% Cl wt. (average value; with C_{14} congeners having 2, 3, 4 and 5 chlorine atoms; C_{15-17} congeners having 3, 4, 5 and 6 chlorine atoms (equivalent to 26.6–50.8% Cl wt.)) substance using anaerobic bacteria from a domestic waste water treatment plant (EC, 2005) which indicated a lack of toxicity to microorganisms. In addition, the toxicity of a C_{14-17}, 52% wt. Cl chlorinated paraffin (average value; C_{14} congeners having 4, 5, 6 and 7 chlorine atoms at least are expected to be present in this substance; C_{15-16} congeners having 5, 6, 7 and 8 chlorine atoms at least are expected and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–58.2% Cl wt.)) has been tested in a 3-hour respiration inhibition test (unpublished study; EC, 2005). No effect on respiration was seen up to the highest concentration tested (2,000 mg/L) (Hoechst AG; as reported in BUA, 1992; EC, 2005). Based on these studies, it is unlikely that substances having higher chlorination levels would be toxic to the microorganisms.

Overall, these screening studies are not considered to be the appropriate type of test for concluding on the persistence potential of UVCB substances such as MCCP. The OECD "Guidelines for the Testing of Chemicals, Revised Introduction to the OECD Guidelines for Testing of Chemicals, Section 3 Part I: Principles and Strategies Related to the Testing of Degradation of Organic Chemicals" (OECD, 2006) indicate that ready biodegradability tests are intended for pure substances and are generally not applicable for complex compositions containing different types of congeners, like UVCB. For an UVCB substance, observed biodegradation may indeed represent the biodegradation of only some of its constituents. However, REACH Annex XIII requires that 'the identification shall also take account of assessment of the PBT/vPvB properties of relevant constituents of a substance and relevant transformation and degradation products'. Consequently, the PBT guidance (REACH Chapter R.11, ECHA, 2017b), indicates that if the test item composition does not consist of similar structures or is not well characterised, it may still contain a certain amount of constituents that are persistent although the amount of easily degradable constituents is high enough to lead to an overall degradation percentage sufficient

to meet the criteria for ready biodegradation. As a consequence, based on the outcome of the screening tests (see Table 24) and in absence of information on the degree of degradation of the different groups of congeners[10] in a test, it can be reasonably assumed that the substances tested (see Table 24) contain potentially persistent congeners at a relevant concentration (≥0.1% (w/w)). For UVCB substances, there are uncertainties related to the screening tests where the contribution of the different congeners of MCCP to the overall degradation is unknown. That is why screening tests without further supplementary information enabling the possibility for the dossier submitter to verify the claims made with regard to the composition of the test substance, i.e. the identity of the individual congener groups and their concentration in the substance as well as on the degree of degradation of the individual congener groups in a test, are considered not sufficient to draw conclusions on the persistence of MCCP as a substance and in particular on the persistence of its different congener groups and individual constituents.

As for the studies listed in Table 24 only information on the carbon chain lengths and average chlorination levels is provided with regard to the composition of the substances tested (except for Unpublished 2018a-d studies), the congener groups present in the testing materials were determined using the methodology described in section '1.2 Composition of the substance'. Accordingly, for this determination a Gaussian distribution of the number of chlorine substituents to the alkane chain with a given carbon number is assumed to describe the distribution of the groups of differently chlorinated congeners (e.g. $C_{14}Cl_y$) around the average percentage of chlorination (Yuan *et al.*, 2017a). The distribution is expected to be centred between the congener groups that have a number of chlorine substituents that is equivalent to just above and below the given average degree of chlorination of the total substance. In the following paragraphs, it is demonstrated that even in those studies where the pass-level for ready biodegradation has been reached the respective studies do not really show that all the congener groups present in the substances tested can be considered to screen in the test 'not P'.

The results of the OECD TG 301D for the C_{14} chlorinated n-alkane, 55.0% Cl wt. and the C_{14} chlorinated n-alkane, 60.2% Cl wt. substances indicate that these substances are potentially persistent (see results in Table 24). Based on the screening test results for C_{14} chlorinated n-alkane, 55.0% Cl wt. and as this substance contains C_{14} congener groups having 4 to 12 chlorine atoms, these congener groups screen as potentially persistent. It is worth noting that C_{14} chlorinated n-alkane, 41.3% Cl wt., C_{14} chlorinated n-alkane, 45.5% Cl wt. and C_{14} chlorinated n-alkane, 50% Cl wt. also contain fractions of C_{14} congener groups (at a relevant concentration ≥0.1% (w/w)) with 5, 6, 7 and/or 8 chlorine atoms as C_{14} chlorinated n-alkane, 55.0% Cl wt. As a conclusion, these substances (C_{14} chlorinated n-alkane, 41.3% Cl wt., C_{14} chlorinated n-alkane, 45.5% Cl wt. and C_{14} chlorinated n-alkane, 50% Cl wt.) cannot be rated as ready biodegradable (respectively rated as 'not P') as they always will contain constituents that belong to groups of congeners that screen 'potentially persistent'.

The results of the OECD TG 301D for the C_{15} chlorinated n-alkane, 51% Cl wt. indicate that this substance is potentially persistent based on a weight-of-evidence approach. Indeed, two out of three studies indicate that less than 60% biodegradation had occurred by day 60 (Unpublished, 2014b and Unpublished, 2018d).

The results of the OECD TG 301D for both the 51.7% and 63.2% Cl wt. C_{14-17} chlorinated n-alkane indicate that these substances are potentially persistent (see results in Table 24). It is worth noting that C_{14-17} chlorinated n-alkane, 51.7% Cl wt. contains C_{14} congener groups having 4, 5, 6 and 7 chlorine atoms; C_{15-16} congener groups having 5, 6, 7 and 8 chlorine atoms and C_{17} congener groups having 6, 7, 8 and 9 chlorine atoms that screen as potentially persistent.

Furthermore, C_{14-17} chlorinated n-alkane, 45.6% Cl wt. contains some congeners (at a relevant concentration ≥0.1% (w/w)) with a similar number of chlorine atoms per molecule than for C_{14-17} chlorinated n-alkane, 51.7% Cl wt. As a conclusion, the substance C_{14-17} chlorinated n-alkane, 45.6% Cl wt. cannot be rated as biodegradable as it will contain congeners that screen potentially

[10] i.e. C_xCl_y, where x is in the range of 14 to 17 and y in the range of 1 to x.

persistent.

In summary, based on all the above evidence, it can be reasonably assumed that all substances presented in Table 24 do contain groups of congeners that screen 'potentially persistent'.

3.1.2.1.3 Simulation tests (water and sediments)

An OECD TG 308 study conducted at 12 °C in the dark using non-radiolabelled C_{14} chlorinated n-alkane, 50% Cl wt. (average concentration; the composition of chlorinated congeners was determined analytically as follows: chlorine content between 35.32–72.98% Cl wt. equivalent to 3 to 14 chlorine atoms per molecule) has been performed in accordance with GLP (Unpublished, 2019c). 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 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*.' The water/sediment volume ratio was between 3:1 and 4:1. However, the minimum sediment layer depth was approximately 2 cm and the minimum sediment dry weight was 5 g (with a maximum of 12.11 g) which is lower compared to the recommendation of the OECD TG 308. The test vessels were very small and unusually shaped (conical bases) 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. It is worth noting 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 (absence of microbial activity) were included to assess the analytical recovery. The recoveries of the fortified sediment samples were in the range 70-90%. Additional vessels were set up for characterisation 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. It is worth noting that based on these measurements, it was not possible to demonstrate that the test media was stabilised during the acclimation period. However, it is not expected that the lack of equilibrium in the test media would have changed significantly the test results as they are referring to total water-sediment system.

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 MCCP. 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 constituent-specific method, which is considered to be reliable (although a radiolabelled study could have produced better data in terms of mass balance and compartment association). 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 in the spiked sand 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 the high and the 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 the test substance for non-labelled analysis are between 70 and 110% of nominal. Values measured in this study indicate that no test substance is unaccounted for. Acceptable variations around these values will likely have been incurred through the extraction process and general handling. It is concluded in the study report that chemical analysis showed no observable biotransformation, and so the total water-sediment half-life was >120 days for MCCP at 12 °C. Congener group-specific analyses were presented for the extracted samples and no significant variation was observed between the concentrations of these extracts (including similar congener pattern), the extracted spiked sand and the original test substance. The concentrations of C_{14} chlorinated n-alkane, 50% Cl wt. (total C_{14}) and the concentrations of each congener group (C_{14} Cl_{3-14}) were measured on days 0, 15, 30, 45, 60, 91 and 120. The total water-sediment DT_{50} values under aerobic conditions for the C_{14} Cl_{3-14} congener groups[11] constituting the test substance have been derived using first-order or bi-phasic models and all the predictions for the best-fit models confirmed that there was no degradation of these congener groups over 120 days at 12°C (see Annex XII). The fact that there was no significant measurable degradation over 120 days suggests that it is unlikely that ≥50% mineralisation or primary degradation would occur over a subsequent 60-day period. Therefore, it can be reasonably assumed that the water-sediment degradation half-lives of C_{14} chlorinated n-alkane, 50% Cl wt. and the C_{14} Cl_{3-14} congener groups of MCCP exceed 180 days. This study is considered to be reliable with restrictions. Based on this study it can be concluded that all constituents (≈ structural isomers) belonging to the $C_{14}Cl_{3-14}$ groups of congeners (equivalent to 35.32–72.98% Cl wt.) are very persistent in sediment (degradation half-lives >180 days).

Other simulation studies

Relatively short half-lives of 12 days and 58 days have been reported in aerobic sediment for two MCCP (^{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). 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 MCCP in oligochaetes (*Lumbriculus variegatus*) and are summarised in EC (2005). The reported degradation was based on the difference between

[11] The composition of the chlorinated congeners of the test substance C_{14} chlorinated n-alkane, 50% Cl. wt. was determined analytically as follows: chlorine content between 35.32–72.98% Cl wt. equivalent to 3 to 14 chlorine atoms per molecule.

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. Both values should have been calculated and reported. It is not known if the authors tried to examine non-extractable residues (NER). As no respective activities have been reported (e.g. application of elevated temperature/pressure or acidic extraction conditions), 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 '3.1.2.1.2 Screening tests', the 35% and 69% Cl wt. substances are expected to contain congener groups that screen 'potentially persistent'.

3.1.2.2 Biodegradation in soil

There is some evidence that adapted microbes can degrade chloroparaffins to chloro-olefins. For example, Heeb *et al.* (2019) investigated the degradation of C_{11-13} 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 MCCP in the environment in acclimated or co-metabolic systems.

3.1.3 Field data

3.1.3.1 Occurrence in sediment

Iozza *et al.* (2008) investigated the levels of chlorinated paraffins, including MCCP, in a dated sediment core from Lake Thun, Switzerland. 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 MCCP 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 congener of MCCP present (accounting for 41 to 64% of the total MCCP). Analysis of the chlorine contents indicated that there was a continuous increase in the chlorine contents of the MCCP present in those parts of the sediment cores representing the last 20 years, with higher chlorine content in recent years (surface layer). The chlorine contents were generally between 53.3% and 56.6% (surface: 56.1%) 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.

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 MCCP 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 might be persistent (in terms of the REACH Annex XIII criteria) in these cores. It should be noted that the analytical method used was ECNI-LRMS. The quantification of CP congener groups was performed following the procedure described by Reth and Oehme (2004). According to Iozza *et al.* (2008), this method allows for a reliable quantification even if the degree of chlorination of the samples and of the reference standards are different. Given recent analytical developments, the accuracy of this technique in terms of quantitation may be uncertain. However, the qualitative detection of MCCP can still be considered to be relevant even if the quantification may present some uncertainties.

A further sediment core was analysed for MCCP 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 MCCP 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 MCCP in the area. The MCCP concentrations in the lower layers were relatively constant.

The carbon chain length and chlorine content distribution of MCCP 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 MCCP used in the area over time.

Chen *et al.* (2011) also found that the chlorine content of MCCP 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 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 MCCP 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. Correspondingly to the data from the Iozza *et al.* (2008) study, the accuracy of this technique in terms of quantitation may be uncertain. However, the qualitative detection of MCCP can still be considered to be relevant even if the quantification may present some uncertainties.

Sediment cores from Lake St. Francis, downstream of Cornwall, Ontario, were found to contain total MCCP 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 MCCP have a half-life in sediments longer than 1 year (Environment Canada 2008). The detection of MCCP in a sediment core from 1972 suggests that MCCP 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.* (2017b). A sediment core from an area with wood-related industry was found to contain MCCP at concentrations of < 6.5–93 ng/g dw. The maximum concentration of MCCP occurred in 2015. However, MCCP 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 MCCP. The oldest sediment section in which they were detected was from 1960. A sediment core taken near a steel factory was found to contain MCCP at concentrations of < 6.5–1200 ng/g dw. In this core, MCCP reached their maximum concentration in the top layer.

It is important to note that MCCP were detected in marine sediments from the Arctic (see section '0'). They were found in marine sediments from the Barents Sea and the Norwegian Sea at concentrations in the range of n.d–2.8 mg/kg dw in top layers (corresponding to ca. 10 years of deposition based on the sedimentation rate) between 2006–2018 (Bakke *et al.,* 2008; Boitsov *et al.*, 2016; Boitsov and Klungsøyr, 2018; Boitsov *et al.,* 2019). As MCCP were found in marine sediments from the Arctic, far away from point sources, these results point towards the persistence of MCCP in marine sediments under aerobic conditions.

3.1.3.2 Concentrations in sludge and soil

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

MCCP concentrations in soil measured by Bogdal *et al.* (2017) show an increase from 1989 to 2014 from six sampling sites in Switzerland. MCCP analysis was performed by GC-ECNI-HRMS. The authors could show that MCCP concentrations in soil increased during the whole time period by a factor of two to three, with the highest concentrations occurring in the last sample from 2014. Bogdal *et al.* (2017) found that the concentrations of MCCP became larger than the concentrations of SCCP in the most recent samples, mainly after 2000. The increasing trend observed in Swiss soil samples is in line with the usage pattern for these substances.

3.1.4 Summary and discussion on degradation

Based on screening and assessment information reported in Section '3.1 Degradation' and in accordance with REACH Annex XIII, a weight-of-evidence (WoE) approach is used in order to conclude on the persistence of MCCP at the level of the investigated congener groups ($C_{14\text{-}17}Cl_{1\text{-}(14\text{-}17)}$). The weight-of-evidence approach applied for each congener group is presented below. It is important to note that all studies used in the below described weight-of-evidence approach have been assessed as reliable (with restrictions), relevant and adequate for the assessment, unless otherwise stated. The results of the OECD TG 308 simulation degradation study described in section '3.1.2.1.3 Simulation tests (water and sediments)' is given a high weight in the WoE and it is considered to provide in combination with the QSAR predictions for potential persistence of MCCP congener groups (see section '3.1.2.1.1 Estimated data') sufficient evidence to conclude that the congeners of MCCP with carbon chain lengths between C_{14} and C_{17} with a chlorination number of 3 or higher are persistent and very persistent (P/vP) in sediment. The QSAR predictions are used as supporting information to the experimental data but are considered to be sufficient to support the conclusion drawn on the persistence of MCCP and its congener groups.

Complex composition of the MCCP and related degradation behaviour of the different congeners leads to some challenges in the persistence assessment. However, combining all the available evidence on the degradability of MCCP and its congener groups, the following can be demonstrated:

An OECD TG 308 study (Unpublished, 2019c) performed on C_{14} chlorinated n-alkane, 50% Cl. wt. indicates that the total water-sediment DT_{50} values for the $C_{14}Cl_{3\text{-}14}$ congener groups[12] constituting the test substance are greater than 120 days at 12°C (under aerobic conditions, see Annex XII). The fact that there was no significant measurable degradation over 120 days suggests that it is unlikely that ≥50% mineralisation or primary degradation would occur over a subsequent 60-day period. Therefore, based on this study (Unpublished, 2019c), it can be reasonably assumed that the $C_{14}Cl_{3\text{-}14}$ groups of congeners are very persistent in sediment (degradation half-lives > 180 days). The outcome of this simulation study is the kind of information that according to REACH Annex XIII shall be considered in determining whether the P criteria (Annex XIII 1.1.1 (d)) or the vP criteria (Annex XIII 1.2.1 (b)) are met and therefore is given high weight in the weight-of-evidence based conclusion on the P-properties of MCCP and their congener groups.

No experimental degradation data for specific C_{15}, C_{16} or C_{17} chloroalkane substances and their congener groups is available while they are expected to be less water soluble (Glüge *et al.,* 2013) and more adsorptive (Gawor and Wania, 2013) than the C_{14} substances. QSAR predictions were used in order to investigate possible trends with respect to persistence among the MCCP congener groups of different carbon chain lengths and different levels of chlorination. Applying the screening P criteria from the PBT guidance (Chapter R.11, ECHA, 2017b), the BIOWIN model predicts that almost all of the congener groups of MCCP ($C_{14\text{-}17}$ congener groups with three or more chlorine substituents at the carbon chain) screen as potentially persistent. Furthermore, the BIOWIN model predicts decreased biodegradation with increase in number of chlorine substituents at the carbon chain, because in the model the negative coefficient for the aliphatic chloride fragment is multiplied with the number of chlorine atoms in the structure. When comparing predictions for congeners with different chain lengths but with the same number of chlorine atoms substituted at the hydrocarbon chain (e.g. $C_{15}Cl_5$ with $C_{17}Cl_5$), the predicted degradation decreases with increase in chain length. This is mainly the result of the coefficient for molecular weight decreasing. Based on the predicted and observed trends in physico-chemical properties of structures of the different MCCP congeners, which are in line with the general scientific knowledge on the expected partitioning behaviour and environmental fate of hydrophobic aliphatic chloroalkanes, it can be reasonably estimated that the $C_{15\text{-}17}$ congeners with the same or higher chlorine contents than the congeners of C_{14} chlorinated n-alkane, 50% Cl. wt. (which contains $C_{14}Cl_{3\text{-}14}$ congeners that all are P/vP) will be equally or more adsorptive to sediment, have lower water solubilities and partition stronger to octanol. They therefore will at least be equally if not more persistent in sediments.

Monitoring data on MCCP, used as supporting information in the WoE, are in line with the outcome of the simulation study and the BIOWIN predictions as they point towards persistence of MCCP in sediments.

Several ready biodegradation screening studies under conditions of enhanced bioavailability have been performed with commercial MCCP product types. Based on the results of the screening tests, it seems that the overall level of degradation appears to decline with increasing levels of chlorination (see Table 24). Overall, these screening studies are not considered appropriate for assessing and concluding on the persistence properties of UVCB substances such as MCCP and their constituents. Indeed, based on the outcome of the screening tests and in absence of information on the degree of degradation of the individual congener groups in the tests, it can be reasonably assumed that the substances tested (see Table 24) contain potentially persistent

[12] The composition of the chlorinated congeners of the test substance C_{14} chlorinated n-alkane, 50% Cl. wt. was determined analytically as follows: chlorine content between 35.32–72.98% Cl wt. equivalent to 3 to 14 chlorine atoms per molecule.

congeners. For UVCB substances, there are uncertainties related to the screening tests where the contribution of the different congeners of MCCP to the overall degradation is unknown. Therefore screening tests without further supplementary information enabling the possibility for the dossier submitter to verify the claims made with regard to the composition of the test substance, i.e. the identity of the individual congener groups and their concentration in the substance as well as on the degree of degradation of the individual congener groups in a test, are normally not sufficient to draw conclusions on the persistence of MCCP as a substance and in particular on the persistence of its individual constituents, respectively different congener groups. That is why the outcomes of the screening tests for MCCP have been given a low weight in the weight-of-evidence assessment.
It is important to highlight that the results of the higher tier degradation simulation study (OECD TG 308, Unpublished, 2019c; Annex XIII 3.2: assessment information) are to be given more weight in the weight-of-evidence assessment than the screening studies of the OECD 301 or 302 series reported in Section '3.1.2.1.2 Screening tests' (Annex XIII, section 3.1: screening information). In the presence of a reliable higher tier study, which, inter alia due to consideration of the sediment compartment reflects environmental conditions wider and thus more realistically than the screening studies, it is not necessary to analyse in detail the potential reasons for potentially inconsistent outcomes of the ready biodegradation screening tests. The outcomes of the higher tier study (Unpublished, 2019c), supersede the screening tests.

Abiotic degradation data indicate that MCCP are not expected to hydrolyse significantly. The predicted atmospheric half-life will vary for the MCCP congener groups according to degree of chlorination, with the estimated half-lives increasing with increasing number of chlorine atoms in the structure (Gawor and Wania, 2013). Based on information from Environment Canada (2008), Gawor and Wania (2013), EA (2019) and UK (2021), MCCP congeners have a range of atmospheric half-lives in the vapour phase between 0.6 to 7.1 days, thus indicating a potential for long-range transport in air for some of the MCCP congener groups. According to Howard *et al.* (1975), direct photodegradation in air for MCCP with 45% wt. Cl and 52% wt. Cl is unlikely to be a significant degradation pathway in the environment. There is no experimental data for indirect phototransformation in air. No information is available on phototransformation potential in water or soil. As a conclusion, abiotic degradation of MCCP and MCCP congeners is not considered to be a significant degradation pathway in the environment.

Monitoring data support findings from experimental and predicted data on biodegradation and abiotic degradation of MCCP congeners and MCCP, as well as on potential long-range transport. The available monitoring data, particularly from sediment core studies, suggest some dechlorination of chlorinated paraffins with high chlorine contents in sediment over time, but they also suggest that degradation in the environment may be slow and provide indirect evidence that MCCP with chlorine contents of ~ 55% by weight can persist in sediments for more than a decade. The detection and/or quantification of MCCP in marine sediments from the Arctic, in locations far away from point sources, point towards persistence of MCCP in marine sediments under aerobic conditions. Finally, concentrations of MCCP in sediment and soil seem to have increased over the last decades. Monitoring data is only used as supporting information in the weight-of-evidence approach for concluding on the degradation potential and persistence properties of MCCP.

Overall weight of evidence based conclusion on the persistence properties of MCCP and their congener groups

As an overall conclusion, based on the above information used in a weight-of-evidence-approach, it is concluded that the $C_{14}Cl_{3–14}$ congener groups of MCCP (equivalent to 35.32–72.98% Cl wt.) meet the 'persistence' criterion (P) and the 'very persistent' criterion (vP) in accordance with Annex XIII, points 1.1.1 and 1.2.1, of the REACH Regulation on the basis of their persistent and very persistent (P/vP) properties in sediment (degradation half-lives > 180 days).

Based on the predicted and observed trends in physico-chemical properties it further can be reasonably estimated that also the $C_{15\text{-}17}$ congener groups of MCCP with the same or higher

chlorine contents than the congeners present in C_{14} chlorinated n-alkane, 50% Cl. wt. (which contains $C_{14}Cl_{3\text{-}14}$ congener groups that all are P/vP) will at least be equally if not more persistent in sediment than the congeners of C_{14} chlorinated n-alkane, 50% Cl. wt. Consequently, it is concluded that also the $C_{15}Cl_{3\text{-}15}$, $C_{16}Cl_{3\text{-}16}$ and $C_{17}Cl_{3\text{-}17}$ congener groups of MCCP meet the 'persistence' (P) and 'very persistent' (vP) criteria of REACH Annex XIII (degradation half-life in sediment > 180 days).

Finally, since MCCP always will contain congener groups with P/vP properties at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet both the 'persistence' (P) and 'very persistent' (vP) criteria of REACH Annex XIII (degradation half-life in sediment > 180 days).
Monitoring data on MCCP support the above conclusions as they point towards persistence of MCCP in sediments.

3.2 Environmental distribution

3.2.1 Adsorption/desorption

MCCP are sparingly soluble in water (water solubility up to 27 µg/L). MCCP have a high log Kow, with values for many constituents predicted to be ≥ 6.5 (see Table 9), depending on the chlorine content and carbon chain length. The log Kow can be used to estimate the organic carbon-water partition coefficient (Koc). EC (2005) derived a Koc value of 588,844 L/kg based on a log Kow of 7 (equation used: log Koc = 0.81 log Kow + 0.10). This is in reasonable agreement with the Koc values determined by Fisk *et al.* (1998a) in sediment (Koc = 103,846 L/kg for the $C_{16}H_{30.7}Cl_{3.3}$ 35% Cl wt. and 175,333 L/kg for $C_{16}H_{20.6}Cl_{13.4}$ 69% Cl wt.), based on ^{14}C measurements. A definitive determination of Koc values using short-chain chlorinated paraffins has indicated that the equation used to derive the Koc value for MCCP as reported in EC (2005) is applicable to all chlorinated paraffins (Thompson *et al*., 1998). The low solubility in water (maximum 0.027 mg/L – see Section 1.3) and the high log Koc values indicate that MCCP are likely to partition to suspended matter and sediment in aquatic environments.

Ma *et al.* (2018), found the C_{14} congener in the particulate phase of seawater. Gawor and Wania (2013) predicted that the association of MCCP constituents with dissolved or suspended particulate phases in the water column depends on the degree of chlorination and the position of the chlorine atoms on the carbon structure. The transition between the dissolved and the suspended particle phases in the water column for MCCP will start for constituents with moderate degrees of chlorination (with ~ 4 chlorine atoms independently of the carbon chain lengths; Gawor and Wania, 2013). It is expected that MCCP constituents with low chlorine atom numbers will preferentially partition to the dissolved phase while MCCP constituents with higher number of chlorine atoms will preferentially partition to the suspended particle phase in the water column. Overall, and based on the Gawor and Wania predictions (2013), the MCCP constituents are expected to be predominantly present in the suspended particle phase in the water column rather than in the dissolved phase.

According to Gawor and Wania (2013), in soil almost all of the constituents of CP (S/M/LCCP) are expected to sorb completely to organic solids. Two transport processes affect the mobility of the CP constituents in soil: evaporation or particle erosion. Generally, the constituents with less number of halogens or smaller carbon structures would evaporate from soils, while others would only undergo particle erosion. As the CP constituents are relatively hydrophobic, most are unlikely to be subject to leaching and reach groundwater, although some SCCP may be sufficiently water soluble. The authors predicted that SCCP and MCCP with 3–4 and 3–5 chlorines respectively, will be subject to both evaporation and erosion in soils. Any constituents of CP with less chlorine atoms are more subject to evaporation, whilst constituents with more chlorines are more subject to erosion in soils. According to EC (2005), vertical movement of MCCP adsorbed onto soil particulates via macropores may provide a transport mechanism in soil.

3.2.2 Volatilisation

Measured data

Campbell and McConnell (1980) experimentally determined a 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, suggesting a low vapour pressure. This study was considered previously in EC (2005) and is also cited in the UK draft proposal to list MCCP as a POP under the Stockholm Convention (UK, 2021).

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 and UK, 2021) and EC, 2005; see values reported in Table 9).
There is no experimental information available on the variation of vapour pressure with carbon chain length and chlorine content for MCCP constituents. 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 MCCP.

Predicted data

Glüge *et al.* (2013) calculated subcooled-liquid vapour pressure for 29 congener groups of MCCP using COSMO*therm*, SPARC and EPI Suite™, and compared the results to experimental data from the literature. A series of recommended property values (see Table 25) were derived with COSMO*therm*, as predictions from this model fitted the experimental data best. These predicted values indicate that vapour pressure is likely to decrease with increasing carbon chain length and chlorine content.

The congener groups of MCCP have a very low vapour pressure at environmentally relevant temperatures.

Table 25: Key physico-chemical property values for MCCP congener groups as recommended by Glüge *et al.* (2013)

Molecular formula	Vapour pressure (Pa) (at 25°C)	Water solubility **(µg/L)**	n-Octanol solubility (g/L)	log Kow
$C_{14}H_{29}Cl_1$	0.11 – 0.12	3.65 – 4.57	274 – 275	7.66 – 7.76
$C_{14}H_{27}Cl_3$	1.3 x 10^{-4} – 0.013	5.02 – 40.4	297 – 412	6.77 – 7.80
$C_{14}H_{25}Cl_5$	7.9 x 10^{-5} – 0.0014	3.86 – 34.4	329 – 550	6.88 – 7.89
$C_{14}H_{23}Cl_7$	<1 x 10^{-6} – 1.5 x 10^{-4}	3.16 – 44.5	219 – 524	6.57 – 7.97
$C_{14}H_{21}Cl_9$	<1 x 10^{-6} – 1.5 x 10^{-5}	2.78 – 272	366 – 560	6.21 – 7.99
$C_{14}H_{19}Cl_{11}$	<1 x 10^{-6}	2.60 – 87.0	431 – 670	6.87 – 8.09
$C_{14}H_{18}Cl_{12}$	<1 x 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 x 10^{-4} – 0.0039	1.56 – 9.88	297 – 403	7.37 – 8.30
$C_{15}H_{27}Cl_5$	7.6 x 10^{-6} – 5.1 x 10^{-4}	1.12 – 13.8	251 – 486	7.14 – 8.41
$C_{15}H_{25}Cl_7$	<1 x 10^{-6} – 5.2 x 10^{-5}	0.93 – 17.0	228 – 484	6.99 – 8.48
$C_{15}H_{23}Cl_9$	<1 x 10^{-6} – 5.6 x 10^{-6}	0.72 – 7.38	300 – 579	7.61 – 8.55
$C_{15}H_{21}Cl_{11}$	<1 x 10^{-6}	0.89 – 68.1	384 – 596	6.88 – 8.54
$C_{15}H_{19}Cl_{13}$	<1 x 10^{-6}	0.50 – 16.1	287 – 639	7.53 – 8.62

Molecular formula	Vapour pressure (Pa) (at 25°C)	Water solubility **(µg/L)**	n-Octanol solubility (g/L)	log Kow
$C_{16}H_{33}Cl_1$	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.

Based upon their low vapour pressure values, MCCP have a low potential for volatilisation to the atmosphere. However, concentrations of MCCP found in air from remote regions indicate that atmospheric transport is occurring. Furthermore, monitoring data (Ma *et al.*, 2018; Jiang *et al.*, 2021; Ma *et al*., 2014) suggest that constituents of MCCP can be found in the gas and in the particulate phases of the atmosphere. The pattern observed for the constituents, respectively the congener groups in the different phases (gas or particle phases), will depend on the degree of chlorination and carbon chain lengths of the congener groups (for further information see monitoring data in section ‘0 3.3.2.1 Concentrations in air’).

3.2.3 Distribution modelling

The Level III Fugacity Model (MCI method) and the STPWIN model of EPI Suite (v. 4.11) (US EPA, 2012) were run for the constituents $C_{14}Cl_6$ (52 % Cl wt.) and $C_{16}Cl_7$ (53 % Cl wt.), using SMILES for one constituent per congener group. These constituents were chosen because the majority of product types have a chlorine content between 45-52 % by weight and the C_{14} chlorinated alkane dominates in the commercial products (EA, 2018). The C_{16} congener was chosen because of its longer carbon chain length so that a comparison between two different chain lengths would be possible. The parameters vapour pressure (2.7×10^{-4} Pa (experimental value) and 1.3 x 10-5 Pa (Glüge *et al.* (2013) respectively) and log Kow (6.4 and 7.07 (ACD Percepta log P methods) respectively) were taken as input to the models. The rest of the parameters used in the model were predicted values from the models within EPI Suite. The values for water solubility and Henry’s law constant were estimated values, and the predictions were in lines with the experimental data and with the recommended calculated ranges proposed by Glüge *et al.* (2013). The connectivity (MCI)-based method of KOCWIN was selected. No half-life data was used as input, as this is lacking for the water and soil compartments. The default emission rate of equal amounts emitted to air, water, and soil was used, with the single level output option.

Table 26: Distribution of MCCP in environmental compartments according to the Level III Fugacity Model (MCI method; US EPA, 2012)

Constituent	$C_{14}Cl_6$ (52 % Cl wt.) Mass amount (%)	$C_{16}Cl_7$ (53 % Cl wt.) Mass amount (%)
Air	0.007	0.003
Water (total)	1.55	0.88
Water	1.03	0.24
Biota	0.13	0.14
Suspended sediment	0.39	0.50
Soil	64.6	56.1
Sediment	33.8	43

Table 27: Modelled removal of MCCP in wastewater treatment plant that uses activated sludge secondary treatment (STPWIN model of EPI Suite (v. 4.11); US EPA, 2012)

Constituent	$C_{14}Cl_6$ (52 % Cl wt.) Removal (%)	$C_{16}Cl_7$ (53 % Cl wt.) Removal (%)
Total removal	93.28	93.87
Total biodegradation	0.77	0.78
Total sludge adsorption	92.51	93.10
Total to air	0.00	0.00

The Level III Fugacity Model shows that MCCP will be distributed mainly to the soil and the sediment compartments once released into the environment (see Table 26). Based on the above predictions (see

Table 27), MCCP will be mainly removed to sludge in a wastewater treatment plant given its high K_{OC} and limited biodegradation potential.

3.2.4 Field data

Monitoring data for MCCP in surface water, sediment, soil, biota, sludge and air are reported in 'Annex III – Summary of environmental monitoring data'.

The available European monitoring data generally show widespread occurrence of MCCP in water (at concentrations up to 4.6 µg/L (particulate)), sediment (at concentrations up to 65 000 µg/kg dw (near Industrial areas in UK)), in soil (at concentrations up to 282 ng/g dw in Norway) and biota (in recent studies: up to 540 µg/kg lipid (liver in 2014-2015) in grey seal, up to 720 µg/kg lipid (muscle in 2013-2017) in eagle owl, up to 1 600 µg/kg lipid (muscle in 2012-2015) in moose and up to 830 µg/kg lipid (muscle in 2012-2016) in grey wolf from Scandinavia; up to 5390 µg/kg ww in Atlantic cod liver from Norway in 2018). MCCP was also found in sludge from Norway at concentrations up to 17 000 µg/kg. In a recent study, MCCP were present at an average concentration of 327 pg/m^3 in air samples from Birkenes in Norway (in 2019).

3.2.5 Summary and discussion of environmental distribution

MCCP are strongly hydrophobic with a low water solubility (up to 27 µg/L) and high log Kow values (log kow ≥6.5). Based on their predicted high log Koc values (up to 588 844 L/kg, derived based on a log kow of 7) MCCP are expected to partition to suspended matter and sediment in aquatic environments.

The distribution modelling shows that MCCP are likely to be associated mainly with the soil and sediment compartments when released to the environment but would also occur in the water compartment (particle and dissolved phases and biota) if released to water. Removal during wastewater treatment processes is estimated to be around 94% mainly by adsorption onto

sludge.

In soil, MCCP are expected to be adsorbed to soil particulates. According to Gawor and Wania (2013), two transport processes affect the mobility of the CP constituents in soil: evaporation or particle erosion. Generally, the constituents with less number of halogens or smaller carbon structures would evaporate from soils, while others would only undergo particle erosion. As the CP constituents are relatively hydrophobic, most are unlikely to be subject to leaching and reach groundwater. According to EC (2005), vertical movement of MCCP adsorbed onto soil particulates via macropores may provide a transport mechanism in soil.

Constituents of MCCP have a very low vapour pressure (1.3 – 2.7 x 10^{-4} Pa at 20 °C for a C_{14-17} chlorinated n-alkane, 52% Cl wt.) at environmentally relevant temperatures. According to Glüge *et al.* (2013), the vapour pressure of MCCP constituents is likely to decrease with increasing carbon chain length and chlorine content. Based upon their low vapour pressure values, MCCP constituents have a low potential for volatilisation to the atmosphere. However, concentrations of MCCP found in air from remote regions indicate that atmospheric transport is occurring. Furthermore, monitoring data (Ma et al., 2018; Jiang et al., 2021; Ma et al., 2014) suggest that constituents of MCCP can be found in the gas and in the particulate phases of atmosphere. The constituents pattern in the different phases (gas or particle phases) will depend on their degree of chlorination and carbon chain lengths.

The available European monitoring data show widespread occurrence of MCCP in surface water, sediment, soil, biota, sludge and air.

3.3 Data indicating potential for long-range transport

Physical-chemical properties of individual chloroalkanes depend on their molecular structure. As a chemical group, chlorinated paraffins have physical-chemical properties similar to legacy persistent organic pollutants (POPs), i.e. low water solubility, semi-volatility and a logarithmic octanol-water partition coefficient (Kow) above 3.

The potential for long-range atmospheric transport has been considered briefly in EC (2005 and 2007). SCCP 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 MCCP appears to be lower than SCCP. This is because MCCP generally have lower vapour pressures and are likely to adsorb more strongly to soil and sediment than SCCP. However, MCCP are a UVCB substance with congeners exhibiting a range of physico-chemical properties. Some congeners of the commercial products may have properties that mean that long-range transport via the atmosphere is a possibility.

3.3.1 Modelling data

The predicted atmospheric half-life will vary for the MCCP congeners according to degree of chlorination with the estimated half-lives increasing with increasing number of chlorine atoms in the structure (Gawor and Wania, 2013). Based on information from Environment Canada (2008), Gawor and Wania (2013), EA (2019) and UK (2021), MCCP congeners have a range of atmospheric half-lives in the vapour phase between 0.6 to 7.1 days, thus indicating a potential for long-range transport for some of the MCCP congener groups (see further information in section '3.1.1.3.1 Phototransformation in air'). According to Howard *et al.* (1975), direct photodegradation in air for MCCPs with 45% wt. Cl and 52% wt. Cl is unlikely to be a significant degradation pathway in the environment. There is no experimental data for indirect phototransformation in air.

Environment Canada (2008) reports vapour pressure (4.5 × 10^{-8} to 2.27 × 10^{-3} Pa (values not given at a consistent temperature)) and Henry's law constant (0.014 to 51.3 Pa.m^3/mol) values for MCCP 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. Table 28 compares vapour

pressure and Henry's law constant of some identified POPs with MCCP as they have been reported by Environment Canada (2008).

Table 28: Volatility of MCCP and some POPs (Environment Canada, 2008)

Substance	Vapour pressure (Pa)	Henry's law constant ($Pa.m^3/mol$)
MCCP	4.5×10^{-8} to 2.27×10^{-3} Pa (C_{14}-C_{17} 42 – 58% Cl wt.) ($1.3 – 2.7 \times 10^{-4}$ Pa at 20 °C (52% Cl wt.), experimental value reported by EA (2018))	0.014 to 51.3 $Pa.m^3/mol$ (C_{14}-C_{17} 37 – 56% Cl wt.)
Lindane	4.3×10^{-3} Pa	0.13 $Pa \cdot m^3/mol$
Heptachlor	3.0×10^{-6} Pa	0.02 $Pa \cdot m^3/mol$
Mirex	2.3×10^{-9} Pa	-

It is worth noting that the OECD *P*ov[13] and LRTP Screening Tool (Wegmann *et al.*, 2009) was not run for MCCP due to uncertainty on the input parameters to the model (such as: the half-lives in air, in water and in soil for which no experimental data are available).

Gawor and Wania (2013), used different quantitative structure–property relationships (QSPR), chemical fate models and the chemical partitioning space to investigate the potential long-range transport and bioaccumulation in humans of complex halogenated substances such as CP. The authors have displayed model results in so called chemical space maps according to partition properties, with partitioning between air and octanol (Koa) on the *x*-axis and between air and water (Kaw) on the *y*-axis. Predicted results for partitioning (at 25 °C) for a relatively large number of constituents of CP have been displayed on the maps as points, forming a so called "cloud" on the map. According to the authors these chemical space maps can be used to identify congener groups with potential for long-range transport and/or bioaccumulation, as well as to predict the partitioning into various environmental compartments and the dominant transport processes for the congeners of mixtures.

For the study, 10% and 1% of the total number of potential constituents of MCCP and LCCP, respectively, were chosen at random using a normal Gaussian distribution. The total number of MCCP constituents was estimated at 123 166 based on the formulae proposed by Shojania (1999) and 12 058 were used in this study. Since there is an increasing overlap in physical–chemical properties at higher chain lengths, this was considered an adequate number of constituents. CP were assumed to hold no more than one chlorine per carbon, as the likelihood for a second chlorine substitution on the same carbon decreases greatly with increasing chain length. Additionally, the chlorination range of these CP (with carbon chain lengths between $C_{10–20}$) was limited to between 30 and 70% (by mass) as this generally had been the range for commercial products. Consideration of the placement of the halogens on the skeletal structure was noted, as steric hindrances imposed by the halogens may prevent the formation of certain structures. Even so the authors noted that constituents that are not likely to exist may be present in the selection.

Gawor and Wania (2013) predicted log Kaw (based on ACD/Absolv (ACD/ADME Suite 5.0) using the LSER equation (Abraham *et al.*, 1994)), log Kow (based on ACD/ADME Suite 5.0) and calculated log Koa (from the log Kow (adjusted to dry octanol) and the log Kaw values) for the constituents of the CP. The authors observed that constituents within CP can vary greatly in partitioning properties. For CP the partitioning constants range over more than fifteen orders of magnitude. The range of predicted log Koa and log Kaw for MCCP was 5.96 – 16.08 and -7.66 –

[13] *Pov* means overall persistence.

1.13, respectively. As the carbon chain length of CP increases, the Koa values increase, i.e. the constituents are getting less volatile. However, the Kaw is relatively unchanged by an increasing carbon chain length, indicating that the water solubility and the vapour pressure of CP changes to a similar extent. The Kaw decreases and Koa increases with increasing degree of halogenation. Constituents with more halogens favour the aqueous and organic phase relative to the gas phase. Relatively high Koa and low to moderate Kaw values for most CP constituents means that they can be expected to associate primarily with organic matter in soils and sediments. Overall, these observations are consistent with expectations, as both laboratory and field studies have observed that generally the "larger" congeners of CP (i.e. those more halogenated or having longer chains) are less water soluble and less volatile, and therefore are more likely to have a high affinity for soils or sediments.

The authors also found out that atmospheric half-lives of CP (estimated with AOPWin v1.92 (EPI Suite, 2011)) increase with the degree of chlorination, whereas the chain length plays less of a role. Gawor and Wania (2013) estimated relatively short degradation half-lives in air of less than two days for most CP (the range was < 1 days to > 5 days), with the constituents with relatively low degree of chlorination having the lowest half-lives in air. Gawor and Wania (2013) divided the constituents into classes of modes of global transport depending on their Koa and Kaw values ("fliers", "multiple hoppers", "swimmers" or "single hoppers"). They classified the heavily halogenated CP such as: SCCP: $Cl_{\sim 9-10+}$; MCCP: $Cl_{\sim 4-6+}$; LCCP: Cl_{4+}, that have log Koa exceeding 10 as "single hoppers". "Single hoppers" are retained in soil or water compartments after particle deposition and would not effectively volatise to undergo "multiple hops" (i.e. repeated cycles of deposition and re-evaporation) to higher latitudes. These constituents would need to undergo LRT without being deposited along the way in order to accumulate in remote locations like the Arctic. Sorbed to aerosol they would be effectively scavenged from the atmosphere by dry and wet deposition. As such, their accumulation potential in the Arctic is quite low, approximately 0–20% of the maximum Arctic Contamination Potential (ACP) value. Analysing the chemical partitioning space maps for MCCP displaying the modes of global transport and the ACP, it can be seen that some constituents of MCCP are in the class of "multiple hoppers" and the Artic Contamination Potential value can be up to 60 % of the maximum value. These constituents correspond to the predicted log Kaw values of above -2 and log Koa values lower than 10 and would be the shorted carbon chain congeners with low degree of chlorination. The authors stated that "multiple hoppers" can undergo gas exchange mostly with terrestrial surfaces and have the potential to accumulate significantly in Artic surface media (Gawor and Wania, 2013). This prediction is confirmed by monitoring data for MCCP.

All MCCP congeners are relatively hydrophobic, and only a very small fraction could possibly be dissolved in raindrops. Nevertheless, wet vapour scavenging may be a relevant deposition process for some SCCP and MCCP, especially at temperatures below 25°C (Gawor and Wania, 2013).

The authors also estimated the metabolic half-lives of CP in fish (estimated with BCFBAF v3.01, EPI Suite™) and by iterative fragment selection (IFS) (Brown *et al.*, 2012). They observed that metabolic half-lives of CP in fish are more governed by the size of the carbon structure and to a lesser degree by the chlorination degree. In addition, their modelling of environmental bioaccumulation potential found that both the size of the carbon skeleton and the number of halogens influence which components will be bioaccumulative, which is illustrated by SCCP, MCCP, and LCCP with ~5–6, ~4–5, and ~4–5 chlorines respectively having the highest potential for bioaccumulation in humans of all the CP congeners. Any CP holding less chlorine would have a small potential to bioaccumulate in humans, according to the model. In general, the constituents with partitioning properties favouring bioaccumulation (high Koa and low Kaw, meaning less volatile and with preference to partition to organic media) tend to also have a higher degradation half-lives in fish. Specifically, SCCP with 12 - 13 carbons and MCCP with ~5–6 and ~6–7 chlorines, respectively, were identified to have the highest combined potential for LRT and bioaccumulation in humans (the so called Arctic contamination and bioaccumulation potential (AC-BAP)) and thus to have the potential to be persistent organic pollutants. Monitoring data tend to confirm this prediction as it has been found that MCCP congener groups with C_{14-15}

and Cl_{4-9} were found in the Arctic (biota; Reth *et al.,* 2006) and in the Antarctic (air; Ma *et al.,* 2014 and Jiang *et al.*, 2021). LCCP with 4 chlorines and 18 carbons were also predicted to have Arctic contamination and bioaccumulation potential (AC-BAPs).

It is worth noting that the QSPR predictions used in this study have considerable uncertainty due to the limited number of experimental values for individual congener groups. As a consequence, the outcome of this study should be considered with caution. The study, however, illustrates that the partitioning properties of the many congener groups of MCCP differ significantly, which in turn will affect the long-range transport, as well as other environmental fate properties of this substance. Therefore, the various congener- groups need to be considered in the LRT assessment.

Ma *et al.,* 2018 estimated the net air–seawater exchange flux and dry deposition of CP in a typical coastal area of China in May and August 2016. The fugacity ratios (log fa/fw) between air and seawater indicated a net deposition process for most CP formula groups.

The authors found that the air–seawater gas exchange of CP was significantly higher than dry deposition in the sampling areas. One of the interesting phenomenon was that the dissolved ∑CP in seawater positively correlates to the wind speed in both seasons, indicating the wind speed is also an important factor influencing the occurrence of CP in seawater (i.e. the increasing of wind speed can increase the air–seawater diffusion).

∑CP in the seawater increased with decreasing salinity in both seasons, indicating the influence of the riverine input of terrestrial sources. Furthermore, a comparison between different sites shows that the diffusion and dry deposition fluxes adjacent to the coastal areas are higher than those in the middle of the sea during the spring, indicating that the contribution from the land sources through atmospheric transport is significant.

For MCCP, the C_{14} congeners dominated in the particle phase of atmosphere and particulate phase of seawater. Generally, the CP congeners with highest deposition flux were Cl_8 congener groups, followed by Cl_7 and Cl_9 congener groups, which is consistent to the CP formula group patterns both in air and seawater samples. The CP congeners with higher volatilisation flux are mostly Cl_5. The result further indicates that the concentration level of CP and the temperature are important factors effecting the air–sea diffusion flux.

Since the temperature might be an important factor in affecting the occurrence of CP in both air and seawater, distribution and air–seawater gas exchange in winter might present some difference from the results of spring and summer.

3.3.2 Monitoring data

As a consequence of the challenges associated with the correct quantification of CP in environmental samples CP concentrations may have a higher uncertainty than concentrations of other POPs reported from the Arctic. Furthermore, the high inter-laboratory variation that has been documented in inter-laboratory comparisons limits the comparability of data between laboratories, for example in assessments of temporal trends.

3.3.2.1 Concentrations in air

Bohlin-Nizzetto *et al.* (2020), presented monthly and annual concentrations of selected environmental contaminants (including S/MCCP) in air at Norwegian background sites in 2019. According to Bohlin-Nizzetto *et al.* (2020), the monitoring stations/observatories have been placed/located, as far as possible, in areas that are not influenced by local sources. Two observatories are used for the monitoring of S/MCCP in air. These are located on the mainland of Norway: Birkenes in southern Norway (58°23'N), and one is located on Svalbard in the Arctic: Zeppelin (78°54'N). S/MCCP were weekly sampled at Zeppelin since 2013 (sampling durations: 48h) and monthly sampled at Birkenes since 2017 (sampling durations: 24h).

Air samples were collected with two types of high-volume air samplers. The samplers consisted of a pump that draws air through the samplers with an average air flow rate of 25 m^3/hour; a glass fibre filter (GFF) that collects the particle-associated compounds; and a set of two pre-cleaned PUF plugs or a set of PUF/XAD/PUF sandwich that collect the gas phase compounds. For S/MCCP data are reported for sum gas- and particle phase (i.e. bulk concentrations). Flow-rate and sampling conditions were digitally monitored and documented (e.g. power failures, etc.) as an integrated part of the sampling and quality control procedure. The sampling methodologies have been optimised to achieve maximum detection while minimising the influence of possible sampling artefacts, such as breakthrough and degradation. In addition, a number of field blank samples followed the yearly sample batch in order to control potential contamination risks. The GFF and PUFs were extracted in the same solvent to obtain the bulk concentration (gas+particle phase) of the individual target compounds.

The filters and the corresponding PUF plugs were extracted separately, but in the same solvent in order to aggregate the sample. Before quantitative analysis, 20 µL of unlabelled tetrachloronaphthalene (TCN, 100 pg/µL) was added as recovery standard (RS). Identification and quantification of SCCP and MCCP was carried out using GC coupled to an Agilent HR qToF (time of flight) in Electron Capture Negative Ion (ECNI) mode. A mass window of ± 20 ppm were used for extraction of the ions for quantification. The lab blanks were obtained by extracting pre-cleaned sampling material (e.g. PUFs, filters, XAD, ABN) in solvent and using the same clean-up and analytical procedures as real samples and field blanks. The LOD was defined as the average blank concentrations plus 3 times standard deviations (SD) of the blank concentrations. The LOQ was defined as the average blank concentrations plus 10 times SD. Values below LOD were used as LOD/2 in further statistical treatment.

Sampling and analysis of the organic contaminants of emerging concern (including S/MCCP) are associated with a bigger uncertainty due to more diffuse sources in laboratories and sampling facilities (e.g. the use of CP has increased again in a lot of different industrial, household products and consumer goods during the last years) that results in a larger risk for contamination. Samples cannot be sampled, stored, extracted and prepared for analysis without any physical contact with a lot of different materials and instruments. This causes a raising number of blank samples exceeding the acceptance level, which in consequence raises the limit of detection for samples analysed in parallel with those blank samples. A sample blank treatment commonly has been used for S/MCCP. The mass of the target compounds in each sample was compared to the average mass in the field blanks (on a site-specific basis). As in other published studies, the blank levels for the SCCP and MCCP were variable and high, resulting in relatively high average blank values (10-50% of detected masses). All samples were therefore blank corrected for the average blanks. Approximately 30% of the measurements for MCCP were below the average blank.

The monitoring data for M/SCCP at Zeppelin are the first measurements of M/SCCP in Arctic air. According to Bohlin-Nizzetto *et al.* (2020), the presented data should be considered as semi-quantitative as the contribution of possible contamination during sampling and analyses have not yet been fully validated. Monthly mean concentrations of S/MCCP in air at Zeppelin in 2019 are reported in Table 29. The annual mean concentration, median and range of SCCP were 230 pg/m^3 (median 225 pg/m^3, range: 21-420 pg/m^3). For MCCP two outliers were observed in 2019 resulting in annual mean concentration of 241 pg/m^3 (median 72 pg/m^3, range <44-3900 pg/m^3). Excluding the two outliers the annual mean concentration for MCCP at Zeppelin was 170 pg/m^3 (median 72 pg/m^3, range <44-720 pg/m^3). The annual mean concentrations measured for SCCP do not show any significant difference between the years (2013-2019). In contrast, the concentrations of MCCP are higher during the last years, indicating an increasing trend for MCCP. As previous years, the concentrations of SCCP are significantly higher than those of MCCP (2-7 times) in a majority of the samples (55%), especially during the summer months. Interestingly, the dominance of SCCP are smaller in 2019 than in previous years. In 2019, the concentrations of MCCP are higher or similar to the SCCP in 42% of the samples, with a dominance of those being observed during the winter period. This is a change compared to all

previous years when only <10% of the total samples had higher or similar concentrations of MCCP than SCCP. This together with the increase of concentrations may suggest higher emission of MCCP.

According to Bohlin-Nizzetto *et al.* (2020), the concentrations of SCCP and MCCP measured at Zeppelin in 2013-2019 are similar to those observed in rural air in Canada, but almost three orders of magnitude lower than recent results from urban to rural sites in China and India (Wang *et al.*, 2013, Chaemfa *et al.*, 2014).

Table 29: Monthly mean concentrations (pg/m^3) of S/MCCP in air at Zeppelin in 2019 (Bohlin-Nizzetto *et al*., 2020)

Zeppelin	Jan.	Feb.	Mar.	Apr.	May	Jun.	Jul.	Aug.	Sept.	Oct.	Nov.	Dec.
SCCP	236	240	125	236	213	198	186	228	241	301	350	175
MCCP	197	324	208	159	169	44	50	73	130	187	271	331

MCCP at Zeppelin were lowest in summer and highest in winter but fluctuating from month to month at Birkenes.

Monthly and annual mean concentrations of MCCP in air at Birkenes in 2019 are provided in 'Annex III – Summary of environmental monitoring data'. The annual mean concentrations at Birkenes in 2019 for SCCP were 220 pg/m^3 (mean and median, range 74-350 pg/m^3). The annual mean concentration for MCCP were lower in 2019 than in 2018; 330 pg/m^3 in 2019 including one outlier (range <95-1500 pg/m^3). Excluding this outlier, the annual mean concentration for MCCP in 2019 was 230 pg/m^3 (range <95-730 pg/m^3). The higher concentrations in 2018 was mainly attributed three extreme concentrations observed in 2018. The concentrations of SCCP are similar at Birkenes and Zeppelin in 2019. The concentrations of MCCP were however higher at Birkenes than at Zeppelin. The detected amount of MCCP were higher than SCCP in ~50% of the samples at Birkenes, similarly to previous years (2017–2018).

Bohlin-Nizzetto *et al.* (2020) concluded that the highest concentrations in air of all the targeted contaminants were observed for cyclic volatile methylsiloxanes, phthalates, polycyclic aromatic hydrocarbons, SCCP/MCCP, and organophosphorous flame retardants.

Jiang *et al.*, (2021) analysed the short-chain chlorinated paraffins (SCCP) and medium-chain chlorinated paraffins (MCCP) in both gas and particle phases at King George Island, West Antarctica (the Chinese Great Wall Station; latitude: 62°12'59"S; longitude: 58°57'52"W), from January 2014 to December 2018.

A total of 120 samples were collected using polyurethane foam (PUF) plugs and glass fibre filters (GFF). CP were quantified using an Agilent 7890B chromatograph in tandem with a 7200 gas chromatography quadrupole time-of-flight (GC-QTOF) mass spectrometer in negative chemical ion (NCI) mode. The quantification of SCCP and MCCP was conducted by four separate injections according to the optimised condition as described in Zeng *et al.* (2011). The authors found that the simultaneous detection of SCCP and MCCP combined with chemical calculation can effectively identify and exclude interferences (Zeng *et al.,* 2011). Two laboratory blanks were processed with a dozen samples to eliminate the effects of matrix interference. Besides, GFF and PUF matrix blanks (n= 10) were also treated as field blanks and analysed in the same way as samples, respectively. The procedural blank levels were used to calculate the method detection limits (MDLs), defined as three times the standard deviation (SD) of the procedural blanks from all batches. The MDLs in this study were 1.93 and 0.26 pg/m^3 for SCCP and MCCP, respectively. The recoveries of the internal standard (chlordane) were in the range of 73–119% (mean: 97%). The mass concentration of gas- and particle-phase CP was reported as the amount of CP in PUF and GFF samples divided by the sampling volume, respectively. All reported concentrations of CP (see Table 30) were corrected by the recovery of the internal standard.

Table 30: CP concentrations (pg/m^3) in atmosphere of King George Island, Antarctica between January 2014 to December 2018 (Jiang *et al.,* 2021)

	Gas-phases (PUF)				Particle-phases (GFF)				Total	
	Min	Max	Mean	SD	Min	Max	Mean	SD	Mean	SD
ΣSCCP	63.1	4060	1070	998	3.48	533	105	118	1170	1040
ΣMCCP	<0.26	27.5	6.33	4.19	<0.26	6.28	1.60	1.59	5.12	3.92
ΣCP	63.1	4080	1070	1000	3.50	536	107	118	1180	1090

The atmospheric levels of MCCP ranged from <0.26 to 27.5 pg/m^3, with a mean value of 5.12 pg/m^3 (particle and gas phases). Concentrations of MCCP found in this study are comparable to those found in the study of Ma *et al.* (2014) where samples were collected in 2013 at the same sampling station in King George Island. An increasing trend was observed in the ratio of MCCP to SCCP from 2014 to 2018. These results showed that the use of MCCP as substitute to SCCP had increased. The congeners pattern of CP in the gas and particle phase was calculated by the authors (Jiang *et al.*, 2021) as follows: for SCCP 91.0% were in the gas and 9.01% in the particle phase species and for MCCP 72.1% were in the gas phase and 27.9% in the particle phase. This indicated that CP preferentially existed in the gas phase in the sampling region. The total CP congener group patterns at the Great Wall Station showed that for MCCP, the congeners with Cl_{7-8} accounted for up to 70.8% in the particle phase. In the gas phase, the most abundant chlorinated congeners of MCCP were Cl_{6-7} (60.8%). Based on the back-trajectory model, Jiang *et al.* (2021) made the assumption that the levels of CP in West Antarctica were affected by the airmass passing through South America, Southern East Pacific, and the Antarctic continent, except the East Pacific.

Jiang *et al.* (2021) concluded that the levels of SCCP or MCCP displayed a slightly increasing pattern from 2014 to 2018. The authors reported that the proportion of CP congeners with longer carbon chains (C_{12-14}) increased over time, especially in the particle phase due to their higher affinity for this phase. A possible reason for this might be the gradual restriction on the use of SCCP by the adjustment of the industrial structure of CP products. As one of the substitute chemicals of SCCP, MCCP might have been used instead and increasingly emitted into the environment.

Ma *et al.* (2014) investigated the concentrations, distribution and gas-particle partitioning of CP in the Antarctic area. Air sampling was conducted from January 16th to February 8th 2013 (in summer), using a high-volume air sampler on a mountain (40 m above ground level) in King George Island, Fildes Peninsula of Antarctica (Great Wall Station, China; latitude: 62°12'59" S; longitude: 58° 57' 52"W).

Twenty four air samples were collected on 48 h intervals. Gas- and particle-phase CP were collected using polyurethane foam plugs (PUF) and glass fibre filters (GFF) respectively. The total suspended particulate (TSP) in air was determined by weighing the mass difference of GFF before and after sampling. The CP concentrations in the gas- and particle-phases were reported by their levels in PUF and filter samples, respectively.

The analysis of the CP was performed on a 5973i triple quadrupole mass spectrometer coupled with a 6890A GC at ECNI mode. The chromatographic peak areas of SCCP congeners were first corrected by removing the interference from MCCP congeners based on the method of Zeng *et al*. (2011). The authors developed an analytical approach based on ECNI-LRMS to minimise mass interferences by simultaneous detection of SCCP and MCCP (Zeng *et al*., 2011). The actual relative integrated signals for each congener were obtained by correcting the SIM signals of [M − Cl]− ions from isotopic abundance and response factors. This method enabled deviations of < 10% for the reference set. The quantifications of SCCP and MCCP were conducted using the procedure described by Reth *et al.* (2005b), respectively. The authors (Reth *et al.,* 2005b) developed a compensation technique, which minimised the influence of the degree of chlorination on the response factors of different CP mixtures, when ECNI-LRMS is employed (with deviations between 7–33% for five independent SCCP control samples). Field blanks and three laboratory blanks were extracted and analysed in the same way as field samples. The MDLs for PUF and GFF were estimated to be 0.1 pg/m and 0.05 pg/m when converted by average volume of 2880

m^3, respectively. The surrogate recoveries of $^{13}C_6$-HCB in all the samples were ranged from 69.5% to 92.4%. The final concentrations of CP reported were corrected by the surrogate recoveries and field blanks.

Twenty-four SCCP formula groups were detected in all samples. However, only eight MCCP formula groups with smaller Koa values, including C_{14} homologue with 4–9 chlorines and C_{15} homologue with 4 and 5 chlorines, could be identified in all samples. The total atmospheric levels of SCCP and MCCP were between the ranges of 9.6–20.8 pg/m^3 (average: 14.9±4.1 pg/m^3) and 3.7–5.2 pg/m^3 (average: 4.5±0.6 pg/m^3), respectively (see Table 31).

Table 31: CP concentrations (pg/m^3) in atmosphere of King George Island, Antarctica between January 16th to February 8th 2013 (Ma *et al.*, 2014)

	Gas-phases (PUF)				Particle-phases (GFF)				Total	
	Min	Max	Arithmetic mean	SD	Min	Max	Arithmetic mean	SD	Arithmetic mean	SD
ΣSCCP	7.8	18.8	13.5	4.0	1.9	2.6	1.7	0.2	14.9	4.1
ΣMCCP	3.0	4.5	3.8	0.6	0.5	0.9	0.7	0.1	4.5	0.6
ΣCP	10.9	23.3	17.3	4.3	1.8	2.8	2.5	0.4	19.4	4.5

Note: sampling volume of 3450 m^3 (mean), ambient temperature at 0°C (mean, range: -5 – 5°C) and TSP concentration of 15.6 µg/m^3.

CP existed mostly in the gas-phase during summertime. The average particle-phase fractions of ΣSCCP and ΣMCCP were 12.9% and 19.0%, respectively. For MCCP, congener groups with less chlorine atoms (Cl_4, Cl_5 and Cl_6) were predominant in the gas-phase with a total contribution of 67.2% (normalised by the total MCCP abundance). However, the fraction of total C_{14} and C_{15} homologues in the particles (93.6%) was significantly higher than that in the gas (77.2%). These results indicated that CP congeners with longer carbon chain and higher degree of chlorination (corresponding to lower sub-cooled vapor pressure values or larger octanol-air partition coefficients (Koa)) had higher affinity to atmospheric particulates. Ma *et al.* (2014) suggested that the mechanism of absorption into organic matter of the aerosol played a much important role on atmospheric partitioning and transferring of CP in remote Antarctic area.

Wu *et al.* (2019) collected 83 air samples between 2012 and 2015 from the Tibetan Plateau in order to investigate the airborne levels and distributions of MCCP. The sampling areas were located at Lhasa and Shergyla Mountain, which is in the south eastern Tibetan Plateau with abundant forest coverage. The sampling campaign was carried out from July 2012 to July 2015. At Shergyla Mountain, sampling sites were 1983 to 4553 m above sea level, and the interval between adjacent sampling sites was 200–300 m (corresponding to different elevation gradients on eastern and western slopes). The Tibetan Plateau is located in the northern Himalayas. On the Tibetan Plateau, due to the sparse human population and the lack of developed industrial activities, POPs have limited local sources. With the polar-like climate and high altitude, the Tibetan Plateau has become, according to the authors, a remote area to investigate the global transport behaviour of POPs.

Air samples were collected by using a passive air sampling technique based on the sorption of gaseous pollutants to the sampling resin XAD-2. Due to this technique, concentrations of MCCP refer to concentrations on the vapor-phase only. Samples analysis was performed by gas chromatography quadrupole time-of-flight (GC-QTOF) mass spectrometry (Agilent Technologies, Santa Clara, USA) in electron capture negative ion (NCI) mode. The quantitation method was on the basis of previous work from Reth *et al.* (2005b) with a few adjustments. The high-resolution mass spectrometer was used to reduce the interference between the SCCP and MCCP. The MDL value was 40 pg/m^3, and the recovery of $^{13}C_{10}$-trans-chlordane for experimental samples was between 76% and 108%. In all the blanks, MCCP levels were lower than 5% of the total MCCP concentrations in air samples, so the final reported data were not blank corrected.

The airborne MCCP concentrations at Shergyla Mountain were in the range of 50–690 pg/m^3, with average annual concentrations of 131 pg/m^3, 337 pg/m^3, 429 pg/m^3 and 421 pg/m^3 from 2012 to 2015, respectively. The MCCP levels at Shergyla Mountain were about 10–100 times higher than the levels at the Antarctic areas (Ma *et al.*, 2014). At Shergyla Mountain, C_{14} and C_{15} were the dominating carbon congener groups of MCCP. For different chlorine-atom congener profiles, $Cl_{7\text{-}8}$ were the dominant chlorine groups. The homologue profiles of MCCP in the atmosphere at Shergyla Mountain were similar to those of the MCCP in atmosphere of South China and Beijing indoor air (Gao *et al.*, 2018), which was also in accordance with the compositions of the major industrial CP products manufactured in China.

At Shergyla Mountain, MCCP concentrations in air increased with altitude, which indicated that MCCP could potentially possess the ability of "mountain cold trapping". The increasing factor for MCCP concentrations, which was defined as the ratio between ΣMCCP at the highest and lowest altitudes on the eastern and western slopes, was between 2.8-5.5 and 1.5–2.8, respectively, while the increasing factor was between 1.5-2.7 and 1.3–2.9 for ΣSCCP (Wu *et al.*, 2017).

According to Wania and Westgate (2008), mountain cold trapping is defined as the increase of POP levels along with the increasing elevation at typical mountain areas due to the repeated temperature-driven air-surface exchanges. The main mechanism of mountain cold-trapping is the temperature-driven difference in the efficiency of precipitation scavenging between lowland and mountain. The chemicals that achieve higher concentrations at higher altitudes than at lower elevations are those that are not efficiently scavenged by precipitation falling at the temperature prevailing at lower elevations, but whose rate of wet deposition increases as an orographically lifted air mass cools (Wania and Westgate, 2008). The susceptibility and ability of chemicals to mountain cold trapping could be predicted by the mountain contamination potential (MCP) model proposed by Wania and Westgate (2008). The MCP is defined as the fraction of the total chemical amount in the mountain environment, which is present in the soils of the two highest altitudinal zones. The MCP of different congener groups is closely related to their equilibrium partitioning coefficients between octanol and air (Koa), and water and air (Kwa) (or Henry's law constant). Based on the MCP calculations, substances with 0 < log Kwa < 6 and 6 < log Koa < 12 have a potential for mountain cold-trapping (Wania and Westgate, 2008).

The MCP for MCCP was estimated between 0.96–7.21 for log Kwa and 10.27–15.89 for log Koa (estimated by the COSMOtherm model and COSMO-RS theory (Glüge *et al.*, 2013)) thus indicating a potential for "mountain cold trapping" for some congeners of MCCP (such as $C_{14}Cl_5$, $C_{14}Cl_7$, $C_{15}Cl_5$, $C_{15}Cl_7$, $C_{16}Cl_5$ and $C_{17}Cl_5$; Wu *et al.,* 2019). Similar results were found while using a second-order polynomial correlation with a log Kwa in the range of 3–6 and a log Koa in the range of 11–15 thus indicating that some congeners of MCCP possessed the mountain cold trapping effect ability (Wu *et al.,* 2019). It is worth noting that Gawor and Wania (2013) predicted a broader range of log Koa values for MCCP (5.96 – 16.08) (see section 3.3.1), thus confirming a potential for mountain cold-trapping. According to Wania and Westgate (2008), the bands of elevated cold-trapping in mountains and Polar Regions are centred around a log Koa of 8 and 10 and a log Kwa of 2 and 4.5, respectively. Thus, it can be concluded that some congeners of MCCP can be enriched in mountains while others can be enriched in Polar Regions. Furthermore, the congeners of MCCP that become enriched in mountains tend to be less volatile than those that are preferentially accumulating in Polar Regions. Based on this conclusion, it can be inferred that congeners of MCCP that can be enriched in mountains and in Polar Regions have half-lives in air greater than two days.

According to Wania and Westgate (2008), many of the chemicals that have been found to become enriched at higher elevations are bioaccumulative. Indeed, the partitioning properties favouring mountain cold-trapping and the partitioning properties favouring bioaccumulation in both fish and bovine milk overlap substantially. Mountain cold trapping could thus result in contaminant exposure of human populations that eat fish from alpine lakes or dairy products from livestock grazing a high altitude. Wildlife may also be affected, even if a substance does not biomagnify up the food chain. That is why based on the outcome of the study of Wu *et al.*

(2019), it can be concluded that congeners of MCCP that can be enriched at higher elevations tend to be bioaccumulative.

Among urban cities, Lhasa is a remote city located in South western China, but it is the most developed city in the Tibetan Plateau. Air samples were also collected in Lhasa to study the distributions and homologue profiles of MCCP, to further compare the possible transport behaviours with the Shergyla Mountain area from 2012 to 2015. The ΣMCCP in the air of Lhasa were in the range of 845–6670 pg/m^3, which were higher than ΣMCCP at Shergyla Mountain. In the atmosphere of Lhasa, C_{14} and C_{15} homologue groups were the dominant carbon groups, and Cl_{7-8} groups were the most dominating chlorine congener groups. The compositions of the MCCP congener groups were consistent with that at Shergyla Mountain and were also similar to the profiles of atmosphere found in urban cities in China (Gao *et al.*, 2018). According to Wu *et al.* (2017), the south east Tibetan Plateau was affected by two types of air currents from South west Asia (Indian monsoon) and from South Asia, jointly during the sampling period based on the back trajectory model. Thus, according to the authors (Wu *et al.,* 2019), the potential CP sources at Shergyla Mountain might be related to South Asia, whereas the air source of CP at Lhasa might be jointly influenced by the local urban CP release and long-range atmospheric transport (LRAT) to some extent.

Wu *et al.* (2019) concluded that the molecular masses of MCCP were higher compared to SCCP, so the LRAT for MCCP was more difficult than that for SCCP, resulting in the relatively lower MCCP concentrations and different trends of abundant homologue groups. MCCP airborne concentrations at Shergyla Mountain and Lhasa both showed an increasing trend from 2012 to 2015, which is also similar to the results of SCCP. According to Wu *et al.* (2019), the increasing trend of MCCP airborne concentrations since 2012 is likely due to the increasing production and usage of CP in China.

3.3.2.2 Concentrations in sediment

Under the MAREANO (Marine AREA database for Norwegian waters) programme, the Norwegian Institute of Marine Research analysed chlorinated paraffins in marine surface sediments (0-2 cm depth) in different locations in the MAREANO area. A pilot study was performed between 2009-2015 in order to assess the need for further follow-up on five substance groups (including chlorinated paraffins). Based on this pilot study, it was decided that further developments of the analytical methods would be needed for chlorinated paraffins (SCCP and MCCP). After improvements of the analytical methods, measurements of chlorinated paraffins in marine sediments were performed each year since 2017 in the Arctic seawaters. The outcome of the pilot study performed between 2009-2015 and the results of the different measurement campaigns from 2017 to 2019 are presented below.

<u>Pilot study performed between 2009-2015 (Boitsov *et al.*, 2016):</u>
A pilot study was performed during 2009-2015 in order to determine the presence and levels of five substance groups (PFAS, chlorinated paraffins, phosphorous flame retardants (PFR), siloxanes and Alkylphenols and alkylphenol-like compounds) in marine sediments from the MAREANO area. The goal of the pilot study was to assess whether there was a need for monitoring and for establishing methodologies (from sampling to reporting) for these new substance groups.

Ten marine surface sediment samples were collected during the MAREANO cruises in the Barents Sea and the Norwegian Sea in the period 2009-2015. The sediment cores were collected with a multicorer and surface sediment samples (0-2 cm depth) were taken out from the cores. The open parts of the Barents Sea have a sedimentation rate around 2 mm/year or lower and it was thought that the sediment core contained about 10 years of deposition. It is noted that the sedimentation rate may be higher in some fjord and coastal areas. All analyses of CP were performed by high-resolution mass spectrometer MS system with negative ion electron capture system (ECNI-HRMS), with methane as CI gas (Boitsov Personal communication, January 2021

(Boitsov, 2021)). The outcome of the marine sediments analysis for chlorinated paraffins (top layers) is reported in Table 32.

Table 32: Concentrations of SCCP and MCCP in marine sediments (µg/kg dw) collected between 2009-2015 in the MAREANO area (including LOD and LOQ values (µg/kg dw); Boitsov et al., 2016).

Samples Number	LOQ	R1261 MC20	R1349 MC416	R1565 MC97	R749 MC20	R739 MC19	R769 MC01	R421 MC033	R682 MC01	R1492 MC56	R1298 MC37
(longitude, latitude and water depth (m))		63°01,88' 04°41,10' 768 m	63°35,44' 5°34,40' 767 m	66°33.31' 08°13.61' 338 m	67°47,09' 08°59,56' 1863 m	67°47,74' 11°09,53' 264 m	68°20,84' 10°04,29' 1964 m	72°08,77' 16°32,81' 385 m	71°27,11' 27°45,34' 403 m	73°35.99' 36°34.60' 258 m	69°53,90' 30°55,09' 314 m
Sampling year		2013	2014	2015	2011	2011	2012	2009	2011	2015	2014
Location		Norskehavet -sør		Norskehavet				Barentshavet			Varanger-fjorden
SCCP	1393	452 (<LOQ)	79 (<LOQ)	107 (<LOQ)	92 (<LOQ)	58 (<LOQ)	514 (<LOQ)	117 (<LOQ)	139 (<LOQ)	100 (<LOQ)	1081 (<LOQ)
MCCP	19	2.9 (<LOQ)	4.6 (<LOQ)	2.3 (<LOQ)	3.4 (<LOQ)	2.8 (<LOQ)	5.3 (<LOQ)	0.8 (<LOQ)	3.1 (<LOQ)	1.8 (<LOQ)	4.1 (<LOQ)

Note: Concentrations below LOQ but above LOD are shown in bold.

Concentrations of SCCP and MCCP in the ten marine sediment samples were all below their limit of quantifications (LOQs). However, SCCP and MCCP were detected in all ten samples. Due to analytical challenges it was recommended to further improve the analytical methods for these substances before considering further monitoring.

Measurement campaigns (from 2017 to 2019):

In all measurement campaigns (from 2017 to 2019), surface sediment samples (0-2 cm depth) were collected with a box corer. All analyses of CP were performed by high-resolution mass spectrometer MS system with negative ion electron capture system (ECNI-HRMS), with methane as CI gas. It is worth noting that analytical methods for SCCP and MCCP significantly improved over the years which explains the difference in value observed for their limit of quantification (LOQ).

In 2019, chlorinated paraffins were analysed from seven locations in the MAREANO area (Boitsov and Sanden, 2020). The sediment samples were collected in April 2019 west of Bjørnøya and in October 2019 in Kvitøyrenna and Kongsfjorden (Svalbard).

Levels of chlorinated paraffins (SCCP and MCCP) in samples from the seven sites were all below their LOQ of 20 µg/kg dw for SCCP and 6.9 µg/kg dw for MCCP.

In 2017-2018, chlorinated paraffins were analysed from eight locations in the MAREANO area (Boitsov *et al.,* 2019). The samples were collected in 2017 South-West of Svalbard and in 2018 in Kongsfjorden (North-West of Svalbard) and Rijpfjorden (North of Svalbard). The LOQs were higher than in 2019 measurements with a LOQ for SCCP and MCCP at 96 µg/kg and 334 µg/kg, respectively.

Levels of chlorinated paraffins (SCCP and MCCP) were mostly below their LOQs. SCCP and MCCP were quantified at one station in Kongsfjorden (Station R1869, latitude: 79°01.19', longitude: 11°24.92', water depth: 346 m) at 105 µg/kg dw for SCCP and 410 µg/kg dw for MCCP. At one station in Rijpfjorden (Station R1872, latitude: 80°02.38', longitude: 22°15.20', water depth: 145 m), only MCCP were quantified at 536 µg/kg dw.

During the 2017 measurement campaign, sediment samples were collected at three sites during the MAREANO cruise in October - November 2017 in the eastern Barents Sea (Boitsov and Klungsøyr, 2018). The LOQs were higher than in 2018 and 2019 measurements with a LOQ for SCCP and MCCP at 1376 µg/kg and 655 µg/kg, respectively. Levels of chlorinated paraffins (SCCP and MCCP) were all below their LOQ, except for MCCP which were quantified at one of the three stations at a level of 2.8 mg/kg dw (Station R1776, latitude: 74°40.94', longitude: 36°06.19'; water depth: 265 m).

Akvaplan-niva project by Bakke *et al.,* 2008 studied contaminants (including chlorinated paraffins) in the Barents Sea surface sediments (0-1 or 0-3 cm) collected from 11 stations in 2006/2007. Sediment samples were collected using box-correr or multicorer. A total of 11 sediment samples were screened for short and medium chain chlorinated paraffins. SCCP and MCCP were analysed using HRGC/HRMS in electron capture negative ion (ECNI) mode. Methane was used as the moderating gas. The [M-Cl]- ion of each formula group were monitored, and the pattern of the formula groups was used for quantification.

SCCP were quantifiable in all sediment samples and up to 92 µg/kg dw. MCCP could only be quantified at 4.8 µg/kg dw in one sample from the Tromsøflaket region (latitude: 71.3193 longitude: 22.4955, water depth: 438 m; sample collected in 2006).

3.3.2.3 Concentrations in biota

The Norwegian Institute for Water Research – NIVA (Green *et al.*, 2019), studied the levels, trends and effects of contaminants (including SCCP/MCCP) in biota along the coast of Norway (from the Swedish border in the south and to the Russian border in the north), as well as Svalbard. Samples were collected during 2018. Investigation of contaminants in Svalbard have been included since 2017. Samples from two species were used; muscle and liver from cod (*Gadus morhua*) caught in the Isfjord and blood and eggs from the common eider (*Somateria mollissima*) found in the Kongsfjord. The Atlantic cods were sampled from 16th August 2017 to 9th November 2018. In Svalbard, the cod samples were investigated at one station (Isfjord) and liver samples were collected from 15 individuals. Contaminants in the Common eider were investigated at one station in Svalbard (Breøyane, Kongsfjord). Blood samples were collected from 15 individuals (two subsamples from each) and eggs from 15 other individuals during the period 16th to 23rd June 2018. All samples are from adult nesting females.

Different analytical methods were used for identifying and quantifying CP by two different laboratories. CP in cod livers were determined by GC-MS (as concerns over the reliability of this analytical method, it complicates interpretation of the results). The LOQ was set to 5−10 ng/g (with an estimation of 50% of uncertainty). Values below the limit of quantification (LOQ) are set to an average of ten random numbers between the LOQ and half of the value of this limit for calculation for use in time trends. Samples for analyses of CP in the blood and eggs (homogenate of yolk and albumin) of the common eider were extracted with a suitable organic solvent. The lipid and other interferences were removed with the use of sulfuric acid and silica SPE (solid

phase extraction) before detection with GC-HRMS or GC-QTOf-MS. The LOQ was set to 0.3–30 µg/kg (with an estimation of >50% of uncertainty).

Concentrations of MCCP in liver of cods and blood and eggs of eider collected in Svalbard in 2017 and 2018 are provided in Table 33. Median concentration of MCCP was 34.62 µg/kg ww in eider blood and 14.0 µg/kg ww in eider eggs from the same station, an increase from 2017. In the study of Green *et al.* (2019), the median concentration of MCCP (14.0 µg/kg ww) in eider eggs from Svalbard in 2018 was higher than in another study of eider from Kongsfjord in Svalbard (mean value of 4.2±4.1 µg/kg ww; samples collected in 2012) (Harju *et al.,* 2013). According to Green *et al.* (2019), Cod from Svalbard had the same level of SCCP and MCCP as cod from some urban areas along the coast of Norway.

Table 33: Median concentrations (µg/kg ww or ng/g ww) of MCCP in cod livers and in eider blood and eggs from Svalbard (Norwegian Arctic) collected in 2017 and 2018 (Green *et al., 2018 and* 2019)

Species and sampling location	Sampling year	Number of samples	Median concentration (µg/kg ww or ng/g ww)	Standard Deviation (µg/kg ww or ng/g ww)	Number of data > LOQ	Minimum and maximum concentrations > LOQ (µg/kg ww or ng/g ww)
Cod (*Gadus morhua*), liver Isfjord	2018	15	56.60	25	15	49.5 – 127
Cod (*Gadus morhua*), liver Isfjord	2017		35.40	19.41	15	24.1 – 94.2
Eider (*Somateria mollissima)*, blood Breøyane, Kongsfjord	2018	15	34.62	72	15	2.36 – 278.96
Eider (*Somateria mollissima)*, blood Breøyane, Kongsfjord	2017		2.50	6.29	15	0.1 – 26
Eider (*Somateria mollissima)*, eggs Breøyane, Kongsfjord	2018	15	14.00	15	14	4.06 – 54.23
Eider (*Somateria mollissima)*, eggs Breøyane, Kongsfjord	2017		8.60	10.89	-	-

Schlabach *et al.* (2018) measured concentrations of SCCP and MCCP in biota from Svalbard and the Island of Røst (Norwegian Arctic). Samples were collected in 2017. Species representing the different parts of the Arctic marine food chain were sampled, including common eider (*Somateria mollissima*), European shag (*Phalacrocorax aristotelis*), kittiwake (*Rissa tridactyla*), glaucous gull (*Larus hyperboreus*) and polar bear (*Ursus maritimus*). Blood was taken from polar bear, while eggs were collected from birds. Chlorinated paraffins were analysed using a GC system coupled to a QToF mass spectrometer operated in electron capture negative ionisation mode (GC-ECNI-

HRMS). The authors estimated that the total measurement uncertainty (due to sampling regime, storage of samples, chemical analysis and data treatment) for new emerging compounds (including S/MCCP) would be in the order of 40 to 50%.
Concentration levels of SCCP and MCCP in Arctic biota are reported in Table 34. In addition, Schlabach *et al.* (2018) measured the concentration levels of MCCP in mink and eggs of common gull from Tromsø area. This information is reported in 'Annex III – Summary of environmental monitoring data'.

Table 34: Concentrations (ng/g ww) of SCCP and MCCP in Arctic biota from Svalbard and the Island of Røst collected in 2017 (Schlabach *et al.*, 2018)

Species and sampling location	Sampling year	Number of samples	Substance	Detection frequency (%)	Average concentration (ng/g ww)	Minimum and maximum concentrations (ng/g ww)
Common Eider *(Somateria mollissima)*, eggs Islands of Kongsfjorden, Svalbard	June 2017	10	SCCP	60%	84	61 – 118
			MCCP	100%	31	13 – 59
European Shag (*Phalacrocorax aristotelis*), eggs Island of Røst	May 2017	5	SCCP	100%	107	34 – 217
			MCCP	100%	150	7.8 – 366
Kittiwake (*Rissa tridactyla)*, eggs Islands of Observasjonsholmen, Kapp Guissez and Krykkjefjellet in Kongsfjorden, Svalbard	June 2017	5	SCCP	100%	48	34 – 69
			MCCP	100%	40	9.3 – 96
Glaucous gull *(Larus hyperboreus)*, eggs Islands of Observasjonsholmen, Kapp Guissez and Krykkjefjellet in Kongsfjorden, Svalbard	June 2017	5	SCCP	100%	48	13 – 71
			MCCP	100%	36	8.6 – 49
Polar bear *(Ursus maritimus)*, blood Svalbard	April 2017	10 (n=5 females and n=5 males)	SCCP	100%	912	40 – 7 300
			MCCP	60%	41	5.1 – 93

Schlabach *et al.* (2018) reported that chlorinated paraffins were detected in all samples of Arctic biota. The authors concluded that in absence of substantial local sources, these findings clearly show that SCCP and MCCP are subject to both long-range atmospheric transport and bioaccumulation.
Concentrations found for MCCP in this study (Schlabach *et al.,* 2018) are quite similar to those found in eggs of Common eider from Svalbard in 2018 (Green *et al.*, 2019). However, concentrations found for MCCP in this study (Schlabach *et al.,* 2018) are higher than to those collected in 2012 in eggs of Kittiwake, European shag, Common eider and in blood of polar bear from Svalbard (Herzke *et al.*, 2013 and Huber *et al.*, 2015). It seems that concentrations of MCCP increased in these species between 2012 and 2017. This trend should be considered with caution due to the difference in analytical methods between these studies and the small size of the samples.

Herzke *et al.* (2013) studied the background concentrations of SCCP and MCCP in Arctic biota from Svalbard (Norwegian Arctic). To be able to distinguish between pollution sources (i.e., long-range transport vs. local sources) and establish a contaminant baseline for future time- and spatial trends, samples were collected at remote locations. Samples were collected in 2012 (except for the ringed seal samples which were collected in 2010). Species representing the different parts of the Arctic marine food chain were sampled, including polar cod (*Boreogadus saida*), Atlantic cod (*Gadus morhua*), Common eider (*Somateria mollissima*), kittiwake (*Rissa tridactyla*), glaucous gull (*Larus hyperboreus*), ringed seal (*Phoca hispida*) and polar bear (*Ursus maritimus*). Plasma was taken from polar bear, ringed seal and glaucous gull, while eggs were collected from kittiwake and eider ducks. Liver was collected from Atlantic cod and whole fish of Polar cod. CP were analysed using GC/HRMS. A surrogate standard (^{13}C POPs mixture) was used for the SCCP and MCCP.

Both SCCP and MCCP were detected in the majority of the Arctic samples with the exception of only 10% detection of MCCP in cod liver, indicating a widespread exposure to these chemicals in the marine Arctic. Concentration levels of S/MCCP in Arctic biota are reported in Table 35. Levels of SCCP were found to dominate compared to MCCP in polar bear and seal plasma, kittiwake eggs, cod liver and polar cod. However, the opposite trend was observed for glaucous gull plasma and eider duck eggs where MCCP were found at higher concentrations.

Table 35: Concentrations of SCCP and MCCP in Arctic biota from Svalbard (Norwegian Arctic) collected in 2010 and 2012 (Herzke *et al.*, 2013)

Species Tissue	Polar bear Plasma (ng/mL; n=20)	Ringed seal Plasma (ng/mL; n=10)	Glaucous gull Plasma (ng/mL; n=12)	Kittiwake Egg (ng/g ww; n=12)	Common eider Egg (ng/g ww; n=12)	Atlantic cod Liver (ng/g ww; n=3)	Polar cod Pooled whole fish (ng/g ww; n=1)
Lipid %	0.9*	0.7*	14.4*	8.1	17.4	50.5	1.7
SCCP	3.99±2.91 (95%)	4.96±2.70 (100%)	3.95±1.99 (75%)	7.83±8.26 (67%)	3.23±1.77 (83%)	10.3±10.7 (100%)	2.28 (100%)
MCCP	2.20±1.84 (95%)	2.91±2.39 (90%)	8.87±9.88 (67%)	4.91±4.88 (100%)	4.24±4.07 (100%)	0.94 (10%)	1.51 (100%)

Note: In brackets percentage of samples above the detection limit, *from literature data

Huber *et al.* (2015) assessed the chemical mixture exposure profiles of seabirds from the Norwegian marine environment by investigating the levels of legacy and emerging pollutants in the eggs of three seabird species (common eider (*Somateria mollisima*), European shag (*Phalacrocorax aristotelis aristotelis*), and European herring gull (*Larus argentatus*)). Seabird eggs from the selected species were collected at two remote islands, Sklinna (65°11°N, 11°00°E) and Røst (67°30°N, 12°00°E) on the Norwegian coast during the breeding season between May 2012 and June 2012.

The sample analyses were performed by high resolution (HR)-GC-MS in EI and NCI mode. Quantification was performed using an internal standard method with isotope labelled compounds. During analysis, solvent injections were done regularly in order to monitor instrument background and carry-over effects. Limit of detections (LODs) were set as a signal to noise of 3:1, if blank contamination appeared, the blank concentration multiplied by three gave the new LOD.

Concentrations of MCCP in bird eggs were found at a much higher frequency (80%) compared with SCCP (40%) with concentrations ranging <0.76–17.5 ng/g ww and <2–4.8 ng/g ww, respectively. This may be attributed to restrictions placed on SCCP production and use in Europe. Furthermore, Huber *et al.* (2015) assumed that a higher detection frequency of MCCP may also be explained by slower metabolic and elimination rates. Longer carbon chain length and higher degrees of chlorination have been shown to slow metabolism and degradation (Fisk et al., 1996 and Madeley and Birtley, 1980 as cited in Huber *et al.,* 2015). Concentrations found for SCCP and MCCP in this study are quite similar to those found in eggs of Kittiwake and Common eider from Svalbard (Herzke *et al.*, 2013).

Reth *et al.* (2006) quantified SCCP and MCCP in liver and muscle from Arctic Char (*Salvelinus alpinus*) and seabirds (little auk (*Alle alle*) and kittiwake *(Rissa tridactyla*) collected at Bear Island (European Arctic) as well as in Cod samples (*Gadus morhua*) from Iceland and Norway. The samples were collected in July 2001. The Bear Island is a small island in the central Barents Sea, Bjørnøya (Bear Island, 74°N, 19°E), which is 500 km away from any known point source.

In this study, the samples were analysed by HRGC-ECNI-LRMS. Quantification was performed according to Reth *et al.* (2005b), which, according to the authors, allows an accurate quantification even if the degree of chlorination of the CP in the sample is different from the chlorine content of the standard. Reth *et al.* (2006) noted that a slight overestimation of the real chlorine content (by ca. 1–3%) cannot be avoided by ECNI-MS. The limits of detection (LODs) were between 0.5 and 1 ng/µl of SCCP and MCCP mixtures and the limits of quantification (LOQs) were between 1.5 and 3 ng/µl at a signal-to-noise ratio of 10:1. Method blanks were below detection limits. The relative distribution of the homologue groups in the standard mixtures was determined five times and the relative standard deviation was less than 10%. Congeners with 10 to 15 carbon atoms and 5 to 10 chlorine atoms were analysed.

SCCP and MCCP were detected in all samples, and the concentrations found in Bear Island are listed in Table 36. MCCP concentrations found in Norway and Iceland are reported in Section 3.4.4.2.

Table 36: SCCP and MCCP concentrations (ng/g wet and lipid weight) in fish and seabirds from Bear Island (Norwegian Arctic; 74°N, 19°E) collected in July 2001 (Reth *et al*., 2006)

Sample No.	Lipid (%)	SCCP concentration (ng/g ww)	MCCP concentration (ng/g ww)	SCCP concentration (ng/g lw)	MCCP concentration (ng/g lw)
Arctic char (*Salvelinus alpinus*), Lake Ellasjøen, n=2					
B1 (liver)	12	27	43	230	360
B3 (muscle)	2	13	47	540	1600
B2 (liver)	12	11	13	89	110
B4 (muscle)	2	7	10	300	440
Little auk (*Alle alle*), Bjørnøya, n=2					
C1 (liver)	10	18	48	190	500
C3 (muscle)	5	7	55	150	1200
C2 (liver)	10	88	370	880	3700
C4 (muscle)	4	16	17	430	450
Kittiwake (*Rissa tridactyla*), Bjørnøya, n=2					
D1 (liver)	5	6	39	110	730
D3 (muscle)	5	5	38	95	720
D2 (liver)	6	44	12	860	240
D4 (muscle)	12	5	5	41	41

In the Arctic char samples from Lake Ellasjøen on Bear Island SCCP and MCCP levels were comparable and ranged between 7 and 27 ng/g ww for SCCP and between 10 and 47 ng/g ww for MCCP. The range of SCCP as well as MCCP was comparable with previously detected sum concentrations of PBDEs and toxaphenes in Arctic char from Bear Island captured also in July 2001 (Evenset *et al.,* 2005 as cited in Reth *et al.,* 2006). In the seabirds, concentrations ranged between 5 and 88 ng/g ww for SCCP and between 5 and 55 ng/g ww for MCCP with one exception of 370 ng/g ww measured in a liver sample from Little auk. CP were detected in both muscle and liver of each species from Bear Island at variable concentrations without any clear trend. S+MCCP lipid weight data were higher for samples from Bear Island than for the cod samples from northwest Europe.

The relative abundance of C_{14} substances was between 55 and 82% (mean 65.8%) and the mean ratio of C_{14}/C_{15} substances was around two (higher mean ratios up to 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 MCCP had between 6 and 9 chlorine atoms per molecule, and the mean chlorine content of the MCCP found was estimated to be 55.85% (range 54.5 - 57.4%).

Reth *et al.* (2006) concluded that even if a higher abundance of C_{10} congeners was observed for the samples from the remote areas, high-chlorinated SCCP as well as MCCP were also present. The authors (Reth *et al.,* 2006) assumed that CP patterns in the Arctic organisms might be a result of exposure to CP transported via the atmosphere as well as via birds and the corresponding bioaccumulation and biomagnification processes. It is worth noting that the sampling size used in this study is small. The results of this study should be considered with caution.

3.3.3 Summary and discussion of long-range transport

Based on their physical-chemical properties, some congeners of MCCP are predicted to have long-range transport potential (LRTP). Indeed, MCCP have similar physical-chemical properties to legacy persistent organic pollutants (POPs).

The study of Wu *et al.* (2019) demonstrated that some congeners of MCCP can be enriched in mountains while others can accumulate in Polar Regions. Furthermore, the congeners of MCCP that become enriched in mountains tend to be less volatile than those that are preferentially accumulating in Polar Regions. Based on this conclusion, it can be inferred that congeners of MCCP that accumulate in mountains and in Polar Regions have half-lives in air longer than two days. The predicted atmospheric half-life will vary for the MCCP congeners according to degree of chlorination with the estimated half-lives increasing with increasing number of chlorine atoms in the structure (Gawor and Wania, 2013). Based on information from Environment Canada (2008), Gawor and Wania (2013), EA (2019) and UK (2021), MCCP congeners have a range of atmospheric half-lives for vapour phase between 0.6 to 7.1 days, thus indicating a potential for long-range transport for some of MCCP congeners.

Gawor and Wania (2013) predicted that MCCP with ~5–6 and ~6–7 chlorines, respectively, were identified to have the highest combined potential for LRT and bioaccumulation in humans (the so called Arctic contamination and bioaccumulation potential (AC-BAP)) and thus to have the potential to be persistent organic pollutants.

Monitoring data tend to confirm this prediction as it has been found that MCCP congeners with $C_{14\text{-}15}$ and $Cl_{4\text{-}9}$ were found in the Arctic (biota; Reth *et al.,* 2006) and in the Antarctic (air; Ma *et al.,* 2014 and Jiang *et al.*, 2021).

MCCP have been detected in various media in the Arctic, including in air from Svalbard (concentrations in the range of <44–720 pg/m^3 in 2019 (particle and gas phases); Bohlin-Nizzetto *et al.,* 2020), in marine sediments from the Barents Sea and the Norwegian Sea (concentrations in the range of n.d–2.8 mg/kg dw in top layers between 2006–2018; Bakke *et al.,* 2008; Boitsov *et al.*, 2016; Boitsov and Klungsøyr, 2018; Boitsov *et al.,* 2019), in terrestrial,

avian and marine biota samples from the Norwegian Arctic between 2001 and 2018, including in top predators such as Polar Bears.
MCCP were also found in air samples from the Antarctic (concentrations in the range of <0.26–27.5 pg/m^3 (particle and gas phases), between 2014 and 2018; Jiang *et al.*, 2021). Concentrations of MCCP found in air samples from the Antarctic were lower than the ones found in the Arctic.

MCCP were also found in air samples from the Tibetan Plateau (at Shergyla Mountain) at high altitude (1983 to 4553 m above sea level) with concentrations in the range of 50–690 pg/m^3 (gas phase; between 2012 and 2015; Wu *et al.*, 2019).

The presence of MCCP at sites remote from known point sources such as the Arctic and Antarctic therefore indicates long-range environmental transport.

Furthermore, monitoring data indicate that concentrations of MCCP have increased during the last decades. This increase was observed in the Arctic air (from 2013 to 2019; Bohlin-Nizzetto *et al.,* 2020)) and in air samples from the Tibetan Plateau (from 2012 to 2015; Wu *et al.,* 2019). In addition, in the Antarctic air, an increasing trend was observed in the ratio of MCCP to SCCP from 2014 to 2018 suggesting that the use of MCCP as substitute to SCCP had increased (Jiang *et al.,* 2021). As described in section '3.4.4.2 Monitoring data in biota', the increase of concentrations of MCCP was also observed in blue mussels from the coast in Norway between 2017–2018 (Green *et al.,* 2019) and in porpoise and dolphin samples from South China Sea between 2004–2014 (Zeng *et al.,* 2015). Furthermore, Iozza *et al.* (2008) indicated that the level of MCCP in a sediment core from Lake Thun in Switzerland showed an increasing trend from 1965 to 2004 (see section '3.1.3.1 Occurrence in sediment'). Similarly, MCCP concentrations in soil measured by Bogdal *et al.* (2017) show an increase from 1989 to 2014 from six sampling sites in Switzerland (see section '3.1.3.2 Concentrations in sludge and soil').

3.4 Bioaccumulation

3.4.1 Screening data

As presented in Section 1.4, congeners of MCCP generally have a low water solubility and experimental log Kow values in the range 6-8, with a "typical" value around 7. MCCP are therefore potentially bioaccumulative (log Kow >4.5).

3.4.1.1 Log Kow

Log Kow Measured data

A non-GLP OECD 123 (slow-stirring method) study was performed (Unpublished, 2019b) with a C_{14} chlorinated n-alkane, 50% Cl wt., containing a range of C_{14} congeners with 4 to 14 chlorine atoms as determined by analytical method. A certificate of analysis for the test substance is not included in the report. All samples were analysed in duplicate using the APCI-TOF-HRMS method, 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 considered to be reliable.

The average log Kow value was 6.58 ± 0.09 at 19 °C. Other chain length constituents of MCCP were not included in this study, so the reported value only represents a proportion of the possible constituents of commercial products. Variation of log Kow 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 Kow value for MCCP 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). The latter study is discussed in more detail below.

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.

Unpublished (2019b) study is considered to be reliable with restrictions.

Two additional studies (Renberg *et al*., 1980; Fisk *et al*., 1998a), were considered in EC (2005). These studies measured the log Kow of four substances with different degrees of chlorination (representing C_{14-17} chlorinated n-alkane 45%Cl wt., C_{14-17} chlorinated n-alkane 52% Cl wt., C_{16} chlorinated n-alkane 35% Cl wt. and C_{16} chlorinated n-alkane 69% Cl wt., respectively)) using either a high performance thin layer chromatography method or a HPLC technique (with radiochemical analysis). The measured log Kow values were in the range 4.7-8.3. No information is provided about the internal standards or reference substances, and so 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 Kow 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 Kow 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 Kow values were based on retention times of HPLC chromatographic peak(s)/band(s) of each substance, and the range of log Kow 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 Kow 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_{14-17}, 46.7% Cl wt.	6.67	(5.57 - 7.90)

When the entire data set was considered, it was apparent that the log Kow 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 Kow increased with increasing chlorine content in a non-linear fashion[14].

The effect of carbon chain length on the log Kow 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

[14] The correlation between chlorination degree and log Kow was found to follow a second order polynomial relationship.

carbon chain lengths in the C_{10} to C_{13} range). It was found that for a given chlorine content, the log Kow values increased at an approximately constant rate for every addition of a carbon (the average increase in log Kow 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 Kow = 0.281 × n + 2.280	R^2 = 0.9967
ca. 60% Cl wt.	log Kow = 0.269 × n + 2.515	R^2 = 0.9979
ca. 65% Cl wt.	log Kow = 0.276 × n + 2.621	R^2 = 0.9774
ca. 70% Cl wt.	log Kow = 0.321 × n + 2.576	R^2 = 0.9812

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

This study used an indirect method for the determination of log Kow. 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 Kow 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.

Log Kow Predicted data

Log Kow values have been predicted with the log P models contained within the ACD Percepta program, ACD/Labs release 2019.2.1 (Advanced Chemistry Development, Inc., 2019) for the following hypothetical MCCP congener- groups $C_{14}Cl_{1-14}$, $C_{15}Cl_{1-15}$, $C_{16}Cl_{1-16}$ and $C_{17}Cl_{1-17}$ and their structural isomers. See 'Annex II – Modelling of log Kow and biodegradation and generation of representative structures for MCCP' for information about the structures used for the log Kow predictions, as well as for the BCF and BIOWIN predictions. ACD Percepta has three methods for predicting log P; the Log P GALAS method, the Log P Classic method and the Log P Consensus method. The Log P Consensus method incorporates both GALAS and Classic predictions, weighing them according to the internal metrics of the corresponding algorithm accuracy and applicability domain, and provide a single "averaged" prediction. Preference has been given to the Log P Consensus method, however, if the predicted log Kow was outside of the lower range of log Kow values which has been recommended by Glüge *et al.* (2013) (see Table 25 and below), then the higher log Kow prediction from the Log P Classic or from the Log P GALAS method has been chosen given that the reliability of the Log P GALAS prediction has been > 0.5. A comparison of the ACD Percepta log Kow predictions against the recommended values by Glüge *et al.* (2013) was undertaken to ensure that the log Kow predictions reported here and used for the BCF predictions are in line with predictions undertaken elsewhere. The log Kow predictions are presented in full in Table 54 of Annex II. The range of the predicted log Kow for $C_{14}Cl_{1-14}$ is 6.2-8.25, $C_{15}Cl_{1-15}$, is 6.63 – 8.76, $C_{16}Cl_{1-16}$ is 7.07-9.28 and $C_{17}Cl_{1-17}$ is 7.33 - 9.8.

The results from the QSAR predictions reflect a similar trend to that observed experimentally in the Hilger *et al.* (2011a) and Unpublished (2019b) studies (described above) and by QSAR predictions in the Glüge *et al.* (2013) study. The predicted log Kow values are generally higher with increasing carbon chain length, which can be seen in the log Kow ranges reported above. The lower and upper log Kow values in the range increase with about 0.4 – 0.5 log units with increase in carbon chain length. Similarly, the log Kow starts increasing at a chlorination level of approximately >65% for all chain lengths, and the highest log Kow are predicted for these congeners. The models predict that the log Kow of the lowest chlorination degrees ($C_{14}Cl_{1-2}$, $C_{15}Cl_1$, $C_{16}Cl_{1-2}$ and $C_{17}Cl_1$) are higher than for congeners with more chlorine atoms and the log Kow starts decreasing around three chlorine atoms. The lowest log Kow are predicted for congeners with approximately 55% chlorine content ($C_{14}Cl_7$, $C_{15}Cl_8$, $C_{16}Cl_7$ and $C_{17}Cl_8$). The predictions also indicate that the log Kow value for the congener groups $C_{14}Cl_{3-11}$, $C_{15}Cl_{3-13}$, $C_{16}Cl_{3-13}$ and $C_{17}Cl_{3-14}$ are relatively independent of the chlorine content. Hilger *et al.* (2011a), Glüge *et al.* (2013) and Unpublished (2019b), have concluded that log Kow values are relatively

independent of chlorine content for a given carbon chain length up to a chlorine content of 55% Cl wt. Log Kow 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.

The predicted log Kow varies for the structural isomers of the same congener group, for example the range for the congener group $C_{15}Cl_3$ is 7.22 - 8.92 (see Table 54 of Annex II for all congeners). The fact that physical-chemical properties of the same congener groups of chlorinated paraffins can differ due to the structural isomers has been discussed in Gawor and Wania (2013) and Glüge *et al.* (2013). The latter study states that the upper and lower boundaries of the ranges reported for the congener groups correspond to different properties of different constitution isomers and, therefore, reflect actual variability of the properties. For the ACD Percepta log Kow predictions it has been observed that there is less variation in the log Kow for structural isomers of the congener groups with higher degree of chlorination. The position of the chlorine atoms on the hydrocarbon chain has an effect on the log Kow, and this effect might be greater for congeners with fewer chlorine atoms substituted at the hydrocarbon chain as compared to congeners with a higher number of chlorine atoms (explaining why there is more variation in predicted log Kow for structural isomers of congener groups with a lower degree of chlorination).

The ACD Percepta log P methods were chosen instead of the KOWWIN model of the EPI Suite™ platform (US EPA, 2012) due to reasons enumerated below. Some studies (Gawor and Wania, 2013 and Glüge *et al.* 2013) have shown that the KOWWIN model compared to other available models yields log Kow predictions for chlorinated paraffins which are less in agreement with experimental values. In the Gawor and Wania (2013) the predecessor to the ACD log P Classic method, ACD/Labs log P of the ACD/ADME Suite 5.0 was chosen to predict the log Kow for constituents of SCCP, MCCP and LCCP since the predicted log Kow derived from this model were judged most similar to the experimental values, based on proximity of data pairs to the 1:1 line and the generally best regression (R^2=0.70 for ACD/Labs, R^2 = 0.57 for KOWWIN (Gawor and Wania, 2013). In the Substance Evaluation of MCCP (EA, 2019), the rapporteur demonstrated that there were substantial differences in the predicted log Kow values by KOWWIN (v. 1.68) to measured values reported by Sijm and Sinnige (1995) and Hilger *et al.* (2011a). They observed that as the carbon chain length and the chlorine content increase, the difference between the predicted values from KOWWIN and the values reported by Sijm and Sinnige (1995) and Hilger *et al.* (2011a) also increase. It was concluded that this analyses casts doubt on the reliability of the KOWWIN predictions.

Issues with the applicability domain of KOWWIN for predicting log Kow for constituents of MCCP have been identified, which affect the reliability of the predictions. The KOWWIN uses a "fragment constant" methodology to predict log Kow and coefficient values of fragments or groups are summed together to yield the log Kow estimate. Although there is currently no universally accepted definition of the model domain, predictions of log Kow estimates may be less accurate for compounds that have more instances of a given fragment than the maximum for all training set compounds (US EPA, 2012). The maximum number of chlorine atoms contained in substances in the training set is six. This means that the MCCP constituents with more than six chlorine atoms exceed the maximum value of chlorine fragments present in the training set and therefore the predictions for those constituents are considered uncertain. The coefficient for the “chlorine-aliphatic attach” fragment is 0.3102 and for every additional chlorine atom in the structure, this value is summed in the calculation to yield the log Kow predictions. The predicted log Kow by KOWWIN (v. 1.68) for many of the for many of the constituents (C_{14} more than ten chlorine atoms, C_{15} more than eight, C_{16} more than five and C_{17} more than two chlorine atoms) are above 9 (maximum log Kow prediction 11.22). Since the training set does not contain any substances with experimental log Kow values of 9 or higher, and the validation set only contains a few, predictions of log Kow in this part of the graph (log Kow > 9) will be more uncertain than predictions at the lower ends. Considering all the above it appears that the KOWWIN model overestimates the log Kow for the MCCP constituents. Gawor and Wania (2013) further noted that the models implemented within EPI Suite predicted physical–chemical properties for substances that differ with respect to skeletal structure and the degree of

halogenation, but rarely discriminate based on the position of halogens on the skeletal structure. The models within ACD/ADME Suite are more sensitive to both the degree and position of halogenation.

Glüge *et al.* (2013) calculated log Kow values for 29 congener groups of MCCP 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 25). 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 Kow values for these congeners is 6.2 – 8.1, which is somewhat higher than the experimental findings.

The log Kow predictions from the ACD Percepta Log P methods are more in agreement with the experimental values reported for some of the congener groups and with the recommended values by Glüge *et al.* (2013) than the log Kow predictions from KOWWIN. This further supports the choice of the ACD Percepta Log P methods.

Log Kow value recommended by the dossier submitter

It is considered that the large number of constituents contained within MCCP will lead to a range of log Kow values, many of which are likely to be equal to or exceed 6.5.

3.4.1.2 BCF predictions

The BCF Baseline model (v. 03.10) of CATALOGIC (v.5.13.1.156) (LMC, 2018) has been used to predict BCF for the congener groups $C_{14}Cl_{1\text{-}14}$, $C_{15}Cl_{1\text{-}15}$, $C_{16}Cl_{1\text{-}16}$ and $C_{17}Cl_{1\text{-}17}$ and their constituents. It has been demonstrated that the congeners of MCCP, and also structural isomers of the same congener group, can have different physical-chemical properties and bioaccumulation potential due to the difference in carbon chain length and number of chlorine atoms, as well as due to the positioning of the chlorine atoms on the carbon chain (Du *et al.,* 2020; Fisk *et al.,* 1996, 1998b and 2000; Gawor and Wania, 2013 and Glüge *et al.* 2013). Therefore, a selection of structures was chosen for the BCF predictions to represent the MCCP congener groups and their constituents, see Annex IV for details. In addition to the general selection, some additional constituents were further selected and modelled for some of the congener groups in order to gain a better understanding of the spread of BCF predictions across a specific congener group. In total 420 structures were used for the BCF predictions (see Annex IV for more details).

The BCF Baseline model of CATALOGIC applies mitigating factors for metabolism and size of the molecule (most relevant for MCCP), as well as for water solubility, synergistic/antagonistic effect and for acids and phenol (the two last not applicable for the MCCP predictions). The model combines a training set of BCF data in fish (826 chemicals) with a metabolic database with documented fish and rat liver transformation maps (for 450 organic compounds)(LMC, 2018). The model uses log Kow predictions from KOWWIN of EPI Suite (v.4.0) as default and the user can input other log Kow values for the predictions. For the BCF predictions log Kow values derived with the log P methods (Consensus, Classic or GALAS) of ACD Percepta for the respective structures were used as input (see Table 54 of Annex II). This was deemed necessary considering that the KOWWIN model of EPI Suite is not the preferred model for predicting log Kow of the MCCP constituents due to the model likely overestimating the log Kow.

The results of the modelling are presented in detail in Annex IV,
Table 61. The congener groups for which at least two constituents have predicted BCF value over the B-criteria threshold of log BCF 3.3 (BCF≈2000) and/or the vB-criteria threshold of log BCF 3.69 (BCF≈5000) have been concluded as having bioaccumulation potential (see

Table 37 below). The only exception to this is the congener group $C_{14}Cl_3$, which was concluded as having bioaccumulation potential due to one predicted value above the threshold of log BCF 3.69 and interpolation from the congener groups $C_{14}Cl_2$ and $C_{14}Cl_4$ which also indicate bioaccumulation potential. The following congener groups have been concluded as having bioaccumulation potential according to the BCF Baseline model of CATALOGIC; $C_{14}Cl_{2\text{-}11}$, $C_{15}Cl_{3\text{-}10}$ and $C_{16}Cl_{5\text{-}10}$. The C_{17} congeners have been concluded as not indicating bioaccumulation potential, even though there are two respective BCF predictions for $C_{17}Cl_6$ and $C_{17}Cl_7$ being borderline B. For the C_{17} chain length the log Kow values are generally higher opposed to the lower chain lengths, with log Kow values around 8 or higher for many of the constituents. This corresponds to the log Kow range of the BCFmax graph for the BCF Baseline model where the BCF values start decreasing due to increasing molecular size and hindered uptake.
The applicability domain check of the predictions yields that 63 % of structures are fully within the applicability domains (parametric, structural, mechanistic and metabolic domain) of the BCF Baseline model (v.03.10). All structures are within the parametric and mechanistic domain of model. As for the structural domain of the model, 89 % of the structures are fully within the domain and 21 % slightly outside the domain (mostly around 5 % unknown fragment, 8 % at the most). 84 % of the structures are fully within the metabolic domain of the model and 16 % slightly outside the domain (mostly around 5 % incorrect fragment) (see
Table 61 in Annex IV for further details). Generally, more of the structures with lower degrees of chlorination are fully within the applicability domain.

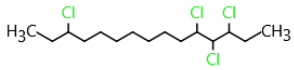
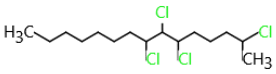
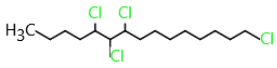
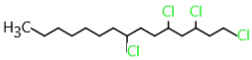
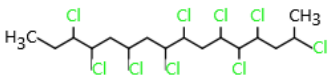
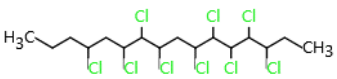
The structures which are out of domain contain a fragment with the methyl group at the end(s) of the carbon chain and a chlorine atom on the second carbon, or on the second and third carbon. This fragment is not fully covered by the training sets of the model. The training sets include some chlorinated paraffin structures with chlorine atoms on the terminal carbon(s), but generally the representation of this class of chemicals is limited in the training sets of the model. The fact that the fragment described above, making up maximum 8 % of the structure, is not fully covered by the model is not perceived as reflecting on the reliability of the predictions to such a degree that the predictions would be invalid. The analyses of all the results have shown that the BCF predictions for structures with this fragment fall within the same range of values as those of similar structures which are fully in domain. The applicability domain has, however, been noted in the analyses of the results, yielding higher value to the BCF predictions that are fully within applicability domain.

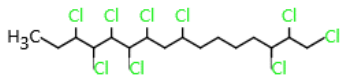
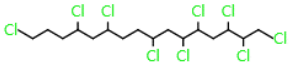
Table 37: Bioaccumulation potential for MCCP congeners according to BCF predictions

Carbon chain length	Number of chlorine atoms																
C14	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
B result for constituents	not B	B	vB	vB	B/vB	vB	B/vB	vB	vB	B	B	not B	not B	not B	-	-	-
% Cl wt.	< 40			40-50		50-55		55-65		> 65			> 70				
B result for fractions				vB		vB		vB		B			not B				
C15	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
B result for constituents	not B	not B	B	B	B	B/vB	B/vB	B	B	B	not B	not B	not B	not B	not B	-	-
% Cl wt.	< 40			40-50		50-55		55-65			> 65						
B result for fractions				B		B		B			not B						
C16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
B result for constituents	not B	not B	not B	not B	B	B	B	B	B	B	not B	not B	not B	not B	not B	not B	-
% Cl wt.	< 40			40-50		50-55		55-65			> 65						
B result for fractions				B		B		B			not B						
C17	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
B result for constituents	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B
% Cl wt.	< 40			40-50		50-55		55-65			> 65						
B result for fractions	not B			not B		not B		not B			not B						

The predicted BCF values for structural isomers of the same congener group can vary significantly. This depends on the log Kow value, on which metabolic transformation the model applies, as well as on the relative effects of the metabolism and size mitigating factors. These in turn depend on the position of the chlorine atoms on the carbon chain. The differences in log Kow for the various constituents also depend on difference in chain length. To illustrate the differences of predicted BCFs, the results for some constituents of congener groups $C_{15}Cl_4$ and $C_{16}Cl_9$ are presented in
Table 38 below.

Table 38: The predicted BCF for isomers of congeners $C_{15}H_{29}Cl_3$ and $C_{14}H_{26}Cl_4$

Constituents	Structure	Log BCF	Mitigating factor Meta-bolism	Mitigating factor Size	Log Kow
$C_{15}Cl_4$ (A)		3.34 (± 0.34)	0.342	0.658	7.47
$C_{15}Cl_4$ (B)		3.0 (± 0.35)	0.1925	0.808	8.15
$C_{15}Cl_4$ (C)		2.64 (± 0.39)	0.586	0.461	7.65
$C_{15}Cl_4$ (D)		1.24(± 0.76)	0.78	0.284	8.15
$C_{16}Cl_9$ (A)		3.47 (± 0.36)	0.183	0.817	7.3
$C_{16}Cl_9$ (B)		3.26 (± 0.38)	0.165	0.835	7.52

Constituents	Structure	Log BCF	Mitigating factor Meta-bolism	Mitigating factor Size	Log Kow
$C_{16}Cl_9$ (C)		2.59 (± 0.44)	0.45	0.433	7.65
$C_{16}Cl_9$ (D)		2.13(± 0.63)	0.613	0.396	7.47

The constituents with methyl groups at both ends of the carbon chain (like $C_{15}Cl_4$ A and B, $C_{16}Cl_9$ A and B) are predicted with the highest BCF values and lowest mitigating factors for metabolism because the predicted transformation only involves omega oxidation of the methyl group(s) and no removal of chlorine. The model applies another transformation, aliphatic C-hydroxylation (hydroxylation of a carbon in the chain) for some constituents (like $C_{15}Cl_4$ (D)) where the chlorine atoms are not positioned on adjacent carbons. Furthermore, for some constituents where the chlorine atoms are not positioned on adjacent carbons, dehalogenation transformation may be predicted yielding lower BCF values (for example for $C_{15}Cl_4$ (D)) due to higher mitigating factors for metabolism. Constituents with chlorine atom at the terminal carbon(s) are predicted by the model to undergo a gluthation conjugation transformation removing chlorine atom(s), hence the metabolism mitigating factors are higher, yielding lower BCF values (like $C_{15}Cl_4$ (C) and (D), $C_{16}Cl_9$ (C) and D)). The reliability of the transformation pathways could not be further strengthened by analogues in the training set, as chlorinated alkane substances in the range of C_{10} to C_{18} in the observed transformation maps dataset are recorded with the parent only (no degradation products).

In the BCF Baseline model (v. 03.10) the predicted metabolism pathway(s) for the MCCP constituents have a greater influence on the observed variation in predicted BCF than the log Kow. Based on experimental studies the model developers have concluded that cytochrome P450-dependent oxidation (involving dehalogenation reaction) and glutathione (GSH)-dependent conjugation are the primary routes in the metabolism of haloalkanes. They summarised that the rate of metabolism of the chlorinated paraffins is influenced by the chain length and/or the degree of chlorination and that the proportion of unmetabolised chlorinated paraffin increased with its degree of chlorination. One study in rats demonstrated that differences between the distribution of SCCP congeners in blood, urine (Cl_5) and faeces (Cl_{8-10}) were more dependent on chlorination degree than on carbon chain lengths and should be dependent on their physicochemical properties, mainly the octanol-water partition coefficient (Kow)(Unpublished, 2020).

The BCF predictions reflect both limited metabolism with omega oxidation of the methyl groups(s) and no chlorine removal, leading to relatively high BCF values, as well as higher degree of metabolism with multiple transformations leading to dehalogenation, which yield lower BCF values. Several experimental data have demonstrated BCF values > 2000 and/or 5000, which reflect limited metabolism. Therefore, the predictions with the low metabolism and relatively high BCF are considered valid and have been used in this analysis.

Several of the BCF predictions indicating bioaccumulation potential are consistent with experimental data based on which some congener groups are concluded as bioaccumulative or very bioaccumulative (see section '3.4.5 Summary and discussion of bioaccumulation'). For example, the congener groups $C_{14}Cl_{5-11}$ are very bioaccumulative based on the results of a fish dietary OECD TG 305 study (reliable without restrictions; Unpublished 2019e) and the BCF predictions for these congener groups are B and vB. A *Daphnia magna* bioaccumulation study

(reliable with restrictions; Castro *et al.*, 2019 and 2020) showed bioaccumulation of the following groups of congeners $C_{14}Cl_{4-9,}$ $C_{15}Cl_{3-9}$, $C_{16}Cl_{2-8}$ and $C_{17}Cl_{2-9}$. Whereas most of the C_{15} and C_{16} congeners were predicted as bioaccumulative (apart from $C_{16}Cl_{2-4}$), the $C_{17}Cl_{2-9}$ congeners have been predicted as not having bioaccumulation potential according to the BCF Baseline model.

The BCF predictions reflect low bioaccumulation potential (BCF values < log BCF 3.3) for the C_{14}-C_{16} congeners with a chlorine content > 65%, as well as for all C_{17} congeners. This is a result of the log Kow values being relatively higher for these congeners, which in the BCF Baseline model reflects decreasing uptake due to increasing size of the molecule. The effect of limited uptake and consequent limited bioavailability due to molecular size and steric hindrance of the larger MCCP congeners have been discussed (Du *et al.*, 2020 and Fisk *et al.*, 1996). However, also larger MCCP structures have been shown to bioaccumulate (Castro *et al.*, 2019 and 2020) and biomagnification potential of LCCP congeners has been observed (Du *et al.,* 2020). The bioaccumulation seems to be more affected by the rate of metabolism, which has been shown to decrease with increasing chlorination content and carbon chain length (Fisk *et al.*, 1996, 1998 and 2000, Unpublished, 2020).

3.4.2 Bioaccumulation in aquatic organisms (pelagic & sediment organisms)

3.4.2.1 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). The method used was based on the OECD TG 305, using a flow-through system. The test substance was a chlorinated n-pentadecane-8-^{14}C (chlorine content was 51% by weight (average); a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: congeners having 5,6,7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 46.2–58.2% Cl wt.)) mixed with a non-radio-labelled C_{14-17}, 51% wt. Cl chlorinated paraffin (average value; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{14} congeners having 4,5,6 and 7 chlorine atoms at least are expected to be present in this substance and C_{15}, C_{16} and C_{17} congeners having 5,6,7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–58.2% Cl wt.). The mixture tested contained 49% of the ^{14}C-labelled component and 51% of the non-labelled component.

A kinetic BCF of 1 087 L/kg was derived for the lower exposure group (0.93 µg/L (measured concentration), 1 µg/L (nominal concentration)) and 349 for the higher exposure group (4.9 µg/L (measured concentration), 5 µg/L (nominal concentration)), based on total radioactivity measurements (so may represent accumulation of metabolites as well as the chlorinated paraffin, so the BCF determined may overestimate the actual accumulation potential of the substance). No lipid data were presented in the original study report, so it was not possible to lipid normalise the BCF (the REACH Guidance recommends normalisation to a 5% lipid content if the data allow). A significant contributing factor to the apparent depuration during this study was growth dilution. The growth-corrected kinetic BCF would be around 1 833 – 2 072 L/kg for the lower exposure group (0.93 µg/L) (see 'Annex V – Growth correction of the BCF for a C_{15}, 51% Cl wt. substance', previously presented in EA, 2010). The growth corrected depuration half-lives were 28 to 36 days which suggests significant concern for bioaccumulation (a depuration half-life around 8-10 days is indicative of a lipid-normalised and growth-corrected BCF above 5000 L/kg according to the analysis in Environment Agency (EA, 2012a)). It is worth noting that given the low water solubility of MCCP 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 underestimate steady-state BCFs. 'Annex VI – Consideration of bioavailability in laboratory bioconcentration tests' at the end of this report contains further discussion on this issue. As it is unclear if the growth-corrected kinetic BCFs estimated in this study are accurate (overestimated based on total radioactivity or underestimated due to possible inaccuracy of measured dissolved concentrations) and as the BCFs were not lipid normalised due to the lack of data, this study is only used as supporting

information in a weight-of-evidence approach for concluding on the bioaccumulation potential of the substance. This study is considered to be reliable with restrictions.

An additional fish bioconcentration study was requested for MCCP under Commission Regulation (EC) No. 466/2008, with a deadline of 30 November 2008. The resulting study (Unpublished, 2010h) was discussed in detail in EA (2010). It was performed in accordance with OECD TG 305 and GLP using Rainbow Trout (*Oncorhynchus mykiss*). The test substance was a ^{14}C-labelled[15] C_{14} chlorinated n-alkane, 45% Cl wt. (average value; congeners having 3,4,5 and 6 chlorine atoms at least are expected to be present in this substance (equivalent to 35.3–52.6% Cl wt.); it was the same substance that was tested in the modified ready biodegradation tests described in Section 3.1.2.1.2).

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) instead of two as recommended in the OECD TG 305. 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±1 °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 1. The resulting BCFs (based on the mean whole body concentration measured at day 35 and the kinetic data) are summarised in Table 39. The mortality in both the solvent control and treated fish was less than 10% at the end of the test.

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 Table 39.

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 39.

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 a kinetic BCF of around 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). It is worth noting that the BCF steady-state cannot be corrected for the growth of fish as no agreed method is available to correct BCF steady-state for growth.

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

Table 39: 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
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.

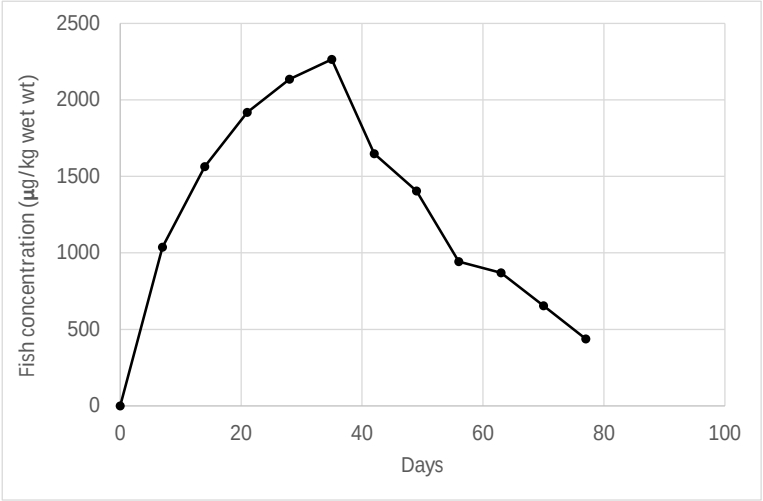


Figure 1: Uptake and depuration curve for a C_{14} chlorinated n-alkane, 45% Cl wt. in Rainbow Trout (redrawn from the data reported in Unpublished, 2010h)

According to OECD TG 305, 'a steady-state is reached in the plot of test substance in fish (Cf) against time when the curve becomes parallel to the time axis and three successive analyses of Cf made on samples taken at intervals of at least two days are within ± 20% of each other, and there is no significant increase of Cf in time between the first and last successive analysis'. The three successive analyses of Cf were confirmed to be within ± 20% of each other. However, based on the curve presented in Figure 1, it seems unlikely that steady-state was reached as the concentrations in fish seem to continue increasing between 21 to 35 days. By using a linear model, it was found that the slope of the curve for the last three points of the uptake phase (at days 21, 28 and 35) was significantly different from zero with a probability of 0.00666 (p<0.05%; Statistic data with the R software are reported in 'Annex VII – Outcome of the statistic of the linear model for the BCF data for C_{14} chlorinated n-alkane, 45% Cl wt. (Unpublished, 2010h) with the statistical software R'). This means that the curve cannot be considered parallel to the time axis. As a consequence, it can be concluded that the steady-state was not reached at the end of the uptake phase (at 35 days) and the real BCF steady-state would have been higher than 3 230 L/kg (lipid normalised). The kinetic BCF is considered to be more reliable than the steady-state BCF, as it provides a statistically more robust value.

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 in the fish tissues. 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. Theoretically the amounts of metabolites present in the fish at any one time will be a balance between their rate of formation from MCCP 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. Thus the 21% found to be incorporated into the tissue may have been the result of assimilative metabolisation of only a part of the taken up parent compound over the entire uptake and depuration period. Besides that, there may have been other polar metabolites that have left the fish via excretion (feces, urine and respiration). Also, the parent compound may have been eliminated from the fish via the excretion route during the depuration phase, the lipid-normalised and growth-corrected kinetic BCF value would still be above 5 000 L/kg, i.e. approximately 11 530 L/kg. Due to the above limitations, this study is considered as reliable with restrictions. Based on this study, it can be concluded that C_{14} chlorinated n-alkane, 45% Cl wt. (average) with 3–6 chlorine atoms per molecule (equivalent to 35.3–52.6% Cl wt.) is very bioaccumulative with an estimated lipid-normalised and growth-corrected kinetic BCF value of ca. 11 530 L/kg (BCF>5 000).

Some additional reported fish BCFs (e.g. from Bengtsson *et al.*, 1979) are summarised in EC (2005), but are either not reliable or unreliable (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 they were not considered further.

3.4.2.2 Dietary studies

A GLP-certified OECD TG 305 dietary study using a C_{14} chlorinated n-alkane, 50% Cl wt. (Unpublished, 2019e) was performed. The test substance was the same as used for the OECD TG 308 study (Unpublished, 2019c), a liquid identified as tetradecane chlorinated 50% and contained a total chlorine content of 50.07% (w/w) (average value; with 3 to 14 chlorine atoms per molecule (equivalent to 35.32–72.98% Cl wt.) as determined by analytical method). It was prepared by chlorination of n-tetradecane 99% and contained no stabiliser. This study is rated as reliable without restrictions. Radiolabelled test material was not used, so it is not possible to assess how much test material was metabolised. However, a sensitive and specific analytical method was used (APCI-QToF-HRMS) for quantifying individual congeners of MCCP and total MCCP. The study results can therefore be assumed to relate to the tested material and not metabolites.

Dietary exposure was chosen because of the very low water solubility of MCCP. 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 measured were within the ranges and limits required by OECD TG 305, with the exception that the fish in the test vessels were kept at a temperature of 11.8 to 12.5°C which is slightly lower than the range 13-17 °C recommended in the OECD TG for this species. The temperature in the control test vessel was monitored continuously and was 11.7 to 12.9°C. 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 was fed food containing nominally 15 µg/g of test substance; and a positive control group that was fed food dosed with nominally 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). Results for the fish group dosed with nominally 15 µg/g of test substance are not provided in the study report as the samples collected were only stored for possible future analysis.

The test and reference substances were incorporated into the fish feed in form of a solution of the substances dissolved in hexane. 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, ten fish were sampled from each of the exposure groups, pooled to make five samples, with two fish per pooled sample. Feeding rates for all groups were maintained at approximately 1.5% of body weight (wet weight). Initial feeding 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 food and fish samples were analysed for HCB using a GCMS method. Analysis of the test substance was performed by an academic laboratory specialising in the analysis of MCCP. The test substance was only analysed in the food and fish samples treated with nominal 15 µg/g of test substance plus 3 µg/g of HCB. Samples from the fish group were pooled (five samples with two fish per pooled sample collected at the same sampling days and for the same exposure groups i.e. control group or treated group), homogenised, lyophilised (freeze dried) and stored at -80 °C prior to shipping to the laboratory for extraction and specific analyses of the test substance using atmospheric pressure chemical ionisation time-of-flight high resolution mass spectrometry (APCI-ToF-HRMS). The effects of freeze-drying are not considered in the study report. The freeze-drying could have led to removal of volatile components but the vapour pressure of 2.7×10^{-4} Pa at 20 °C indicates that volatile losses would not be significant. Congener-specific analysis of fish and food samples was conducted and the values summed-up to obtain the total test substance concentration (see Figure 2). The method detection limit for total test substance (sum of all congeners) was 0.071 µg/g. The $C_{14}Cl_6$ to $C_{14}Cl_{11}$ groups of congeners showed a similar relative pattern of concentrations built-up and decline during the uptake and depuration phases in fish as the total substance C_{14} chlorinated n-alkane, 50% Cl wt. The concentrations of the $C_{14}Cl_3$ congeners in fish remained below the detection limit at all time points and the $C_{14}Cl_4$, $C_{14}Cl_{12}$, $C_{14}Cl_{13}$ congeners were present at concentrations close to the detection limit. The $C_{14}Cl_{14}$ concentrations in fish were detected (at a concentration equal to the limit of detection) at depuration day 3 only.

The chemical analyses appears to be well performed. The analytical report states that the accuracy, precision and reproducibility of the substance-specific analytical technique were evaluated, as well as the recoveries of the test substance from fish tissue. The external calibration produced acceptable relative standard errors (29%). The repeatability of the instrumental analysis was tested by repeatedly injecting (five times in total) 1 ng/µL of the C_{14-17} mixture (52% Cl wt., which corresponds to the external standard used for the calibration) during the run; for which the relative standard deviation (RSD) was 2.9%. The repeatability of the extraction was tested by extracting the spiked fish samples in triplicate, for which the RSD was 8%. The method detection limit (MDL) was calculated by the average blank plus three times the standard deviation. The average level of total C_{14} from the procedural blanks was 0.029 µg/g, resulting in an MDL of 0.071 µg/g.

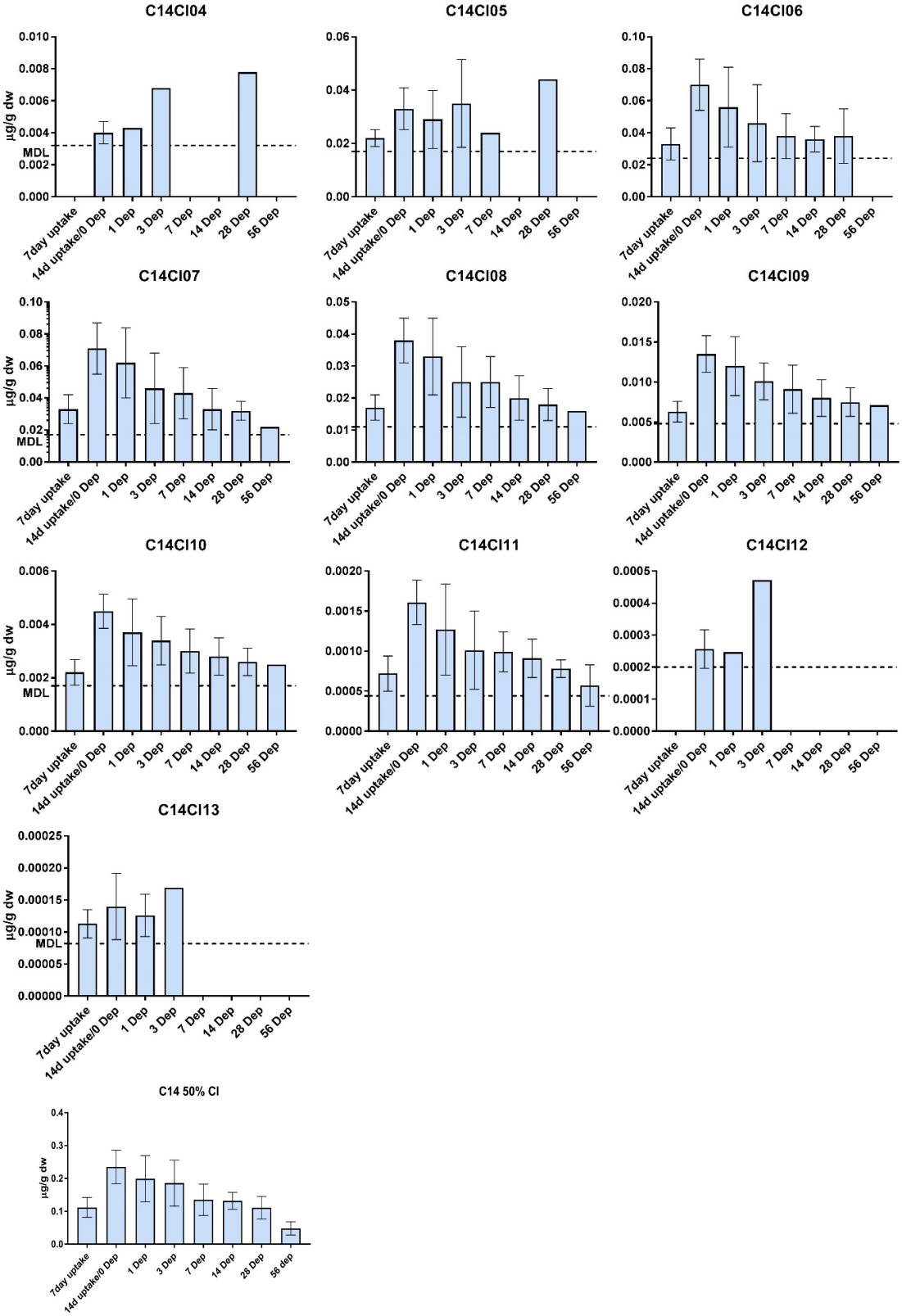


Figure 2: Concentrations (µg/g ww) of individual congeners of C_{14} (including total congener concentrations) in rainbow trout fish tissue collected at different uptake and depuration days above method detection limits (Unpublished, 2019e)

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.

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.

A large number of concentrations in fish tissue 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 low concentrations 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 and a statistical outlier on day 28 was excluded from the calculations. The influence of these replacements on the depuration rate constant (k_2; $days^{-1}$) and statistical fit (R^2; unit less) was assessed and reported in the final study report.

Dietary biomagnification factors for total C_{14} chlorinated n-alkane, 50% Cl wt. and HCB were presented in the final study report (Unpublished, 2019e). 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 0.468. No dietary BMFs were reported in the final study report (Unpublished, 2019e) for individual C_{14} congeners while congener-specific analyses of fish and food samples concentrations were provided.

The kinetic, growth corrected and lipid normalised biomagnification factors (BMF_{kgL}) for individual MCCP congeners and the total test substance (or C_{14} chlorinated n-alkane, 50% Cl wt.) were calculated using the bcmfR R-package and following the recommendations from OECD TG 305 (including recommendations from the Guidance document on Aspects of OECD TG 305 on Fish Bioaccumulation (OECD, 2017)). Detailed information on how the BMF_{kgL} values were calculated (including input parameters for the calculations) are available in 'Annex VIII – Calculations performed on the dietary BMF study (Unpublished, 2019e) '.

No statistically significant difference in the fish weight data analysis between the test (uptake phase and depuration phase) and control data was found. All the data (test uptake phase, test depuration phase and control) were pooled and an overall fish growth rate constant for the study (k_g) was calculated as the overall slope of the linear correlation.

As the overall growth rate constant (k_g) was larger than the depuration rate constants (k_2) for $C_{14}Cl_5$ and $C_{14}Cl_{7\text{-}11}$ congeners the depuration rate growth corrected constants (k_{2g}) derived from these values were all negative ($k_{2g} = k_2 - k_g$). As a consequence and based on the recommendations of the OECD TG 305, an alternative approach (i.e. mass approach) to the method for correcting growth dilution was used in order to avoid having negative k_{2g} values. However, even after applying the mass approach, all k_{2g} values derived for $C_{14}Cl_5$ and $C_{14}Cl_{7\text{-}11}$ (using linear regressions) were negative thus indicating a lack of depuration in *Oncorhynchus mykiss.* As the depuration rate growth corrected constant (k_{2g}) was negative for these congeners, the BMF derived from this negative k_{2g} was also negative. As the mass approach did not work in this case, the bcmfR R-package was re-run for $C_{14}Cl_5$ and $C_{14}Cl_{7\text{-}11}$ assuming a less conservative scenario corresponding to a lack of growth dilution where the depuration rate (k_2) was not corrected for growth ($k_g=0$ and $k_2=k_{2g}$) while in the normal scenario the depuration rate (k_2) is growth corrected as follows: $k_{2g} = k_2 - k_g$. This scenario ($k_g=0$ and $k_2=k_{2g}$) overestimates the depuration rate and consequently the estimated BMF value will be underestimated thus corresponding to the less conservative scenario. The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB.

For the $C_{14}Cl_6$ group of congeners, the "mass approach" was not applied as its k_2 value (0.02302) was higher than the overall fish growth rate constant for the study (kg =0.018794). The BMF for $C_{14}Cl_6$ group of congeners was directly derived using the bcmfR R-package following the

“normal” approach (cf. the “growth rate constant subtraction method for growth correction” as described in the OECD TG 305).

It is worth noting, that BMF value could not be derived for $C_{14}Cl_3$, $C_{14}Cl_4$, $C_{14}Cl_{12}$, $C_{14}Cl_{13}$ and $C_{14}Cl_{14}$ as these congeners either were not detected and/or not enough frequently detected during the depuration phase.

Conclusion

Based on the BMF_{kgL} values derived for the different MCCP congeners, the corresponding fish BCFs were calculated for the different MCCP congeners (including total substance) using the 15 models within the OECD TG 305 BCF estimation tool (Excel® spread sheet Version 2). Inputs and outputs from the OECD TG 305 BCF estimation using growth and lipid-corrected values are presented in ‘Annex VIII – Calculations performed on the dietary BMF study (Unpublished, 2019e) ’.

Table 40 presents the outcome of the calculations of the BMF_{kgL} values with the bcmfR R-package (including input parameters) and corresponding BCF values estimated with 15 models within the OECD TG 305 BCF estimation tool (Excel® spread sheet Version 2). The results indicate BCF values for $C_{14}Cl_{5\text{-}11}$ congeners of MCCP and C_{14} chlorinated n-alkane, 50% Cl wt. well above 5 000 L/kg. Based on this study it can be concluded that C_{14} $Cl_{5\text{-}11}$ congeners of MCCP (corresponding to 47.91–67.62% Cl wt.) and C_{14} chlorinated n-alkane, 50% Cl wt. are very bioaccumulative (>5000 L/kg) in rainbow trout.

Table 40: Summary Table – Outcome of the calculations of the BMF_{KgL} values with the bcmfR R-package (including input parameters) for MCCP congeners and total substance and corresponding BCF values estimated with 15 models within the OECD TG 305 BCF estimation tool (Excel® spread sheet Version 2)

	$C_{14}Cl_3$	$C_{14}Cl_4$	$C_{14}Cl_5$	$C_{14}Cl_6$	$C_{14}Cl_7$	$C_{14}Cl_8$	$C_{14}Cl_9$	$C_{14}Cl_{10}$	$C_{14}Cl_{11}$	$C_{14}Cl_{12}$	$C_{14}Cl_{13}$	$C_{14}Cl_{14}$	C_{14} chlorinated n-alkane, 50% Cl wt.
Mean lipid fraction in fish (%) (same value for all congeners)	5.793	5.793	5.793	5.793	5.793	5.793	5.793	5.793	5.793	5.793	5.793	5.793	5.793
Mean lipid fraction in food (%) (same value for all congeners)	16.35	16.35	16.35	16.35	16.35	16.35	16.35	16.35	16.35	16.35	16.35	16.35	16.35
Mean measured concentration of the test substance in the food or C_{food} **(µg/g** ww of food) or (mg/kg ww of food)	0.01	0.53	3.93	5.90	3.90	1.47	0.44	0.14	0.06	0.03	0.01	0.01	16.43
Food ingestion rate constant (I) (g food/g fish/day or kg food/kg fish/day) (same value for all congeners)	0.0150	0.0150	0.0150	0.0150	0.0150	0.0150	0.0150	0.0150	0.0150	0.0150	0.0150	0.0150	0.0150
Growth rate constant (k_g) (day^{-1})	0.018794	0.018794	0 (less conservative scenario)	0.018794	0.018794 Or 0 (less conservative scenario)	0 (less conservative scenario)	0 (less conservative scenario)	0 (less conservative scenario)	0 (less conservative scenario)	0.018794	0.018794	0.018794	0.018794
Best fit model used for the	-	-	Box-cox power	Log-transfor	Untransformed model	Log-transforma	Box-cox power	Log-transforma	Log-transfor	-	-	-	Untransformed

	$C_{14}Cl_3$	$C_{14}Cl_4$	$C_{14}Cl_5$	$C_{14}Cl_6$	$C_{14}Cl_7$	$C_{14}Cl_8$	$C_{14}Cl_9$	$C_{14}Cl_{10}$	$C_{14}Cl_{11}$	$C_{14}Cl_{12}$	$C_{14}Cl_{13}$	$C_{14}Cl_{14}$	C_{14} chlorinated n-alkane, 50% Cl wt.
calculation of k_2, k_{2g} and BMF_{KgL}			transformation model	mation model		tion model	transformation model	tion model	mation model				model
Depuration rate constant (k_2) (day^{-1})	Not derived	Not derived as only two data points available. However, a lack of depuration cannot be excluded	0.0021 Not statistically different from zero (Student t-test)	0.02302	0.026786	0.01244	0.01044	0.00962	0.01163	Not derived as only two data points available. However, a lack of depuration cannot be excluded	K_2 not derived as only data points for two days are available. However, a lack of depuration cannot be excluded	K_2 not derived as these congeners were only detected at depuration day 3	0.02741
Depuration rate corrected for growth (k_{2g}) (day^{-1})	Not derived	Not derived	0.0021 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.00422	0.00799 or 0.026786 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.01244 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.01044 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.00962 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.01163 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	Not derived	Not derived	Not derived	0.00861
BMF_{KgL}	BMF not derived as these congeners were not detected	BMF not derived. However, high BMF value cannot be ruled out due to a potential	0.6673 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.47292	0.42977 Or 0.12823 (less conservative scenario with $k_g=0$	0.31626 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.47684 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.54647 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.33104 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	BMF not derived. However, high BMF value cannot be ruled out due to a	BMF not derived. However, high BMF value cannot	BMF not derived as these congeners were only	0.33303

	$C_{14}Cl_3$	$C_{14}Cl_4$	$C_{14}Cl_5$	$C_{14}Cl_6$	$C_{14}Cl_7$	$C_{14}Cl_8$	$C_{14}Cl_9$	$C_{14}Cl_{10}$	$C_{14}Cl_{11}$	$C_{14}Cl_{12}$	$C_{14}Cl_{13}$	$C_{14}Cl_{14}$	C_{14} chlorinated n-alkane, 50% Cl wt.
		lack of depuration			and $k_2=k_{2g}$)					potential lack of depuration	be ruled out due to a potential lack of depuration	detected at depuration day 3	
BCF estimates (15 models)		High BCF value cannot be ruled out	All BCFs > 5000 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	All BCFs > 5000	All BCFs > 5000 Or All BCFs > 2 000 and BCFs > 5 000 (11 out of 15 models) (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	All BCFs > 5000 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	All BCFs > 2 000 and BCFs > 5 000 (14 out of 15 models) (using the less conservative scenario with $k_g=0$ and $k_2=k_{2g}$; and a log Kow of 6.86 for the constituent)	All BCFs > 5000 (less conservative scenario with $k_g=0$ and $k_2=k_2$)	All BCFs > 5000 (less conservative scenario with $k_g=0$ and $k_2=k_2$)	High BCF value cannot be ruled out	High BCF value cannot be ruled out		All BCFs > 5000

Benchmark approach

A benchmark approach is used in order to compare the laboratory BMF values for MCCP and MCCP congeners (Unpublished, 2019e) with the laboratory BMF values for substances identified as SVHC based on their vPvB properties. Based on BMF values for rainbow trout reported in Table 41, it seems that MCCP and congener groups of MCCP have BMF values at the higher end of the range of values for the SVHC substances having vB properties. Compared to the other chlorinated substance in the table below, i.e. Dechlorane Plus, the depuration rate constants fall within a similar range. The benchmark exercise supports the outcome of the Unpublished (2019e) study which shows that $C_{14}Cl_{5\text{-}11}$ congeners of MCCP and C_{14} chlorinated n-alkane, 50% Cl wt. are very bioaccumulative (>5000 L/kg) in rainbow trout.

Table 41: Comparison of laboratory BMF values in Rainbow Trout (*Oncorhynchus mykiss*) for MCCP, MCCP congeners and SVHC substances identified as vPvB

	Log Kow	Assimilation efficiency α (%)	Half-life growth corrected (days)	Depuration rate constant (K_2) (day^{-1})	BMF	BCF (L/Kg)	Reference
C_{14} chlorinated n-alkane, 50% Cl wt.	6.58	6.8	80.4	K_2 = 0.0274	BMF_{KgL} = 0.33	BCF_{KgL} > 5 000	Unpublished, 2019e
$C_{14}Cl_5$	6.32	3.2	337. 9	K_2 = 0.0021	BMF_{KgL} = 0.67	BCF_{KgL} > 5 000	Unpublished, 2019e
$C_{14}Cl_6$	6.66	4.7	164.1	K_2 = 0.0230	BMF_{KgL} = 0.47	BCF_{KgL} > 5 000	Unpublished, 2019e
$C_{14}Cl_7$	6.59	8.1	86.7	K_2 = 0.0268	BMF_{KgL} = 0.43	BCF_{KgL} > 5 000	Unpublished, 2019e
$C_{14}Cl_8$	6.66	9.3	55.7	K_2 = 0.0124	BMF_{KgL} = 0.32	BCF_{KgL} > 5 000	Unpublished, 2019e
$C_{14}Cl_9$	6.86	11.8	66.4	K_2 = 0.0104	BMF_{KgL} = 0.48	BCF_{KgL} > 5 000	Unpublished, 2019e
$C_{14}Cl_{10}$	5.98	12.4	72.1	K_2 = 0.0096	BMF_{KgL} = 0.55	BCF_{KgL} > 5 000	Unpublished, 2019e
$C_{14}Cl_{11}$	6.34	9.1	59.6	K_2 = 0.0116	BMF_{KgL} = 0.33	BCF_{KgL} > 5 000	Unpublished, 2019e
D4	6.49	40	105	K_{2g} = 0.0066	BMF_{KgL} = 0.47–4.6		ECHA, 2015a ECHA, 2018a
D5	8.023		74	K_{2g} ~0.0094	BMF = 0.63-3.9 (depending on normalisation)		ECHA, 2018a
o-Terphenyl vPvB constituent of Terphenyl, hydrogenated (EC Number: 262-967-7)	5.52				BMF_{KgL} = 0.59	BCF = 12 993 BCF_{KgL} = 6 219 ± 1 647 (estimated based on BMF_{KgL} of 0.59)	ECHA, 2018b
		20	8.1	K_2 = 0.085	BMF_{KgL} = 0.2	BCF_{KgL} =3513–7 694 (estimated based on BMF_{KgL} of 0.2)	
Benz[a]anthracene	5.91				BMF = 0.001		ECHA, 2017d
Dechlorane Plus	≥9	~0.8-2 (anti-	30–40	K_{2g} = 0.010 –	BMF_{KgL} = 0.01 –	BCF > 5 000	ECHA, 2017e

	Log Kow	Assimilation efficiency α (%)	Half-life growth corrected (days)	Depuration rate constant (K_2) (day^{-1})	BMF	BCF (L/Kg)	Reference
		DP) ~1.6-7.5 (syn-DP)	(anti-DP) 50—70 (syn-DP)	0.013 (syn-isomer) and K_{2g} = 0.017 – 0.023 (anti-isomer) (lipid-normalised)	0.023 (anti-isomer) BMF_{KgL} = 0.046 – 0.062 (syn-isomer)	(estimation based on long depuration half-life)	
C_{12}-PFCA	9.363 (estimated log P with ACD/Labs)				BMF = 0.43± 0.062 (juvenile rainbow trout (carcass))	BCF = 18 000 (in juvenile rainbow trout (carcass), measured in a study with aqueous exposure) BCF_K = 5 761—8 210 (estimated based on elimination rate and BMF value; in juvenile rainbow trout (carcass)) BCF = 18 000 (in juvenile rainbow trout (liver) measured in a study with aqueous exposure) BCF_K = 7 927—8 575 (estimated based on elimination rate and BMF value; in juvenile rainbow trout (liver))	ECHA, 2012a
C14-PFCA	10.8				BMF=1.0 ± 0.25	BCF = 23 000 (in	ECHA, 2012b

	Log Kow	Assimilation efficiency α (%)	Half-life growth corrected (days)	Depuration rate constant (K_2) (day^{-1})	BMF	BCF (L/Kg)	Reference
	(estimated log P with ACD/Labs)				(juvenile rainbow trout (carcass))	juvenile rainbow trout (carcass) measured in a study with aqueous exposure) BCF_K = 17 835– 19 294 (estimated based on elimination rate and BMF value; in juvenile rainbow trout (carcass)) BCF = 30 000 (in juvenile rainbow trout (liver) measured in a study with aqueous exposure) BCF_K = 17 835– 19 294 (estimated based on elimination rate and BMF value; in juvenile rainbow trout (liver))	
C11-PFCA	7.2 (estimated with COSMOtherm)				BMF= 0.28 ± 0.04 (juvenile rainbow trout (carcass))	BCF = 2 700 (in rainbow trout (carcass) measured in a study with aqueous exposure) BCF_K = 5 848– 6 326 (estimated based on elimination rate	ECHA, 2012c

	Log Kow	Assimilation efficiency α (%)	Half-life growth corrected (days)	Depuration rate constant (K_2) (day^{-1})	BMF	BCF (L/Kg)	Reference
						and BMF value; in juvenile rainbow trout (carcass)) BCF = 4 900 (in juvenile rainbow trout (liver) measured in a study with aqueous exposure) BCF_K = 5 246– 5 675 (estimated based on elimination rate and BMF value; in juvenile rainbow trout (liver))	

Note: BCF_K means kinetic bioconcentration factor; BCF_{KgL} means lipid normalised, growth corrected kinetic bioconcentration factor; BMF_{KgL} means lipid normalised, growth corrected kinetic biomagnification factor; K_{2g} means growth corrected depuration rate constant.

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 considered 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 MCCP 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 but might also include metabolites. 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 congeners likely to be present in MCCP (the method of manufacture of MCCP means that it is unlikely that a chlorine atom will be present on both the terminal and adjacent carbon atoms). Furthermore, for two of the studies (Fisk *et al.*, 1998b; and Fisk *et al.*, 2000), it is important to note that the measured concentration of test substance in the fish only considers concentration in the carcass (whole fish minus liver and gastrointestinal tract). Monitoring data in biota indicate that MCCP can be found in the liver of snakes, frogs, seabirds and cod (Du *et al.,* 2019 and 2020; Green *et al.*, 2019; Reth *et al.,* 2006 and Herzke *et al.,* 2019), that is why, it is most likely that the concentrations measured in the carcass only lead to an underestimation of the concentration in the fish tissues, subsequently an underestimation of the BMF values. According to Fisk *et al.* (1996), fish concentrations reported in the study and used for deriving BMF values are referring to whole-body fish concentrations.

The metabolism rate constants for the substances tested were estimated (Unpublished, 2013). 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[16].

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. However, these findings seem to be in agreement with the predictions made by Gawor and Wania (2013). The authors (Gawor and Wania, 2013) estimated the metabolic half-lives of CP in fish (estimated with BCFBAF v3.01 (EPI Suite™) and by iterative fragment selection (IFS) (Brown *et al.*, 2012). They observed that metabolic half-lives of CP in fish are more governed by the size of the carbon structure and to a lesser degree by the chlorination degree. For example, half-lives estimated for LCCP exceed 1000 days, compared to 10 to 100 days for SCCP. For all the CP, it is the less volatile components (high Koa and low Kaw) with a higher degree of halogenation that have the potential to significantly bioaccumulate in humans. These compounds preferentially partition into organic media, including organism lipids. The modelling of environmental bioaccumulation potential found that both the size of the carbon skeleton and the number of halogens influence which

[16] 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).

components will be bioaccumulative, which is illustrated by SCCP, MCCP, and LCCP with ~5–6, ~4–5, and ~4–5 chlorines respectively having the highest potential for bioaccumulation in humans of all the CP congeners. Any CP holding less chlorine would have a small potential to bioaccumulate in humans, according to the model. In general, the congeners with partitioning properties favouring bioaccumulation tend to also have higher degradation half-lives in fish (Gawor and Wania, 2003).

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 MCCP are summarised in Table 42 (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 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 (2019e) was used to derive a growth-corrected and lipid-normalised BMF value.

Table 42: Summary of dietary accumulation data for MCCP

Substance	Concentration in food (µg/kg)	Feeding rate (% body weight)	Assimilation efficiency - **α**[c] (%)	Growth corrected depuration rate constant (10^{-2}/d)	Growth corrected depuration half-life (days)	Kinetic dietary BMF[d]	Reference
$C_{14}H_{26}Cl_4$ (42.3% Cl)	92	Not given	33	1.8	39	1.7	Fisk *et al.* (1998b)
$C_{14}H_{25}Cl_5$ (a) (47.9% Cl)	66	Not given	51	1.3	53	3.6	Fisk *et al.* (1998b)
$C_{14}H_{25}Cl_5$ (b) (47.9% Cl)	54	Not given	46	1.5	46	2.9	Fisk *et al.* (1998b)
$C_{14}H_{24}Cl_6$ (a) (52.6% Cl)	63	Not given	130	2.4	29	5.0[e]	Fisk *et al.* (1998b)
$C_{14}H_{24}Cl_6$ (b) (52.6% Cl)	40	Not given	27	1.6	43	1.6	Fisk *et al.* (1998b)
^{14}C - $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl (average); with Cl_{5-8} equivalent to a range of 47.9-59.9% Cl wt., based on a Gaussian distribution, as considered by the dossier submitter)	1 300	1.5	10	1.2	58	0.43	Fisk *et al.* (2000)
^{14}C - $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl (average); with	13 000	1.5	11	1.7	41	0.27	Fisk *et al.* (2000)

Substance	Concentration in food (µg/kg)	Feeding rate (% body weight)	Assimilation efficiency - α[c] (%)	Growth corrected depuration rate constant (10^{-2}/d)	Growth corrected depuration half-life (days)	Kinetic dietary BMF[d]	Reference
Cl_{5-8} equivalent to a range of 47.9-59.9% Cl wt., based on a Gaussian distribution, as considered by the dossier submitter)							
C_{14} chlorinated n-alkane 50% Cl wt. (average; with Cl_{3-14} equivalent to a range of 35.32–72.98% Cl wt., determined by analytical method)	16 430	1.5	6.77	0.861	80	0.33	Unpublished (2019e), BMF & depuration re-assessed for the purpose of this report
^{14}C - $C_{16}H_{31}Cl_3$ (34.1% Cl with $Cl_{3.3}$ (average); with Cl_{2-5} equivalent to a range of 24.1–44.5% Cl wt., based on a Gaussian distribution, as considered by the dossier submitter)	29	1.5	33	1.4	50	1.07	Fisk *et al.* (1996)
^{14}C - $C_{16}H_{31}Cl_3$ (34.1% Cl with $Cl_{3.3}$ (average); with Cl_{2-5} equivalent to a range of 24.1–44.5% Cl wt., based on a Gaussian distribution, as considered by the dossier submitter)	296	1.5	35	1.9	37	0.90	Fisk *et al.* (1996)
^{14}C - $C_{16}H_{21}Cl_{13}$ (69% Cl with $Cl_{13.4}$ (average); with Cl_{12-15} equivalent to a range of 66.6–71.6% Cl wt., based on a Gaussian distribution, as considered by the dossier submitter)	21	1.5	30	1.2	58	0.72	Fisk *et al.* (1996)
^{14}C - $C_{16}H_{21}Cl_{13}$ (69% Cl with $Cl_{13.4}$ (average); with Cl_{12-15} corresponding to a range of 66.6–71.6% Cl wt.,	198	1.5	9.4	1.1	63	0.44	Fisk *et al.* (1996)

Substance	Concentration in food (µg/kg)	Feeding rate (% body weight)	Assimilation efficiency - **α**[c] (%)	Growth corrected depuration rate constant (10^{-2}/d)	Growth corrected depuration half-life (days)	Kinetic dietary BMF[d]	Reference
based on a Gaussian distribution, as considered by the dossier submitter)							
^{14}C - $C_{16}H_{21}Cl_{13}$ (69% Cl with $Cl_{13.4}$ (average); with Cl_{12-15} equivalent to a range of 66.6–71.6% Cl wt., based on a Gaussian distribution, as considered by the dossier submitter)	2 000	1.5	11.4	0.9	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 as reported in Table 42 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. Dietary BMF data reported in Table 42 indicate that depuration from fish is relatively slow and BMFs above one are estimated for C_{14} chlorinated paraffins with four and six chlorine atoms per molecule (corresponding to chlorine contents of approximately 42–53% by weight). In contrast, a growth-corrected and lipid-normalised BMF value of 0.333 was obtained by evaluation of results from the most recent OECD TG 305 study for C_{14} chlorinated n-alkane, 50% Cl wt (Unpublished, 2019e). BMFs are estimated to be close to one for C_{16} chlorinated paraffins with two and five chlorine atoms per molecule (chlorine content approximately 24.1–44.5% by weight). At higher chlorine contents than these the BMF is below one for both the C_{14} and C_{16} substances. According to the PBT guidance (Chapter R.11; ECHA, 2017b), if a BMF is found to be <1, it cannot be considered as a good discriminator for concluding substances not to be (very) bioaccumulative according to the BCF criteria of Annex XIII. 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 chlorine atoms on the terminal carbon and on adjacent carbon atoms. These types of structures are likely to be presented in smaller amounts in commercial MCCP than structures with a different chlorine positioning to this and hence they may not represent the more typical structures.

As well as BMF data, these feeding studies provide information on the growth-corrected depuration half-life of MCCP (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 fish BCFs have been calculated using this tool based on relevant data from the Fisk *et al.* (1996), Fisk *et al.* (1998b), Fisk *et al.* (2000) and Unpublished (2019e) studies as shown in 'Annex IX – Analysis of bioaccumulation using fish dietary studies' and 'Annex VIII – Calculations performed on the dietary BMF study (Unpublished, 2019e) . 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 MCCP 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 5 304 to 126 000 L/kg and 13 000 to 140 000 L/kg can be estimated for C_{14} (including C_{14} 50% Cl wt.) and C_{16} chlorinated paraffins, respectively. An analysis has also been carried out by estimating the non-growth-corrected BCF. In this case, the non-growth-corrected BCF is estimated to be of the order of 2 566 to 45 000 L/kg for the C_{14} chlorinated paraffins (including C_{14} 50% Cl wt.), 8 000 to 62 000 L/kg for the C_{16} chlorinated paraffins, and a maximum 31 111 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). Thus, indicating a high to very high level of bioaccumulation while the BCFs predicted are expected to be under-estimated by using this less conservative approach ($k_g=0$).

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 MCCP 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 0.00861 day^{-1}, corresponding to a half-life of 80.45 days (Unpublished, 2019e). 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. Due to the uncertainties reported above, the outcome of the Fisk *et al.* studies are used as supporting information in a weight-of-evidence approach for concluding on the bioaccumulation potential of these substances.

In Fisk *et al.* (2000), the depuration rate constant for $C_{18}H_{31.4}Cl_{6.6}$ (48.64% Cl wt.) is 0.0076 and 0.0088 day^{-1}, which is equivalent to a growth-corrected depuration half-life of 79 to 91 days. The corresponding BMF values were 0.81 and 0.93. 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. LCCP would therefore be expected to have a BCF above 5 000 L/kg.

3.4.2.3 Other supporting data

Daphnia magna

Castro *et al*. (2019); Castro (2020) investigated bioaccumulation potential in the cladoceran water flea *Daphnia magna*. 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)[17]. Detailed composition of the test material is provided in Figure S6 of the supplementary information and further details were provided by the lead author (Castro M, Personal Communication, 2020 and 2021).

Study description and results

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 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

[17] 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 and a C_9-C_{30} 52% Cl wt. product from China.

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 (green algae *Pseudokirchneriella subcapitata*) (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 concentration of algae (when added) was 4 µC/mL (approximately $3x10^5$ algae cells/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.

After the 48-hour uptake period, 10 daphnids per replicate were collected and after the 24-hour depuration, 25 daphnids per replicate were collected (Castro M, Personal Communication, 2020). Any dead animals were 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 homogenised 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. A total of 224 chlorinated paraffin congener groups from C_9Cl_3 to $C_{31}Cl_{12}$ were used to identify the congener group pattern for all the test materials used in the study. Chlorinated paraffin congener group patterns of all the samples fitted well those of the test materials (R^2 > 0.80). Chlorinated paraffin pattern recognition was done by analysing the relative individual congener response and quantification was based on the sum of these instrumental responses. Thereafter, chlorinated paraffins in individual samples were quantified with the respective test material with no pattern deconvolution.

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 and for Cereclor S45 they were respectively 172 ± 57% and 144 ± 43% for daphnid and water samples. The high average recoveries 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 concentrations of Cereclor S45 in Daphnia after 48-hour uptake via water only were in the range 0.31 - 1.15 ng/µg dry weight with a mean of 0.66 ng/µg dry weight (Castro M, Personal Communication, 2020). At the end of the depuration period, the Daphnia concentrations of Cereclor S45 were all below the LOD.

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. The supplementary information to the paper indicates that the water content of a fed juvenile Daphnia magna (3-4 days old), from the same culture as used in the study, was 90%.

Mortality did not exceed 10% in any of the controls or treatment groups (Castro M, Personal Communication, 2020).

Steady-state BCF values were calculated based on the total concentration in Daphnia exposed via water at steady-state divided by the freely dissolved water concentration (average concentration 1.2 µg/L). Steady-state BAF values were calculated based on the total concentration in Daphnia exposed via water and food at steady-state divided by the freely dissolved water concentration (average 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 43.

Table 43: MCCP bioaccumulation data for *Daphnia Magna* (Castro *et al.*, 2019 and Castro, 2020)

Parameter	Result
Log BCF (dry weight, steady-state)	5.7 ± 0.19 L/kg dw
Log BCF (wet weight, steady-state)	~4.7 L/kg ww[b]
Log BCF (lipid normalised, steady-state)	7.0 ± 0.19 L/kg lipid
BCF (lipid normalised, steady-state)	10 000 000 L/kg lipid
BCF (wet weight, steady-state)	~50119 L/kg ww[b]
Log BAF (dry weight, steady-state)	5.6 ± 0.1 L/kg dw
Log BAF (wet weight, steady-state)	~4.6 L/kg ww[b]
Log BAF (lipid normalised, steady-state)	6.7 ± 0.1 L/kg lipid
BAF (wet weight, steady-state)	~39810 L/kg ww[b]
Uptake rate constant, k_u	1.1×10^5
Uptake rate constant via respiration only (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).

b – Results re-calculated based on a Daphnia water content of 90%, (Castro M, Personal Communication, 2020).

After one week's exposure, the amount of MCCP adsorbed to the Daphnia 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). Thus, the study results show that accumulation was taking place and, despite the large surface/volume ratio compared with larger organisms, adsorption of MCCP to the body surface was only a minor contribution to the concentration measured in Daphnia.

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. The authors consider that 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. Another consideration is that bioavailability might be reduced by adsorption to uneaten food.

The highest steady-state log BCF values measured in the study were observed for the C_9-C_{14} 70% Cl wt. Huels 70C product (SCCP) (Log BCF = 6.0 ± 0.44 L/kg dw or 7.4 ± 0.44 L/kg lipid). The lowest values were obtained for the LCCP product, CP-42 (Log BCF = 5.4 ± 0.23 L/kg dw or 6.7 ± 0.23 L/kg lipid). MCCP had the shortest depuration half-life of the five products tested. 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, CP-42. It was speculated that this could have been explained by metabolism of low chlorine content chlorinated paraffins. 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.

Evaluation of the study
The study is well performed, and it is considered to be reliable with restrictions. The study indicates very high steady-state BCFs and BAFs in *Daphnia magna*, well above 5000. However, the exact values of the BCF and BAF results should be treated with caution for reasons listed below:

- There is no standard internationally recognised test guideline for *Daphnia* bioaccumulation. The study followed an adapted version of OECD TG 305 for fish bioaccumulation, but in the absence of a ring-test with *Daphnia*, the reliability and reproducibility of the method is unknown.

- Although the dissolved concentration of MCCP was below the water solubility limit (27 µg/L), it is not clear whether 48 hours gave sufficient time for all soluble congeners to fully dissolve. However, Figure S6 in the Supplementary information to Castro *et al.*, 2019 reports a 90% similarity between the congener patterns found in the test material and in the Daphnia, which suggests that this was sufficient time at least for a majority of congeners.

- Only a single water concentration value is presented, (1.18 µg/L with a standard deviation of 0.41 µg/L; Castro M, Personal Communication, 2020) which was measured in the absence of test organisms. It is not clear how this differs from the actual exposure concentration in the presence of organisms or how variable this might have been over the duration of the test.

- *Daphnia* are very small organisms and only 10 or 25 organisms were collected for each measurement. This could affect the reliability of concentration measurements, which would also have been affected by the analytical recovery rate exceeding 100%. The sensitivity of the results to variations in the measured concentrations is unclear.

- There is some uncertainty in the derived kinetic data (rate constants, depuration half-life and time to 95% steady state). The depuration kinetics are based on an LOD value as levels in daphnids were below the LOD at the end of the study. Since the actual concentration in the organisms at the end of the depuration period may have been lower, the depuration rate constant could have been higher. The depuration rate is used directly to estimate the uptake rate. As noted by the authors, since static conditions were used, the concentration of MCCP in water after 24 h depuration would not have been zero, which complicates the interpretation of depuration.

- The authors claim that steady-state in the organisms was achieved after 48 hours. The duration of the uptake and depuration phase was based on a pilot screening study using test material CP-52 that lasted 72 h. 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.

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, it is not clear 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. Due to the above limitations, this study is used as supporting information in a weight-of-evidence approach for concluding on the bioaccumulation potential.

Information on specific congeners

Figure S6 in the Supplementary information to Castro *et al.,* 2019 shows the congener pattern observed in the test material Cereclor S45 and in the Daphnia after aqueous exposure. The lead author has provided more detailed congener profiles and information on the relative contribution of each congener to the total sum of MCCP used for quantification (Castro M, Personal Communication, 2020 and 2021). Specific standards were not used for every individual congener, so the quantification of individual congeners is not possible, and the results give a semi-quantitative indication of the relative contribution of each congener to the total MCCP. The absence of a specific congener in the given figure does not necessarily mean that it was not present in the sample.

A comparison of the congener patterns found in the test material Cereclor S45 with those found in Daphnia after aqueous exposure shows that some congeners were detected in Daphnia but not in the test material. The congeners which are not detected in the commercial product mainly fall at the extremes of the Cl distribution. These congeners may not have been detected because of the limitations of the semi-quantitative method in detecting congeners present at lower concentration compared to the other congeners that lie in the middle of the Cl distribution (e.g. $C_{14}Cl_5$).

Congeners detected in both the test material Cereclor S45 and in Daphnia after aqueous exposure were:

- $C_{14}Cl_4$, $C_{14}Cl_5$, $C_{14}Cl_6$, $C_{14}Cl_7$
- $C_{15}Cl_3$, $C_{15}Cl_4$, $C_{15}Cl_6$, $C_{15}Cl_7$, $C_{15}Cl_8$
- $C_{16}Cl_3$, $C_{16}Cl_4$, $C_{16}Cl_5$, $C_{16}Cl_6$, $C_{16}Cl_7$, $C_{16}Cl_8$
- $C_{17}Cl_3$, $C_{17}Cl_4$, $C_{17}Cl_5$, $C_{17}Cl_6$, $C_{17}Cl_7$, $C_{17}Cl_8$

Since the above congeners were found in both the test material and Daphnia, the BCF from this study is considered relevant for the bioaccumulation assessment of each of these congeners.

The following congeners were not detected in the test material Cereclor S45 but were detected in Daphnia after aqueous exposure:

- $C_{14}Cl_8$, $C_{14}Cl_9$

- $C_{15}Cl_5$, $C_{15}Cl_9$
- $C_{16}Cl_2$
- $C_{17}Cl_2$, $C_{17}Cl_9$

Since the above congeners were detected in Daphnia after aqueous exposure, the BCF from this study is also considered relevant for the bioaccumulation assessment of each of these congeners as it suggests accumulation in these organisms. As explained above, non-detection of a group of congeners in the test material does not necessarily mean that it was not present in the test material. Alternatively, the above congeners may have been formed by transformation of the test material and then accumulated in Daphnia.

Mytilus edulis

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:

Madeley and Thompson, 1983
Bioaccumulation was assessed as part of a 60-day GLP-certified toxicity study (Madeley and Thompson, 1983). The test substance was a commercial C_{14-17} chlorinated n-alkane, 52% Cl wt. product (average value; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{14} congeners having 4, 5, 6 and 7 chlorine atoms at least are expected to be present in this substance; C_{15-16} congeners having 5, 6, 7 and 8 chlorine atoms at least are expected and C_{17} congeners having 6,7,8 and 9 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–58.2% Cl wt.)). It was mixed with a small amount of radiolabelled chlorinated paraffin (n-pentadecane-8-^{14}C, 51% wt. Cl ((average); a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: congeners having 5,6,7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 46.2–58.2% Cl wt.)). A flow-through test system with filtered natural seawater (salinity 35 ‰ , pH 8.1-8.3, dissolved oxygen 6.15-8.0 mg/l) at 15±1°C was employed. Acetone, at a concentration of 500 ppm (v/v) or 0.5 ml/L, was present in the test and a solvent control containing acetone at the same concentration was run. 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). The organisms were fed with algae (*Platymonas suecica*) at a rate of 1.01-1.11×10^9 cells/day. The algae were continuously dosed to the in-flowing dilution water. There was no significant mortality of the mussels (<10% of mortality) as a result of exposure to either concentration of chlorinated paraffins for 60 days. A reduction in filter feeding activity was seen at the higher test concentration. No effects on mean shell length were seen in either of the two exposure concentrations when compared to the control populations (data on tissue weights were not reported). According to Madeley and Thompson (1983), the analytical method used to measure the parent compound is recognised to be relatively inaccurate, but it was the only available analytical technique specific for chlorinated paraffins at that time. The analytical method used for the parent compound did not differentiate between all individual chlorinated paraffins; it broadly distinguished between short and intermediate chain (C_{10-17}) lengths on the one hand and long chain (C_{20-30}) lengths on the other hand. 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 of the mixture of commercial C_{14-17} chlorinated n-alkane, 52% Cl wt. product and the radiolabelled chlorinated paraffin (n-pentadecane-8-^{14}C, 51% wt. Cl) (quantification of chlorinated paraffins was performed by Thin layer Chromatography)) or 2 856 L/kg (based on ^{14}C-measurements of the radiolabelled chlorinated paraffin (n-pentadecane-8-^{14}C, 51% wt. Cl)). These BCF values have been corrected for concentration of CP_{10-17} found in mussels at the start of the study (assuming

that the volume of the mussels has not significantly changed during the study). It is worth noting that as the pre-contamination level was low (0.180 µg/g ww) it does not change significantly the BCF values: 2 181 L/kg (based on parent compound analysis of the mixture of commercial C_{14-17} chlorinated n-alkane, 52% Cl wt. product and the radiolabelled chlorinated paraffin (n-pentadecane-8-^{14}C, 51% wt. Cl) or 2 855 L/kg (based on ^{14}C-measurements of the radiolabelled chlorinated paraffin (n-pentadecane-8-^{14}C, 51% wt. Cl)). 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.

Based on the information available in the study, it was not possible to check whether steady-state was reached at the end of the 60 days exposure period. However, in the below study of Renberg *et al.* (1986), steady-state was reached in mussels after 14 days of exposure. In addition, it is worth noting that depuration was not studied. The percent lipids of the mussels was not reported. In this study Madeley and Thompson (1983) may have underestimated the true BCF, because it was 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 particles. These data are therefore BAF values. Due to the uncertainties around exposure to / dosing of the test substance (above the water solubility and with possibility of significant over or underestimation of BAF) and the analytical method for the parent compound, this study is not considered to be reliable. However, it is reported here as the outcome of this study is in line with the below study from Renberg *et al.* (1986) which suggests that congeners of MCCP are bioaccumulating in mussels.

Renberg et al. (1986)

Renberg *et al.* (1986) tested a ^{14}C-labelled C_{16} chlorinated n-alkane, 34.1% Cl wt. (with 2 to 5 chlorine atoms per molecule equivalent to a range of 24.1–44.5% Cl wt. and based on a Gaussian distribution (as considered by the dossier submitter); the average formula was given as $C_{16}H_{30.7}Cl_{3.3}$). This study is considered as reliable with restrictions. The mussels (*Mytilus edulis*) used in the test had a mean length of 3.0±0.5 cm and a mean wet weight of 0.5±0.1 g and were allowed to attach to glass plates for approximately one week prior to the start of the test. 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 mussels were fed with a suspension of green algae before the start of the test but they were not fed during the bioaccumulation study. The exposure consisted of a 28-day uptake phase (depuration was not studied) and two samples of wet tissue from three mussels were sampled on each of day 1, 3, 7, 14, 21 and 28 of the study. The concentration in water was also determined at the same time as in the mussels. Levels of CP were calculated from the radioactivity measurements taking into account the known specific activity of the labelled CP-preparations. 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[18] (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 of between 540 and 705 µg/kg wet weight after 14 days exposure. A BCF steady-state and a BCF statistically determined were reported. For statistical determination the following exponential function was used:

CFt = BCF (1-exp(-Kt)) where CFt is defined as $C_{0:t}/C_{w:t}$; where $C_{0:t}$ and $C_{w:t}$ are the concentrations of the bioconcentrating substances in the organism and water, respectively, at time *t (days)* and *K* is the uptake rate constant and BCF is the asymptotic value.

[18] The mean value of 0.11 µg/L was calculated based on the mean concentration values in water as reported in Table II (Renberg *et al.,* 1986) and used for deriving BCF values.

The authors concluded that the BCF steady-state for the C_{16} chlorinated paraffin was 6 920 L/kg and 7 090 L/kg (statistically determined) with a standard error of 1 100 L/kg and confidence limits[19] of 4 620-9 570 L/kg. The BCF for the control substance was around 13 800 L/kg. The extractable fat in the mussels was measured and a mean value of 1.87% was calculated. According to Renberg et al. (1986), this value is in close agreement with the literature figure of 1.9% (Diem and Lentner, 1971). The BCF values for C_{16} chlorinated paraffin were corrected for a lipid content of 1.9% and they were equal to 7 031 L/kg (BCF steady-state) and 7 204 L/kg (BCF statistically determined) with confidence limits of 4 694–9 723 L/kg. The radioactivity measurements does not distinguish between parent compound and possible metabolites and tissue-bound residues. Therefore, the results could indicate uptake, accumulation and elimination of metabolites rather than the parent compound. The BCF of 7090 L/kg (which corresponds to a BCF of 7 204 L/kg (corrected to a lipid content of 1.9%)) probably represents the upper limit of the true bioaccumulation factor of the chlorinated paraffin. Furthermore, there is a possibility that at least some of the exposure of the organisms resulted from direct ingestion of the substance adsorbed to food particles. These data are therefore BAF values. Based on the above limitations, this study is used as supporting information in a weight-of-evidence approach for concluding on the bioaccumulation potential of the substance.

Lumbriculus variegatus

An experiment to investigate the uptake of medium-chain chlorinated paraffins by oligochaetes (*Lumbriculus variegatus*) from sediment has been carried out (Fisk *et al.*, 1998a). The chlorinated paraffins used were synthesised by chlorination of ^{14}C-hexadecane (labelled in the 1-position for the 34.1% wt. Cl product, and uniformly labelled for the 69% wt. Cl product), and had the following average formulas: $C_{16}H_{31}Cl_3$ 34.1% wt. Cl (with 2-5 chlorine atoms per molecule equivalent to a range of 24.1–44.5% Cl wt. and based on a Gaussian distribution (as considered by the dossier submitter); average: 3.3 chlorine atoms per molecule) and $C_{16}H_{21}Cl_{13}$ 69% wt. Cl (with 12-15 chlorine atoms per molecule equivalent to a range of 66.6–71.6% Cl wt. and based on a Gaussian distribution (as considered by the dossier submitter); average: 13.4 chlorine atoms per molecule). The sediment used had the following composition: 76% sand, 21% silt and 3% clay; organic carbon content 1.3-1.5% of dry weight.

For each exposure concentration, 36 jars were filled with spiked sediment to provide a 100:1 organic carbon:oligochaete lipid ratio (15 animals per jar) and the jars were placed in flow-through aquaria maintained at 11.6°C. The uptake period of the experiment was for 14 days (this was extended to 21 days in some cases), followed by a 42 day depuration period, where the animals were placed in clean sediment. Analysis of the concentrations present in sediment, interstitial water and the oligochaetes was by ^{14}C measurements performed by liquid scintillation counter (LSC) after a variety of extraction methods. Biota-sediment bioaccumulation factors were determined both from the rates of uptake and depuration, and also the equilibrium concentrations found in the organisms and sediment (equilibrium was reached within 14-21 days). For the determination of the bioaccumulation factors, concentrations in the organisms were normalised to the worm lipid content and the sediment concentrations were normalised to the organic carbon content (also corrected for loss of ^{14}C (possibly by biodegradation or metabolism)) as determined by the difference between toluene-extractable and total ^{14}C measurements. The results of the analysis are shown in Table 44.

Table 44: Uptake and accumulation of ^{14}C-labelled chlorinated paraffin by *Lumbriculus variegatus* (Fisk *et al.*, 1998a)

Substance	Sediment conc. at 14 days (µg/kg dry wt)	Sediment organic carbon content[b] (%)	Pore water conc. (µg/L)	Lipid conc.[c] (%)	Uptake rate constant (g/g/d)	Depuration rate constant (d^{-1})	Depuration half-life (days)	BSAF or Kinetic BAF[d]	Steady-state BAF[d]
$C_{16}H_{31}Cl_3$ (34.1% wt. Cl)	47.1	1.4	-	2.5	9.3×10^{-2}	2.1×10^{-2}	33	4.4	0.7
	135	1.3	0.1	2.3	7.6×10^{-2}	-[a]	-[a]	-[a]	
$C_{16}H_{21}Cl_{13}$ (69% wt.	264	1.5	0.1	2.0	1.3×10^{-2}	2.3×10^{-2}	30	0.6	0.2

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

Cl.)									

Note:
a) The depuration data for this treatment did not show a significant linear relationship with time.
b) On a dry sediment weight basis.
c) Mean lipid concentration of exposed organisms.
d) BAF is the bioaccumulation factor – defined as [concentration in organisms (µg/kg lipid (wet wt.))]/[concentration in sediment (µg/kg organic carbon (dry wt.))]. Kinetic BAF based on rate of uptake and rate of depuration. 'Steady-state' BAF based on concentration measurements in organism and sediment at equilibrium (14 days).

A biota-sediment accumulation factor (BSAF) of 4.4 (or 9.16 if lipid normalised to 5% lipid content) was determined for a C_{16} chlorinated n-alkane, 34.1% Cl wt. (with 2-5 chlorine atoms per molecule) and the BSAF for a C_{16} chlorinated n-alkane, 69% Cl wt. (with 12-15 chlorine atoms per molecule) substance was lower at 0.6 (or 1.5 if lipid normalised to 5% lipid content). According to the PBT guidance (REACH guidance Chapter R.11; ECHA, 2017b), lipid and organic carbon normalised BSAF values of 0.5 and higher are an indication of high bioaccumulation thus suggesting that $C_{16}H_{31}Cl_3$ 34.1% wt. Cl and $C_{16}H_{21}Cl_{13}$ 69% wt. Cl have a high bioaccumulation potential. For the determination of concentrations in the worms, the organisms were not cleansed of gut contents prior to analysis so this may have led to a significant overestimation of the actual concentration in the organism and hence the actual uptake of the substances. Due to the uncertainties around the BSAF value (possibility of significant overestimation of the BSAF), this study does not allow a conclusion.

3.4.3 Bioaccumulation in terrestrial organisms (soil dwelling organisms, vertebrates)

3.4.3.1 Soil dwelling organisms

Thompson *et al.* (2001) determined the uptake of a n-pentadecane-8-^{14}C, 51% Cl wt. substance (average; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{15} congeners having 5,6,7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 46.2–58.2% Cl wt.)) by earthworms (*Eisenia fetida*) from soil as part of an earthworm toxicity study. This study is considered reliable with restrictions. The substance had a radiochemical purity of >96.6% w/w and was mixed with a commercial C_{14-17}, 52% Cl wt. (average: 51.9% Cl wt.; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{14} congeners having 4,5,6 and 7 chlorine atoms at least are expected to be present in this substance; C_{15-16} congeners having 5,6,7 and 8 chlorine atoms at least are expected and C_{17} congeners having 6,7,8 and 9 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–58.2% Cl wt.)) to give nominal test concentrations of 100, 320, 1,000, 3,200 and 10,000 mg/kg dry weight (dw) in the test soil. The purity of the commercial C_{14-17}, 52% wt. Cl substance was 99.06% w/w with 0.67% w/w of C_{10-13} and 0.16% w/w of C_{18}. The soil used was an artificial soil consisting of 10% sphagnum moss peat, 70% quartz sand, 20% kaolinite clay and 0.25% calcium carbonate. The soil had an organic carbon content of 4.7%, a pH of 6.66-7.09 and was maintained at moisture content of 26% (a soil wet weight:dry weight ratio of 1.35) throughout the test. The test system was maintained at 20±1°C with a controlled photoperiod of 16 hours light:8 hours dark with a 20 minutes transition period. At the start of the test, four replicates of 10 adult worms each were exposed to the test substance in 500 g of soil (with a depth of ca. 6 cm). Four replicates vessels were included for the control and solvent (acetone) control. After 28 days, the remaining adult worms were removed and any cocoons present were allowed to hatch over the following 28 days. The concentration of the chlorinated paraffin present in the soil phase (on days 0, 28 and 56), the adult worms (on day 28) and the hatched juvenile worms (on day 56) was determined by a radiochemical method. Before radiochemical analysis, the adult and juvenile worms were purged for their gut content.

The mean measured concentrations in soil at the start of the test ranged from 84 to 95% of the nominal values. On Day 28, the mean measured concentrations in soil ranged from 74 to 90%

of the nominal and on Day 56 the range was 64 to 92% of nominal. The measured concentrations in soil over the day 0 to day 28 period were, on average, 87% of the nominal concentration. This value was used to correct the nominal concentrations of 320 and 3,200 mg/kg dw, for which no analysis was undertaken, to give 'equivalent measured concentrations' of 280 and 2,800 mg/kg dw respectively. At Day 28, no mortality of the parent worms was observed in the control, solvent and at the test concentrations ≤ 1,000 mg/kg dw in the test soil. Mortality at 3,200 and 10,000 mg/kg dw in the test soil was 2.5% and 15%, respectively (mortality ≥ 12.5% is statistically significant ($p=0.05$) compared to the mortality in the solvent control). A significant decrease in the weight of the parent worms was observed at Day 28 at the nominal concentrations of 3,200 and 10,000 mg/kg dw compared with the solvent control (a decrease of weight of -15% and -34%, respectively). The test results at 10,000 mg/kg dw are considered to be not reliable. No significant effect on the weight of the adult worms was observed at the test concentrations ≤ 1,000 mg/kg dw in the test soil on Day 28.

Earthworm-soil accumulation factors (BAFs) were calculated based on the ratio of the concentration of the test substance in the earthworm (mg/kg ww or mg/kg dw) and the concentration of the test substance in the soil (mg/kg ww or mg/kg dw). BAFs of 2.4 (based on ww concentrations) and 10.8 (based on dw concentrations) for adults; and 2.3 (based on ww concentrations) and 10.2 (based on dw concentrations) for juveniles were determined at the lowest nominal concentration tested (100 mg/kg dw) for C_{15} chlorinated n-alkane, 51% Cl wt. The BAFs as calculated directly from the ratio of concentration in earthworm/concentration in soil decreases with increasing concentration in soil. Although limited in number, the data appear to show that at high concentrations, the concentration in earthworm is not dependent on the bulk concentration of the substance present in soil. A possible explanation of this finding is that the uptake by the earthworm may be mostly via the pore water, and at the high soil concentrations used in this study, the pore water becomes saturated with the test substance. In the risk assessment report (EC, 2005), the concentration of the substance in the soil pore water was estimated to be 2.9 µg/L, 32.5 µg/L or 336 µg/L at equilibrium (at soil concentrations of 79, 900 and 9,300 mg/kg dry weight respectively). As the upper limit of the water solubility of MCCP is around 27 µg/L (see Section 1.4), it is possible that at the high concentrations used in this study, the soil pore water could have become saturated with the chlorinated paraffin. The other possible mode of uptake of the substance by earthworms from soil is direct ingestion of soil-bound substance. If direct ingestion of soil-bound substance was a major uptake route, then the concentration of substance present in the earthworm would be expected to be directly related to the soil concentration. The available information appears to indicate that this route of uptake is negligible compared with uptake via pore water.

The interpretation of these results is complicated by the fact that the measurements are based on ^{14}C-determinations that could include metabolites of the test substance in addition to the parent compound. It is worth noting that metabolism of MCCP by the sediment-dwelling oligochaete, *Lumbriculus variegatus*, has been demonstrated in the study of Fisk *et al.* (1998a). Therefore, the results could indicate uptake, accumulation and elimination of metabolites rather than the parent compound. As a consequence, the BAFs reported in this study probably represent the upper limit of the true bioaccumulation of the chlorinated paraffin in the earthworms. In addition, it was not possible to calculate the BSAFs of the worms (corresponding to the BAFs normalised for the worm lipid content and the soil total organic carbon content) as the worm lipid content was not reported in the study. In addition, it is unclear if the steady-state was reached at the end of the test as the concentrations in the worm tissues were only reported at Day 28 for the adults and at Day 56 for the juveniles. Furthermore, the depuration was not studied. Due to these limitations, this study is used as supporting information in a weight-of-evidence approach for concluding on the bioaccumulation potential of the substance.

Nicholls *et al.* (2001) reported the concentrations of SCCP and MCCP 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.

3.4.3.2 Plants

A study investigating the actual accumulation of medium-chain chlorinated paraffins in roots of carrot (*Daucus carot*a) has been carried out (Thompson *et al.*, 2005). Further details can be found in EC (2007). The substance tested was ^{14}C-labelled 52.48% wt. chlorinated n-pentadecane (average; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{15} congeners having 5,6,7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to 46.2–58.2% Cl wt.) that was produced as a mixture with unlabelled C_{14-17}, 52.48% wt. chlorinated paraffin (average value; C_{14} congeners having 4,5,6 and 7 chlorine atoms at least are expected to be present in this substance; C_{15-16} congeners having 5,6,7 and 8 chlorine atoms at least are expected and C_{17} congeners having 6,7,8 and 9 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–58.2% Cl wt.)).

The soil used in the test consisted of a mixture of 50% sterilised Surrey loam and 50% gravel. The soil was characterised as follows: pebbles (particle size 64-4 mm) – 4.6%, granules (particle size 4-2 mm) – 40.4%, very coarse sand (particle size 2-1 mm) – 5.0%, coarse sand (particle size 1-0.5 mm) - 0.9%, medium sand (particle size 0.5-0.25 mm) – 1.0%, fine sand (particle size 0.25-0.125 mm) – 3.0%, very fine sand (particle size 0.125-0.063 mm) – 3.5% and silt/clay (particle size <0.063 mm) – 41.7%. The soil had an organic carbon content of 2.0% and a pH of 6.6-7.3.

The test substance was added to the soil in a two-stage process. Firstly, a solution of the substance in acetone was added to a sample of dried, powdered, sewage sludge from a treatment plant treating primarily domestic wastewater. The acetone was then allowed to evaporate. After this, the spiked dried sewage sludge (175 g) was mixed into the soil (35 kg dry weight) in a 41.5 litre cylindrical container (the container was rotated at approximately 21 revolutions per minute for one hour) in two batches, and the two batches were then combined prior to use. The weight of sewage sludge therefore accounted for 0.5% of the total dry soil. Two nominal exposure concentrations were prepared in this way, 1 mg/kg dry weight and 10 mg/kg dry weight. A control soil was prepared in the same way.

The tests were carried out using rectangular containers (one per treatment) with a volume of 32.8 litres. The depth of soil in the containers was approximately 130 mm. The base of the containers had multiple perforations and the bottom of the container was covered with horticultural capillary matting. The containers were placed on a further layer of capillary matting within individual containment trays. This system was used as it allowed any test substance that was leached from the soil to be retained and drawn back into the soil with the irrigation water. Water (dechlorinated tap water) was provided primarily by sub-irrigation through this matting (the matting was kept wet by daily additions of water), but additional water was provided as necessary as a fine mist to the soil surface. During the test, illumination was provided by an array of 22 fluorescent lights (light intensity ~17,500 Lux at the soil surface) operating on a 16 hours light and 8 hours dark photoperiod. The temperature was maintained at 20±2°C during the study.

The experiment was initially started one day after spiking the soil. The soils were initially planted with 70 seeds per treatment but this series of experiments was terminated 21 days after planting owing to insufficient numbers of viable seedlings in all treatment groups, including the controls. Following termination of this series no further water additions were made to the soil prior to re-seeding the soils.

Two days prior to re-seeding the soils (55 days after the spiked soils were originally prepared) the soils were mixed to full depth. The soils were then re-seeded with 127 seeds per treatment (57 days after the soils were originally prepared), and watering was recommenced. This was taken as day 0 of the growth phase of the study.

Soil samples were analysed for the presence of total radioactivity on day -57 (i.e. immediately after spiking the soil), day -2, day 28 and day 70 of the study. On each sampling occasion, a total of three soil samples (taken from the front, middle and back of the test vessel) were taken for each treatment group, and one soil sample was taken from the control group. Four carrot plants from each treatment group were randomly selected for analysis on day 42, 50, 60 and 70. The roots were washed and dried prior to analysis. The analytical method used to determine the total ^{14}C-residues in the soil was changed during the study. The samples taken on day -57 were extracted twice with acetone and the acetone extract was analysed for ^{14}C. For day -2, the analytical procedure was modified as other analyses carried out on day -10 and -8 suggested that the acetone extraction procedure was no longer recovering all of the radioactivity in the soil. The modified method involved directly combusting a dried, powdered, sub-sample of soil and determining the amount of $^{14}CO_2$ evolved. In addition, powdered samples were also extracted using an alternative solvent system (two extractions with hexane, followed by two extractions with ethyl acetate and finally two extractions with dichloromethane). For this method the total radioactivity in the combined extracts, and also the residual ^{14}C remaining in the soil after extraction, was determined. Based on this, it was concluded that analysis by direct combustion of the soil was preferable and this method was used for the subsequent time-points.

The total radioactivity in the carrot roots was determined by combustion analysis. As the maximum weight of tissue that could be contained within one combustion cone was ~1 g, multiple cones each containing a sub-sample of the root, were used for the larger roots. Up to day 70, the total root was analysed in this fashion. However, by day 70 the large size of some of the roots precluded such analysis, and so in cases where the total root weight exceeded 10 g sub-samples of the upper, middle and lower portions of the root were taken for analyses.

For the experiment at the lower treatment level, both the mean concentrations in the soil and the concentrations in the roots could not be determined reliably (although the level of radioactivity was above the analytical detection limit in some samples, the level in other samples at each time point was below the analytical detection limit). Therefore, it was not possible to derive reliable accumulation factors from the data for this treatment level. For the higher treatment level, the concentration in the roots of the carrots was found to be highest on day 42 and then decreased until the last sampling time (day 70). As the measured concentration in soil was reasonably constant over this period, this suggests that the rate of accumulation of ^{14}C-label from the soil was slower than the rate of growth of the carrots. Another explanation for this is that the rate of uptake from the soil declined as the carrots grew larger resulting from a decrease in the surface area to volume ratio. The mean measured concentration in soil over the day -2 to day 70 period was 4.9 mg/kg dry weight (equivalent to 4.34 mg/kg wet weight (by using a soil wet dry ratio of 1.13)). The mean root concentration was 0.38 mg/kg fresh weight at day 42, 0.25 mg/kg fresh weight at day 50, 0.20 mg/kg fresh weight at day 60 and 0.13 mg/kg fresh weight at day 70. Using the mean measured concentration in soil of 4.34 mg/kg wet weight, and the mean concentration of radiolabel in the roots, the bioaccumulation factor (concentration in root (mg/kg fresh weight)/concentration in soil (mg/kg wet weight)) can be estimated as 0.088 at day 42, 0.058 at day 50, 0.046 at day 60 and 0.030 at day 70. The mean bioaccumulation factor over days 50-70 was 0.045 for C_{15} chlorinated n-alkane, 52.48% Cl wt, thus suggesting that the accumulation in carrots seems to be low. It should be noted that at day 42, the weight of the carrot roots was approximately 1 g, well below the size that would be consumed as food. That is why, the mean BAF was derived from Days 50 to 70 when the carrot roots weight was in the range 5–27 g.

As indicated above, the analytical method was changed part way through the study as the extraction with acetone alone did not appear to recover the expected amount of radiolabel from the soil (i.e. the levels measured by this approach were below the nominal concentration; the actual levels measured by this method were not given other than for day -57). One interpretation was that the substance was becoming more tightly bound to the soil during the study potentially leading to a reduced bioavailability to the plants. However, it should be noted that when the analytical method was changed to be based on combustion of the soil, the concentration was found to be relatively constant throughout the experiment (no statistically significantly

differences ($p=0.05$) were found in the levels measured from day -2 to day 70). Since these direct measurements of the total amount of radiolabel present in the soil were also below the nominal concentrations, there is no conclusive evidence for a decline in extractability of the substance from the soil over the course of the experiment.

The interpretation of these results is complicated by the fact that the measurements are based on ^{14}C-determinations that could include metabolites of the test substance in addition to the parent compound. As a consequence, the bioaccumulation factors reported in this study probably represent the upper limit of the true bioaccumulation of the chlorinated paraffin in the carrots. The bioaccumulation potential of MCCP in carrots has been calculated using a mean measured value of the concentration in soil (mean value in soil was 4.9 mg/kg dw between day -2 to day 70 period) which might have biased the BAF values calculated. The BAF values were not growth corrected while carrots significantly grew during the test. In addition, it is unclear if the sewage sludge from a treatment plant treating primarily domestic wastewater and used in this test were not contaminated by MCCP as it is expected that MCCP will bind to sludge given its high K_{OC} (See Section 3.2.3). Furthermore, only the root exposure was considered in this study while foliar exposure would have been a relevant additional route of exposure. Indeed, due to the long-range transport potential of MCCP, surface deposition by atmospheric transport represents a relevant route of exposure for plants. Due to these limitations, this study does not allow a conclusion to be made.

Iozza *et al.* (2009a and 2009b) showed that MCCP were present in samples of spruce needles from the European Alps. MCCP were 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.

3.4.3.3 Mammalian and bird data

Yuan and de Wit (2018) and Yuan *et al*. (2019) analysed biota samples from Sweden for chlorinated paraffins with a chain length up to C_{30} using APCI-QTOF-MS. Numerical values are provided in 'Annex III – Summary of environmental monitoring data'. In the terrestrial food web, bank voles were found to contain the lowest amounts of MCCP among the studied species. The detected concentrations of MCCP 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). MCCP 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. This study was not evaluated.

A consideration of the main experimental data for bioaccumulation potential in mammals was given in EC (2007) and the conclusions are repeated here for completeness (further information on toxicokinetic data is available in section 4.1). Mammalian studies using radiolabelled MCCP 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). 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. In the study by CXR Biosciences Ltd (2005a), it was 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 (see section '4.1 Toxicokinetics (absorption, metabolism, distribution and 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 MCCP 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). In a follow-up study (Thomas *et al.*, 2003) MCCP was detected 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 congeners of MCCP present in samples of human breast milk from Bavaria (Hilger *et al.* 2011b).

Li *et al.* (2017) determined the concentration of SCCP, MCCP and LCCP 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. MCCP 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).

The European Food Standards Agency (2020) quotes levels of MCCP between < LOQ (5.5 µg/kg lipid) to 112 µg/kg lipid in human breast milk across 11 European countries collected between 2014 and 2016; and sampled as part of the WHO/UNEP Coordinated Survey of Human Milk for Persistent Organic Pollutants.

3.4.4 Field data

It is important to note that there are analytical challenges associated with the detection and quantification of MCCP. Therefore, detections of MCCP in biota and the environment are considered valid but quantitative information, when available, should be treated carefully as the reliability of the information might depend on the analytical method used in the study.

3.4.4.1 Field bioaccumulation data

Herzke *et al.* (2013) studied the background concentrations of SCCP and MCCP in Arctic biota from Svalbard (Norwegian Arctic) (see the description of this study in section 3.3). The trophic position (TP) for each species was calculated relative to the species representing the lowest position. The authors made the assumption that isotopic enrichment was constant among trophic positions and of the order 3.4 ‰ according to Post (2002). Trophic magnification factors (TMFs) were calculated as the antilogarithm of the slope (b) of the linear regression between log concentration (lw) and the samples TP in the case of CP. The estimation of the TMFs results in values ranging between 2.3 for the SCCP and 2.0 for the MCCP, indicating a biomagnifcation potential for the S/MCCP. The R^2 coefficient of determination for the linear correlation between log concentration and trophic position varies between 0.52 for SCCP and 0.31 for MCCP. According to Herzke *et al.* (2013), the estimated TMFs have to be treated with caution since the traditionally tissue type (muscle) used in TMF studies could not be used. Instead plasma, liver and egg samples were available which are characterised by a much shorter turnover rate and those only reflect the short-term exposure rather than the long-term one. In addition, exact sampling dates is unknown so that temporal variability is unknown.

de Wit *et al.* (2020) studied chlorinated paraffins (SCCP, MCCP and LCCP) in Baltic Sea biota at different trophic levels to determine their concentrations and biomagnification potential. Nine species (1 mollusc, 2 fish, 3 birds and 3 marine mammals) were sampled: blue mussel (*Mytilus edulis*), viviparous eelpout (*Zoarces viviparus*), common eider (*Somateria mollissima*), Atlantic herring (*Clupea harengus*), common guillemot (*Uria aalge*), white-tailed eagle, grey seal, harbor seal (*Phoca vitulina*) and harbor porpoise. Samples used for analysis by dichloromethane (DCM)-enhanced APCI-Orbitrap-HRMS and by APCI-QTOF-MS were collected in 2015 or 2016, except for harbor seal (2012–2016), grey seal (2006–2010), harbor porpoise (2006–2012) and one pooled herring sample (2014). Mean concentration values found in the different species are provided in 'Annex III – Summary of environmental monitoring data'. SCCP, MCCP and LCCP were found in all Baltic species studied with MCCP being the predominant CP group. In general, the distribution pattern of CP was similar across all species, with the ΣCP being composed of SCCP (31–38%), MCCP (48–54%) and LCCP (13–15%). The highest mean concentration value of MCCP was found in the liver of harbor seal (390 ng/g lw). Mean ΣCP concentrations were highest in liver of harbor seals, porpoises, eiders, grey seals, and in sea eagle eggs as previously reported (Yuan *et al.*, 2019). Eelpout and mussel contained lower concentrations of SCCP and MCCP, similar to those in herring muscle and liver, in seal and porpoise blubber, and in guillemot and eider eggs. According to de Wit *et al.* (2020), CP were found in higher concentrations in liver than in other tissues, possibly due to liver being the site of metabolism.

The biomagnification potential for the predator and prey species from the same general areas of the Baltic Sea were calculated using the mean lipid normalised concentrations of specific CP (de Wit *et al.*, 2020). For CP, ratios of mean lipid weight concentrations of SCCP, MCCP and LCCP between possible predator-prey pairs range from 1.5–5.0 for SCCP, 0.40–3.1 for MCCP and 0.90–3.3 for LCCP. The highest ratios for MCCP were seen for harbor seal/herring (2.4) and sea eagle/guillemot pairs (3.1). Lower BMF values for MCCP were found in: guillemot/herring pairs (0.4), sea eagle/eider pairs (1.1), grey seal/herring (1.4) and Harbor porpoise/herring (1.8). These BMF values should be considered with caution as the predators and their potential prey were not collected at exactly the same sites or times, and no biogeochemical trophic position proxies were available to determine trophic level. In addition, the temporal trends of the CP in the Baltic Sea are unknown. These BMF values provide indicative information only and are used as supporting information in the bioaccumulation assessment of MCCP.

Du *et al.* (2020) investigated the occurrence of chlorinated paraffins (CP) in two snake species, the terrestrial short-tailed mamushi snake (*Gloydius brevicaudus;* n=7) and the semi-aquatic red-backed rat snake (*Elaphe rufodorsata*; n=9), from paddy fields in the Yangtze River Delta, China (located in the junction between Jinshan District in Shanghai and Jiaxing City in Zhejiang province, close to Hangzhou Bay). SCCP, MCCP and LCCP were analysed by APCI-QTOF-MS in liver, muscle and adipose tissues (abdominal fat) of the two snake species. The samples were collected in October 2011, well after the breeding season. Black-spotted frog *(Pelophylax nigromaculatus;* n=45 (3 pools of female frogs and 2 pools of male frogs)), the major prey of red-backed rat snake, was collected from the sampling site in the same time period (on 25th September, 4th October and 22nd October 2011 (Zhou Y. personal communication, October 2020)). The frog muscle samples were analysed by APCI-QTOF-MS. CP were quantified using a pattern-deconvolusion algorithm. The biomagnification potential of CP through the black-spotted frog–red-backed rat snake food chain was determined. LODs and LOQs were calculated as average blank levels (n=10) and three or ten times the SD of the blank. The LOQ mainly reflects the background levels of CP groups in the laboratory environment. The blank levels of MCCP were 2.4±1.8 ng. Following spiking experiments (n=3) of 2 µg MCCP (57.0% Cl wt.), a recovery of 85±15% (mean±RSD) was observed for MCCP (Zhou Y. personal communication, October 2020).

Concentrations of MCCP in liver, muscle and adipose tissues of the two snake species are provided in 'Annex III – Summary of environmental monitoring data'. Comparable concentrations of MCCP in muscle tissues for the two snake species were found in Du *et al.* (2018). Du *et al.* (2020) found the highest concentrations of MCCP in the Short-tailed Mamushi snake muscle (up to 14,000 ng/g lw (average value)). For both snake species the average lipid

weight concentrations were found in the order: muscle > liver > adipose (the same pattern is found for LCCP). Furthermore, a similar pattern is found for frogs based on average lipid weight concentrations: muscle > liver > eggs (Du *et al.,* 2019). According to Du *et al.,* (2019), for frogs no significant differences were found among lipid normalised concentrations of liver, muscle and egg tissues ($p>0.05$). The MCCP congener group patterns for all snake tissues were dominated by C_{14} followed by C_{15}. For both snakes, the overall lipid weight concentrations were in the order SCCP > MCCP > LCCP > vSCCP. The tissue-specific CP burdens for the two snake species were calculated. Higher proportions of MCCP burdens were found in red-backed rat snake muscle (36%) and adipose tissues (59%). For Short-tailed Mamushi, MCCP proportions were 76% in muscle and 19% in adipose tissues. For both snake species, there is a general shift to the right in the C_nCl_m patterns (meaning an increase in chain length and degree of chlorination) going from liver to muscle and then adipose tissue, with shorter chain, lower chlorinated CP more predominantly in liver, more MCCP with higher chlorination degree accumulating in muscle, and more MCCP and LCCP with similar or somewhat higher chlorination degree accumulating in adipose tissue. This indicates a successive loss of shorter chained, lower chlorinated CP and enrichment of longer chained and more highly chlorinated CP from liver to muscle and then adipose tissue. These results may indicate a combination of differential metabolism in the liver removing shorter, lower chlorinated CP preferentially to MCCP and LCCP with higher chlorination degrees, differential accumulation in muscle lipids because of different hydrophobicity of CP groups and later differential accumulation and storage in adipose.

Concentrations found in frog muscles and red-backed rat snake muscles were used for calculating BMF values. As the adipose tissue was not analysed in the frog study it was not possible to calculate a BMF based on concentrations in the adipose. The $\delta^{13}C$ difference between red-backed rat snake and black-spotted frog was 1.07 ‰ , which indicates that these two species were feeding in the same food web. In addition, the $\delta^{15}N$ difference between them was 1.97 ‰ (an average difference in $\delta^{15}N$ of 3.4 ‰ between adjacent trophic levels has been suggested to be remarkably constant among different types of consumers (Vander Zanden and Fetzer, 2007)). BMF values were calculated based on lipid normalised concentrations in the muscle tissues from the two species, having similar lipid contents (frog muscle: 0.56±0.06% and snake muscle: 0.76±0.12%). A mean BMF of 1.78 (mean BMF values for 35 congeners range from 0.21 to 2.8; see Table 45) was calculated for MCCP based on the mean lipid weight concentrations found in the muscles of red-backed rat snake (n=9) and back-spotted frog (n=45) from a total of 35 congeners of MCCP ($C_{14}Cl_{3\text{-}11}$, $C_{15}Cl_{3\text{-}11}$, $C_{16}Cl_{3\text{-}11}$ and $C_{17}Cl_{4\text{-}12}$). The percentage of BMF values >1 for MCCP congener groups was 94% (33 out of 35 congeners had mean BMFs > 1, $C_{17}Cl_4$ and $C_{17}Cl_{12}$ had mean BMFs <1). The highest BMF value of 2.8 was found for the $C_{15}Cl_{11}$ (66% Cl wt.) congener. In general, the BMFs decreased slightly in the order of vSCCP > SCCP > MCCP > LCCP, with respective mean values of 2.2, 1.9, 1.8 and 1.7. The highest BMF value of 4.5 was found for the $C_{18}Cl_{10}$ (59.26% Cl wt.) congener. In addition, BMF values were calculated based on lipid normalised concentrations in the liver tissues from the two species. It is worth noting that the frog liver functions as a storage organ of glycogen and fat to a greater extent than for other vertebrates, which is supported by the much higher lipid content in frog liver (frog liver: 22.6±8.2% and snake liver: 1.28±0.53%). That is why the BMF values in the liver are interpreted in combination with BMF values in the muscle tissues. All the BMF values reported in Table 45 for the different congeners of MCCP ($C_{14}Cl_{3\text{-}11}$, $C_{15}Cl_{3\text{-}11}$, $C_{16}Cl_{3\text{-}10}$ and $C_{17}Cl_{4\text{-}10}$) in the liver of the red-backed rat snake and back-spotted frog are all above 1. Based on the combination of the lipid normalised BMFs >1 in the muscles and livers of a snake-frog predator-prey relationship for MCCP congeners it seems that $C_{14}Cl_{3\text{-}11}$, $C_{15}Cl_{3\text{-}11}$, $C_{16}Cl_{3\text{-}10}$ and $C_{17}Cl_{5\text{-}10}$ have B and vB properties. Regarding $C_{17}Cl_4$ and $C_{17}Cl_{12}$ for which mean lipid normalised BMFs in the muscles of snakes-frogs are <1, it cannot be excluded that these congeners have B/vB properties as it has been shown for instance that a BCF of 2000 corresponds to a lipid normalised BMF of 0.1 in a dietary bioaccumulation studies with carp (ECHA, 2017b). Regarding $C_{16}Cl_{11}$, while the BMF value in the muscle of snakes-frogs is >1, no concentration was detected in the liver of snakes. As a consequence, no conclusion can be drawn regarding the B/vB properties of these three congeners ($C_{16}Cl_{11}$, $C_{17}Cl_4$ and $C_{17}Cl_{12}$).

It is worth noting that the BMF values reported in Table 45 are based on the muscle and the liver tissues and as a consequence, they do not refer to the whole body weight of the snakes and frogs. BMF values in the muscles and livers of the snakes-frogs both indicate that biomagnifcation of congeners of MCCP occurs in snakes. According to Herzke *et al.*, (2013), the muscle tissue is considered to be relevant compared to other tissue type such as plasma, liver and eggs which are characterised by a much shorter turnover rate and those only reflect the short term exposure rather than the long term one. It is worth noting that lipid normalised concentrations of MCCP in snake and frogs follow the same pattern with highest concentrations of MCCP found in the muscles (muscle > liver > adipose for the snakes and muscle > liver > eggs for frogs). It is noted that the sample size of the snakes is small compared to the one for the frogs. While this study is considered to be reliable with restrictions, due to above mentioned limitations, this study is used as supporting information in a weight-of-evidence approach for concluding on the bioaccumulation potential of the substance.

Table 45: Lipid normalised BMF values for MCCP congeners based on mean lipid weight concentrations found in the muscle and in the liver of the red-backed rat snake (n=9) and back-spotted frog (n=45) (Zhou Y. personal communication, October 2020)

MCCP congeners	Log Kow values (estimated by the Moriguchi log P (Mlog P) model from the VEGA platform)	Mean lipid normalised BMFs in muscle of snakes-frogs	Mean lipid normalised BMFs in liver of snakes-frogs
$C_{14}Cl_3$ (35.3% Cl wt.)	6.68	1.36	5.33
$C_{14}Cl_4$ (42.3% Cl wt.)	6.92	1.58	5.36
$C_{14}Cl_5$ (47.9% Cl wt.)	7.15	1.78	4.74
$C_{14}Cl_6$ (52.6% Cl wt.)	7.38	1.89	4.29
$C_{14}Cl_7$ (56.5% Cl wt.)	6.69	1.73	4.39
$C_{14}Cl_8$ (59.9% Cl wt.)	6.91	1.50	4.99
$C_{14}Cl_9$ (62.8% Cl wt.)	7.12	1.19	5.19
$C_{14}Cl_{10}$ (65.4% Cl wt.)	7.33	1.72	4.60
$C_{14}Cl_{11}$ (67.6% Cl wt.)	7.54	2.33	1.33
$C_{15}Cl_3$ (33.8% Cl wt.)	6.92	1.89	3.98
$C_{15}Cl_4$ (40.6% Cl wt.)	7.15	1.87	4.30
$C_{15}Cl_5$ (46.2% Cl wt.)	7.38	2.21	3.38
$C_{15}Cl_6$ (50.8% Cl wt.)	7.6	1.78	3.53
$C_{15}Cl_7$ (54.8% Cl wt.)	7.82	1.94	3.40
$C_{15}Cl_8$ (58.2% Cl wt.)	7.12	1.92	3.20
$C_{15}Cl_9$ (61.1% Cl wt.)	7.33	1.99	2.20
$C_{15}Cl_{10}$ (63.7% Cl wt.)	7.54	2.78	1.70
$C_{15}Cl_{11}$ (66.0% Cl wt.)	7.75	2.86	3.50

MCCP congeners	Log Kow values (estimated by the Moriguchi log P (Mlog P) model from the VEGA platform)	Mean lipid normalised BMFs in muscle of snakes-frogs	Mean lipid normalised BMFs in liver of snakes-frogs
$C_{16}Cl_3$ (32.3% Cl wt.)	7.15	1.81	5.57
$C_{16}Cl_4$ (39.0% Cl wt.)	7.38	2.82	3.69
$C_{16}Cl_5$ (44.5% Cl wt.)	7.6	1.78	2.69
$C_{16}Cl_6$ (49.2% Cl wt.)	7.82	1.74	3.76
$C_{16}Cl_7$ (53.2% Cl wt.)	8.03	1.63	2.96
$C_{16}Cl_8$ (56.6% Cl wt.)	8.25	1.62	2.98
$C_{16}Cl_9$ (59.6% Cl wt.)	7.54	1.54	1.83
$C_{16}Cl_{10}$ (62.2% Cl wt.)¨	7.75	2.41	1.58
$C_{16}Cl_{11}$ (64.5% Cl wt.)	7.95	1.83	<1*
$C_{17}Cl_4$ (37.6% Cl wt.)	7.6	0.91	3.97
$C_{17}Cl_5$ (43.0% Cl wt.)	7.82	2.44	2.71
$C_{17}Cl_6$ (47.7% Cl wt.)	8.03	1.65	3.02
$C_{17}Cl_7$ (51.6% Cl wt.)	8.25	1.63	3.56
$C_{17}Cl_8$ (55.0% Cl wt.)	8.45	1.70	3.62
$C_{17}Cl_9$ (58.0% Cl wt.)	8.66	1.92	1.67
$C_{17}Cl_{10}$ (60.7% Cl wt.)	7.95	2.51	2.06
$C_{17}Cl_{12}$ (65.1% Cl wt.)	8.34	0.21	<1*

*No concentration detected in the liver of snakes.

Du *et al.* (2020) observed that the biomagnification potential of CP congener groups seems to be related to both hydrophobicity and molecular size of these chemicals. vSCCP and SCCP have moderate molecular size and thus, lower hydrophobicity is probably a predominant factor driving biomagnification. For LCCP and MCCP congener groups, although the hydrophobicity is high, the large molecular size may increase the difficulty to cross membranes and limit their bioavailability and biomagnification potential. However, as reported by Du *et al.* (2020), a laboratory study of *Daphnia magna* showed that SCCP, MCCP and LCCP were readily bioconcentrated from water and bioaccumulated from dietary exposure and that this was more dependent on the chlorination degree of the CP than on the carbon chain length (Castro *et al*. (2019); Castro (2020)). In this study, some LCCP congener groups were also more bioaccumulative than SCCP congener groups. Thus, the higher BMFs for some specific LCCP, as observed in Du *et al.* (2020), may be related to their chlorination degree instead of their carbon chain length.

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 MCCP.

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 MCCP 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 MCCP 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 MCCP 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 congeners 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.

3.4.4.2 Monitoring data in biota

The available monitoring data for MCCP in biota are summarised in 'Annex III – Summary of environmental monitoring data'. When considering these data, it is important to recognise that the analysis of MCCP in environmental samples is challenging. 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:

- The Norwegian Institute for Water Research – NIVA (Green *et al.*, 2019), studied the levels, trends and effects of contaminants (including SCCP/MCCP) in biota along the coast of Norway (from the Swedish border in the south and to the Russian border in the north), as well as Svalbard. Samples were collected during 2018. Chlorinated paraffins (CP) were analysed in liver of cod from 13 stations, in blue mussel from 11 stations, and in blood and eggs of eider from one station. Blue mussel (*Mytilus edulis* and potentially other *Mytilus* species such as *M. trossulus,* and *M. galloprovincialis),* dogwhelk (Nucella lapillus), Atlantic cod (*Gadus morhua*) and the common eider (*Somateria mollissima*) were the targeted species for studying concentrations in CP. The blue mussel samples were collected from 3rd September to 20th November 2018. This is within the OSPAR guidelines and considered to be outside the mussel spawning season. The Atlantic cods were sampled from 16th August 2017 to 9th November 2018. The common eider blood samples were collected from 15 individuals (two subsamples from each) and eggs from 15 other individuals during the period 16th to 23rd June 2018. All samples are from adult nesting females.

CP were determined by GC-MS. Concerns regarding the reliability of this analytical method complicates the interpretation of the results. The LOQ was set to 5−10 ng/g (with an estimation of 50% of uncertainty). Values below the limit of quantification (LOQ) are set to an average of ten random numbers between the LOQ and half of the value of this limit for calculation for use in time trends.

In general, the concentrations of MCCP in blue mussel were lower than in cod and ranged from 2.81 to 170.0 µg/kg w.w (median values for mussels) and from 56.6 to 124.5 µg/kg w.w (median values for cods). Blue mussel from Bodø harbour had the highest median concentrations of MCCP (170.0 µg/kg w.w). The median concentration of MCCP in blue mussel increased from 2017 to 2018 (Green *et al.*, 2018 and 2019). Median concentration of MCCP was highest in cod from Austnesfjord in Lofoten (124.5±72 µg/kg w.w). According to Green *et al.* (2019), the source of the MCCP in Lofoten might be the local airport. In addition, a significant upward trend was found for MCCP in cod liver from Bømlo from 2017 to 2018 in the Outer Selbjørnfjord. The trend in cod were also significant when the data was adjusted for fish length. On the contrary, the median concentration of MCCP in liver of cod from Ålesund harbour (842 µg/kg ww in 2017 and 114 ±225 µg/kg ww in 2018) and from the Inner Oslofjord (498 µg/kg ww in 2017 and 106 ±25 µg/kg ww in 2018) have decreased from 2017 to 2018 (Green *et al.*, 2019). The authors (Green *et al.,* 2019) provided a comparison to other studies and reported concentrations of MCCP in cod liver from the Inner Oslofjord found by (Ruus *et al.,* 2019) that were ranging from 102.5 to 750.3 µg/kg ww, as well as MCCP concentrations in freshwater fish from 2017 in the range 8.24 to 51.50 ng/g ww found by Jartun *et al.,* 2018. Concentrations of MCCP in blue mussels and in liver of cod collected in coastal waters of Norway are provided in 'Annex III – Summary of environmental monitoring data'. Concentration of MCCP found in the cod liver and in blood and eggs of eider from Svalbard (Norwegian Arctic) are reported in Section 3.3.

- The Norwegian Institute for Air Research – NILU (Herzke *et al.*, 2019), investigated the occurrence of plastic additives (such as plasticisers like SCCP and MCCP) in liver samples from seabirds as a possible indication of exposure to marine plastic litter/ microplastic. Liver samples from 10 herring gulls (*Larus argentatus*) (five females and five males (adults)) were sampled in Skulsfjord in Troms, Northern Norway in January 2017. The whole stomach and samples of liver tissue were collected from each individual. Extraction with using a mixture of acetone/cyclohexane (1/1 v/v). The organic extract was evaporated and treated 2-4 times with 3-4 mL of concentrated sulfuric acid to remove the lipids. Extracts were measured using GC/HRMS.

  Chlorinated paraffins dominated the analytical results with mean (min-max) concentrations in the liver of herring gulls (n=10) at 210 (<156–698) ng/g ww for SCCP and 87.8 (<63–372) ng/g ww for MCCP. The Environmental quality standard (EQS) established by the Norwegian Environment Agency for MCCP in biota is 170 ng/g ww (Miljødirektoratet, 2016). In this study, 6 out of 10 liver samples exceeded the EQS established by the Norwegian Environment Agency for MCCP. Similar elevated concentrations of S/MCCP were detected in liver from cod sampled in harbours along the Norwegian coast (Green *et al.*, 2018, see data in 'Annex III – Summary of environmental monitoring data'); cod is an important prey to the herring gull and likely a source of the findings reported in this study. According to the authors (Herzke *et al.*, 2019), the considerable concentrations of S/MCCP in herring gull liver are most probably caused by exposure via direct intake of plastic, through the food chain if the prey has been exposed to plastic or through direct intake of the additives via water and air. No correlation was found between S/MCCP findings in gull liver and the occurrence of plastic in their stomach. However, only limited incidences of ingested plastic were found (as only two of the investigated individuals contained plastic in their stomachs).

- Reth *et al.* (2006) found MCCP in Cod liver samples (*Gadus morhua*) from Northern Norwegian coast (in Lofoten, 68°08′N/13°33′W, collected in 2004) and from Iceland (in South of Iceland, Vestmannaeyjar, 63°28′N/20°15′W, collected in 2003 and in North of Iceland, Akureyri, 65°74′N/18°09′W, collected in 2003). MCCP were detected in all samples. MCCP concentrations

in the Cod samples from Norway and Iceland were between 7 and 47 ng/g ww (median of 17 ng/g ww). The CP concentrations obtained in this study were lower than those previously reported for fishes from the North- and Baltic Sea (Reth et al., 2005a,b). Further detail information on this study is reported in Section 3.3.2.4.

The occurrence of chlorinated paraffins (SCCP, MCCP and LCCP) in wildlife species from paddy fields in the Yangtze River Delta, China was investigated by Du *et al.* (2019) and Du *et al.* (2018). These studies are discussed below:

- Du *et al.* (2019) investigated the occurrence of chlorinated paraffins (CP) in black-spotted frog *(Pelophylax nigromaculatus;* n=69) from paddy fields in the Yangtze River Delta, China. The samples were collected in 2011. Among 69 individuals, 45 muscle samples, 12 male frog liver samples, 12 female liver samples together with 12 paired frog egg samples were collected. SCCP, MCCP and LCCP were analysed by APCI-QTOF-MS in liver, muscle and unfertilised eggs (collected from the ovaries of maternal frogs) of the frogs. CP were quantified using a pattern-deconvulsion algorithm. For blank control, one procedural blank was included in every five samples to monitor background level. LODs and LOQs were calculated as average blank levels (n=9) plus three or ten times the SD of the blank. Following spiking experiments (n=3) of 2 µg MCCP (57.0% Cl wt.), a recovery of 86±15% (mean±RSD) was observed for MCCP.

  Concentrations of MCCP in frog liver, muscle and eggs are provided in 'Annex III – Summary of environmental monitoring data'. High detection frequencies were found for MCCP (100%) in all frog samples. The highest concentrations were found in the liver of the frogs (up to an average of 69±47 (31-190) ng/g ww). In both frog liver and egg samples, the concentrations decreased in the order of SCCP > MCCP > LCCP, contributing to 79%, 18% and 3% of the total CP levels, respectively. However, MCCP were the dominants CP groups (43%) followed by SCCP (41%) and LCCP (16%) in the pooled muscle samples. The frog liver samples contained significantly higher CP levels than the eggs and muscle samples. The lipid content of liver tissues (22.63±8.18%) was much higher than that of muscle (0.56±0.06%) and egg tissues (9.87±2.26%). Moreover, no significant differences were found among lipid normalised concentrations of liver, muscle and egg tissues ($p>0.05$). Therefore, according to Du *et al.* (2019), the higher accumulation of CP in the liver may be driven by the lipid enrichment and/or hepatic sequestration caused by the induction of hepatic microsomal binding proteins. Among MCCP, C_{14} was the most abundant alkane chain-length group in all samples contributing to 63.9% of MCCP, followed by C_{15} (19.0%). According to the authors, the dominance of C_{14} for MCCP may be due to the prevalence of this group in CP commercial products manufactured and/or used in China. In addition, the authors stated that C_{14} has shorter carbon chain length and smaller molecular size among MCCP group, resulting in higher bioavailability potentials. The frog liver and frog egg samples shared close CP congener group patterns while pooled muscle samples had different ones. Frog liver and eggs samples were enriched in SCCP (C_{10-11}), while frog muscle samples tend to have higher proportions of longer chain groups (C_{13-14}).

  No significant correlations were found between total CP levels and lipid contents, suggesting that other factors (such as bioaccumulation pathway and metabolism) than lipid content might influence liver CP deposition in frogs.

  Furthermore, Du *et al.* (2019) assessed the potential sexual difference of CP accumulation and CP potential maternal transfer. No significant differences in hepatic MCCP levels were observed between male and female frogs ($p>0.05$). However, for the pooled muscle samples, the mean concentrations of MCCP in the males were 38 ng/g ww which are 7.6 times higher than those in the females. The female frog muscles were enriched in short chain CP groups (C_{10-12}) while male frog muscles tended to accumulate a higher proportion of long-chain CP (C_{13-17}). Most of the CP congener groups (92.4%) detected in female liver tissues were also detected in the paired eggs, highlighting the maternal transfer of CP in frogs. In female frogs, liver is the chamber to produce the vitellogenin, a precursor protein of egg yolk. In the process of yolk deposition in oocytes, lipophilic contaminants bind to the different lipoproteins including very low-density lipoproteins and high-density ones (such as vitellogenin), and then transport from maternal liver to eggs. Therefore, the CP concentration ratio of eggs to the paired maternal

liver (ratio of lipid-normalised concentrations) was used to evaluate the extent to which CP were subjected to maternal transfer in frogs. The mean ratios of MCCP for black-spotted frogs was 0.52 with a range of ratios between 0.077−0.83. Among the CP, LCCP had the highest mean ratio of 0.71 (with a range of ratios: 0.14−1.6) followed by MCCP (0.52) and SCCP (0.35; with a range of ratios: 0.086−1). It is noteworthy that LCCP were more easily transferred to the next generation. The outcome of this study should be considered with caution due to small sample sizes and due to high variability in test results.

- 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 in 2011: 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 'Annex III – Summary of environmental monitoring data'. 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 MCCP > SCCP > LCCP, except in birds where SCCP were found to be more abundant. MCCP appears to be widely dispersed in wildlife at the sampling locations. The concentrations refer to specific tissues (rather than whole body), the sampled species were not necessarily part of the same food web (e.g. some are terrestrial rather than aquatic feeders) and there is no information about dietary concentrations. It is therefore not possible to draw firm conclusions about trophic magnification from this study.

- Zeng *et al.* (2015) examined the temporal trends of SCCP and MCCP in blubber samples of 50 finless porpoises (*Neophocaena phocaenoides*) and 25 Indo-Pacific humpback dolphins (*Sousa chinensis*) collected from the South China Sea between 2004 and 2014.

  Indo-Pacific humpback dolphin (*Sousa chinensis*) and finless porpoise (*Neophocaena phocaenoides*) are two resident cetacean species in the South China Sea that are the top predators in the marine food chain. Finless porpoise and Indo-Pacific humpback dolphin are two resident types of continental shelf cetacean species distributed around Hong Kong in the South China Sea. Finless porpoises have resident populations distributed in the southern and eastern waters of Hong Kong, while Indo-Pacific humpback dolphins are commonly found in the northwestern waters of Hong Kong adjacent to the Pearl River Delta (PRD), a highly developed industrial region of south China. The blubber of adult finless porpoises (*n* = 50) and adult Indo-Pacific humpback dolphins (*n* = 25) was sampled from stranded animals. It should be noted that there are possible limitations in this collection program, including the availability of sample sizes from the two top marine predators and the possibility that use of stranded animals might skew the results to highly contaminated individuals that may be dying as a result of contaminant exposure.

  Instrumental analysis and qualitative identification of SCCP ($C_{10–13}Cl_{5–10}$) and MCCP ($C_{14–17}Cl_{5–10}$) were carried out by GC-ECNI-LRMS. Interferences from CP congeners with five carbon atoms more and two chlorine atoms less were quantitatively calculated by chemical calculation procedure. Quantifications of total SCCP and MCCP were conducted according to Reth *et al.,* (2005b). Both SCCP and MCCP in blanks were below or close to the limits of detection, and the reported concentration of CP was not blank-corrected. Recoveries for surrogate standard MCCP (57% Cl) standards were determined by three replicates with spiked fish oil samples (these samples were from a lake in the Tibetan Plateau, China), and the values were in the range of 79–98%, respectively. The MDLs were estimated to be about 40 and 60 ng/g for ∑SCCP and ∑MCCP, respectively. The repeatability of the analysis was assessed by analysing three duplicate samples, with relative standard deviation ≤10%.

  Elevated levels of SCCP ($C_{10–13}Cl_{5–10}$) and MCCP ($C_{14–17}Cl_{5–10}$) were detected in all blubber samples of both cetacean species, from 2004 to 2014, suggesting that CP are ubiquitous pollutants in the south China marine environment. Generally, ∑MCCP were higher than ∑SCCP in all porpoise and dolphin blubber samples within every sampling year. The C_{14} group was the

most abundant homologue (range 41–51%, overall average 44%) in finless porpoises, which is typical of the composition of MCCP in technical mixtures. A slightly higher proportion of C_{14} in 2004–2010 was observed than in 2011–2014. MCCP congeners with 6–8 chlorines predominated in different sampling years. Similar to the MCCP homologue pattern in porpoises, C_{14} was the most abundant homologue group in dolphins but accounted for a greater proportion (range 50–65%, overall average 56%) within MCCP. There were no significant changes in the MCCP homologue pattern observed in dolphins.

Total SCCP (∑SCCP) concentrations ranged from 280 to 3900 ng/g dry weight (dw) in porpoises and from 430 to 9 100 ng/g dw in dolphins, while total MCCP (∑MCCP) concentrations ranged from 320 to 8 600 ng/g dw in porpoises (with an overall mean of 3 200 ng/g dw) and from 530 to 23000 ng/g dw in dolphins (with an overall mean of 6200 ng/g dw) (see Table 46). Significantly higher concentrations were present in dolphins than porpoises due to their exposure levels in their living habitats.

Table 46: Concentrations of SCCP and MCCP (ng/g dw) in the blubber samples of finless porpoises (n=50) and Indo-Pacific humpback dolphins (n=25) from 2004 to 2014 in Hong Kong, South China (Zeng *et al.*, 2015)

	Finless porpoise				Indo-Pacific humpback dolphins			
	Mean ±SD	Median	range	Average contribution (%)	Mean ±SD	Median	range	Average contribution (%)
Lipid %	65 ± 23	67	18–93	-	49 ± 19	47	14–90	-
C_{13}	230 ± 160	210	21–580	13	570 ± 590	310	78–2100	23
ΣSCCP	1800 ± 1000	1800	280–3900	100	2500 ± 2300	1900	430–9100	100
C_{14}	1400 ± 910	1300	160–3700	44	3400 ± 3600	2500	300–12000	56
C_{15}	850 ± 600	780	67–2300	27	950 ± 1000	630	62–3300	15
C_{16}	570 ± 440	480	58–1700	18	920 ± 1000	700	65–3800	15
C_{17}	360 ± 250	330	30–960	11	850 ± 950	640	41–3500	14
ΣMCCP	3200 ± 2200	2900	320–8600	100	6200 ± 6500	4600	530–23000	100

No significantly gender-associated concentration differences of SCCP and MCCP were observed in either cetacean species (p > 0.05). Therefore, male and female samples were pooled for temporal trend analysis for dolphins and porpoises, respectively. Statistically significantly temporal increasing trends of ∑SCCP and ∑MCCP have been observed in both porpoise (R^2 = 0.59 for SCCP and 0.56 for MCCP, p < 0.05) and dolphin samples (R^2 = 0.82 for SCCP and 0.84 for MCCP, p < 0.05) from 2004 to 2014. Increase rates were of 170% for ∑SCCP and 280% for ∑MCCP from 2010 to 2014. Temporal trends of both elevated SCCP and MCCP levels in finless porpoise are in good agreement with the history of CP production and usage in China over the past 10 years and also in accordance with the increasing trends of CP deposition concentrations in recent sediment layers of sediment core from the Pearl River Delta (Chen *et al.*, 2011).

Temporal trends in dolphins further reflect the influence of production and usage on the bioaccumulation of CP in marine mammals. An apparent temporal shift trend from SCCP to MCCP was also observed in CP accumulation profiles. Zeng *et al.* (2015) predicted that ∑SCCP and ∑MCCP concentrations will double from 2014 to 2022 and from 2014 to 2021, respectively, if it is assumed that the rate of usage of SCCP and MCCP remains constant (and by using linear regression equations).

- Bennie *et al.* (2000) reported levels of MCCP up to around 80 µg/g wet weight (ww) in blubber samples from stranded Beluga Whales *(Delphinapterus leucas)* from the St. Lawrence River, Canada (samples collected between 1987–1991), although the analytical method (low resolution GC-NCI-MS) may have been affected by the possible presence of co-eluting interfering organochlorine substances[20].

- Basconcillo *et al.* (2015) measured short and medium chain polychlorinated n-alkanes in top predatory fish from nine freshwater bodies across Canada in 2010–2011.

  Sample analysis was performed by GC system coupled to a Thermo Scientific double focusing sector high resolution mass spectrometer. The mass spectrometer was operated in the negative ion chemical ionisation (NICI) mode with Argon as the reagent gas. SCCP and MCCP were present in the procedural blanks (SCCP = 0.9 ± 0.5 ng/g ww, n = 8; MCCP = 0.6 ± 0.3 ng/g ww, n = 9) at significantly lower concentrations than sample concentrations. All samples were blank corrected.

  SCCP and MCCP were detected in top predatory fish from all sampled collected in Canada. The highest concentrations of MCCP (11–12 ng/g ww) were found in lake trout from industrialised and populated areas such as Lake Huron, Lake Erie and Lake Ontario. Concentrations of MCCP in fish from Lake Athabasca, Lake Superior, the Saint Lawrence River and Kejimikujik Lake ranged from 4 to 6 ng/g ww. Concentrations of MCCP in fish from Lake Kusawa and Columbia River were the lowest with a concentration of 1 ng/g ww. MCCP levels reported by Harju *et al.* (2013) in polar cod from Svalbard (1.51 ng/g ww (referring to whole fish and analysed by GC/HRMS) and collected in 2012 were very similar to MCCP levels in lake trout from Kusawa Lake. $C_{14}H_{24}Cl_6$ and $C_{14}H_{23}Cl_7$ were the most abundant MCCP homologue groups in fish from most Canadian sites. $C_{14}H_{23}Cl_7$, $C_{14}H_{22}Cl_8$ and $C_{14}H_{21}Cl_9$ were abundant groups in fish from more industrialised and populated areas in Canada such as Lake Erie, Lake Ontario and the Saint Lawrence River.

  The results showed that fish from sites impacted mostly by atmospheric sources contained higher concentrations of SCCP than MCCP while the opposite was observed in sites impacted by industrialisation.

  Concentrations of SCCP in Lake Ontario lake trout collected in 2011 decreased 6.6-fold compared to 2001, however no significant differences were observed for MCCP. Furthermore, in lake trout from Lake Ontario the ratio of SCCP/MCCP decreased from 2001 to 2011 showing a shift towards MCCP.

- 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 MCCP were detected, C_{14} chlorinated paraffins were the predominant congeners found in samples from Lake Michigan. However, samples from Lake Ontario generally showed that C_{15} congeners were present at similar, and in several cases higher, concentrations than the C_{14} congeners in those samples. An indication of potential variability is that the mean concentration of MCCP in Lake Trout from Lake Ontario reported by two different papers

[20] A gas-chromatography-low resolution negative ion mass spectrometry method was used. Although no comparison was carried out for MCCP, 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.

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

- 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 'Annex III – Summary of environmental monitoring data'. In the marine food web, concentrations of MCCP 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 concentrations refer to specific tissues (rather than whole body), the sampled species were not necessarily part of the same food web, and there is no information about dietary concentrations. It is therefore not possible to draw firm conclusions about trophic magnification from this study.
- Several studies have indicated that MCCP 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, MCCP are present in a wide range of organisms living and feeding in locations that are close to input sources (industrial areas, urban areas). MCCP 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 MCCP detected in environmental samples, although advances in analytical methodologies have meant that this has been possible in some of the more recent studies. Based on the new studies, C_{14} chain lengths are frequently the predominant congeners of MCCP found in biota (Houde *et al.,* 2008; Basconcillo *et al.,* 2015; Zeng *et al.,* 2015 and Du *et al.,* 2019), followed by C_{15} chain lengths (Du *et al.,* 2019). These findings are in line with the congener pattern found in commercial products.

Furthermore, it seems that concentrations of MCCP have increased during the last decades. The increase of concentrations of MCCP was observed in blue mussels from the coast in Norway between 2017–2018 (Green *et al.,* 2019) and in porpoise and dolphin samples from South China Sea between 2004–2014 (Zeng *et al.,* 2015). A similar increase trend in concentrations of MCCP was observed in the Arctic air (from 2013 to 2019; Bohlin-Nizzetto *et al.,* 2020) and in air samples from the Tibetan Plateau (from 2012 to 2015; Wu *et al.,* 2019; see section ' 3.3 Data indicating potential for long-range transport for further information).

3.4.5 Summary and discussion of bioaccumulation

Chloroalkanes are neutral organohalogen compounds, so bioaccumulation is likely to involve simple partitioning to lipid storage tissues. The degree of bioaccumulation of the congeners will depend on their hydrophobicity (which is reflected by their high octanol-water partition coefficients, log Kow ≥ 6.5) and potential to be metabolised. As described in Section 3.4.1, log Kow 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 (above 55% Cl wt.), the log Kow increases with increasing chlorine content in a non-linear fashion.

The Fisk *et al.* (1996, 1998 and 2000) studies concluded that the potential for metabolism decreases with increasing carbon chain length and chlorine content, and that it appears that the relationship of bioaccumulation and carbon chain length and chlorine content of chlorinated alkanes is complex. Gawor and Wania (2013) modelled environmental bioaccumulation potential and found that both the size of the carbon skeleton and the number of halogens influence which components will be bioaccumulative.

BCF predictions by the BCF Baseline Model of CATALOGIC for MCCP constituents reflect significant differences in predicted BCF for isomers. The difference is a result of difference in the log Kow of the isomers, as well as what metabolic transformation(s) the model has applied, which in turn is dependent on the positioning of the chlorine atom(s) in the structure. The predictions suggest that the position of the chlorine atoms influences the bioaccumulation

potential. For some structures only oxidation of the methyl groups(s) at the ends of the carbon chain(s) are predicted, leading to less mitigation by the factor of metabolism and higher BCF values. Dehalogenation transformation may be predicted for some congeners where the chlorine atoms are not positioned on adjacent carbon atoms yielding lower BCF values due to predicted higher rates of metabolism. Structures with chlorine atom(s) at the terminal carbon(s) are predicted by the model to undergo a gluthation conjugation transformation removing chlorine atom(s), hence the metabolism mitigating factors are higher, yielding lower BCF values. Due to the limited number of chlorinated paraffins in the training sets of the model and generally the limited amount of available information on observed metabolic transformations for chlorinated paraffins it is difficult to establish how well the predicted transformations reflect metabolism in organisms. Based on experimental data, the developers of the model concluded that cytochrome P450-dependent oxidation (involving dehalogenation reaction) and glutathione (GSH)-dependent conjugation are the primary routes in the metabolism of haloalkanes. They further summarised that the rate of metabolism of the chlorinated paraffins is influenced by the chain length and/or the degree of chlorination and that the proportion of unmetabolised chlorinated paraffin increased with its degree of chlorination (Unpublished, 2020).

Toxicokinetic data on mammals using radiolabelled MCCP indicate 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. Following oral administration (diet, gavage) of CP (including MCCP) to rats the major route of excretion was the faeces with only a small proportion excreted in urine and expired air. The highest initial concentrations of radioactivity were found in the liver, kidneys and ovaries. Highest concentrations of radioactivity were seen in the adipose tissue at 7 days. In general, the elimination of radioactivity from the adipose tissue was slower than for the other three tissues. It was shown that the elimination rate from the adipose tissue decreased with increasing carbon chain length and chlorination degree (EFSA, 2020). A similar picture regarding distribution and elimination was seen in mice administered radiolabelled MCCP orally (gavage) and/or by intravenous injection.

The fish studies with rainbow trout indicated that CP were rapidly accumulated and had high assimilation efficiencies from food and that the depuration half-lives increased with increasing carbon chain length and chlorination degree (EFSA, 2020). MCCP have been demonstrated to have relatively long elimination or depuration half-lives in fish and mammals (growth corrected depuration half-lives in the range of 29–80 days in rainbow trout (Fisk *et al.* (1996, 1998b and 2000) and Unpublished, 2019e) and half-life up to 8 weeks in abdominal fat of rats (Birtley *et al.*, 1980)). These long elimination half-lives mean that significant concentrations of the substance may remain within an organism for several months, possibly years, after cessation of emission.

In laying Japanese quail given MCCP orally, the highest concentration was recovered in tissues with high metabolic activity and/or high cell turnover rate (e.g. liver, intestinal mucosa, spleen, bone marrow and oviduct). High levels were also seen in the gall bladder and the kidney, as well as in lipid-rich tissues such as the outer layers of the yolk of the growing follicles, in the uropygial gland epithelium and fat.

In addition, CP (including MCCP) have been detected in human blood and milk samples which indicates that CP are absorbed to some extent in humans and detection of CP in umbilical cord blood and placenta indicates that CP can be transferred to the foetus (EFSA, 2020; Xia *et al.* 2017; Wang *et al.* 2018b).

The available (limited) field bioaccumulation studies for MCCP are equivocal: trophic magnification factors below and above 1 have been derived.

Despite the general uncertainty in available monitoring data due to analytical methods, MCCP are present in a wide range of organisms living and feeding in locations that are close to input

sources (industrial areas, urban areas). MCCP have also been detected in samples from remote regions, including the Arctic, and also in top predators. These data provide supporting evidence that MCCP are taken up by organisms in the environment. Only limited information is available on the actual carbon chain length distribution and chlorine contents of MCCP congeners detected in environmental samples, although due to advances in analytical methodologies this has been possible in some of the more recent studies. Based on the new studies, C_{14} chain lengths are frequently the predominant congeners of MCCP found in biota (Houde *et al.,* 2008; Basconcillo *et al.,* 2015; Zeng *et al.,* 2015 and Du *et al.,* 2019), followed by C_{15} chain lengths (Du *et al.,* 2019). These findings are in line with the congener pattern found in commercial products.

Furthermore, it seems that concentrations of MCCP have increased during the last decades. The increase of concentrations of MCCP was observed in blue mussels from the coast in Norway between 2017–2018 (Green et al., 2019) and in porpoise and dolphin samples from South China Sea between 2004–2014 (Zeng et al., 2015). A similar increase trend in concentrations of MCCP was observed in the Arctic air (from 2013 to 2019; Bohlin-Nizzetto et al., 2020) and in air samples from the Tibetan Plateau (from 2012 to 2015; Wu et al., 2019; see section ‘
3.3 Data indicating potential for long-range transport for further information). Iozza *et al.* (2008) indicated that the level of MCCP in a sediment core from Lake Thun in Switzerland showed an increasing trend from 1965 to 2004 (see section ‘3.1.3.1 Occurrence in sediment’). Similarly, MCCP concentrations in soil measured by Bogdal *et al.* (2017) show an increase from 1989 to 2014 from six sampling sites in Switzerland (see section ‘3.1.3.2 Concentrations in sludge and soil’).

Weight-of-evidence (WoE) approach:

Based on screening and assessment information reported in Section 3.4, a weight-of-evidence approach is used in order to conclude on the bioaccumulation potential of MCCP and their constituents at the level of the congener groups-assessed. The outcome of the weight-of-evidence approach applied for each congener group of MCCP is presented below. Further details on the weight (or confidence level) given to each experimental data and to the QSAR predictions in the weight-of-evidence approach are provided in ‘Annex X – Experimental and modelling data used as part of a weight-of-evidence (WoE) approach in order to conclude on the bioaccumulation potential of the congener groups of MCCP. It is important to note that all studies used in the below described weight-of-evidence approach have been assessed as reliable (with or without restrictions), relevant and adequate for the assessment. The results of the studies having a high weight in the WoE are considered to provide sufficient evidence to conclude congener groups of MCCP as B and/or vB. QSAR predictions are only used as supporting information to the experimental data.

It is important to note that for an UVCB substance, observed bioaccumulation may represent bioaccumulation of only some of its constituents. As the testing material of most of the bioaccumulation studies contained several groups of congeners of MCCP and no analysis was performed at the level of the congener groups for the majority of bioaccumulation studies, it is difficult to identify whether only (a) specific group(s) of congeners present in the substance tested are responsible for the bioaccumulation observed in a study or whether the congener groups all contributed equivalently. That is why QSAR predictions have been used to estimate congener specific bioaccumulation potential and to support the conclusion for each congener group based on a weight-of-evidence approach. However, some studies included identification of the congener groups present in the test material, and sometimes also in the organism tested. Due to analytical limitations it was not always possible to calculate for this latter group of studies congener group specific bioaccumulation values. Nonetheless, the studies for which congener group specific bioaccumulation values were derived or for which groups of congeners were present in the organism tested gave further confidence in the bioaccumulation potential of specific congener groups.

It has to be noted that the same group of congeners can be found in testing materials having different average chlorination levels. This is due to the fact that for a given testing material, the

chlorine numbers are considered normally distributed, the centre of the normal distribution corresponds to the average chlorination degree of the testing material. Please refer to section '1.2 Composition of the substance', for further information on the methodology used in order to determine the groups of congeners present in the testing materials when this information was not available.

All the congener groups mentioned in the conclusion section below were present in the testing materials of the studies used in the weight-of-evidence. For the *Daphnia magna* study (Castro *et al*., 2019 and Castro, 2020), congeners mentioned hereafter were detected in the Daphnia but not necessarily in the testing material. Detection in *Daphnia magna* is considered as relevant information as it suggests accumulation in these organisms. If a group of congeners was not detected in the test material it does not necessarily mean that it was not present in the test material. It is observed that the congeners which are not detected in the commercial product mainly fall at the extremes of the Cl distribution. These congeners may not have been detected because of the limitations of the semi-quantitative method in detecting congeners present at lower concentration compared to the other congeners that lie in the middle of the Cl distribution. Alternatively, the above congeners may have been formed by transformation of the test material and then accumulated in *Daphnia magna.*

Conclusion on the B-properties of the C_{14} chlorinated n-alkanes:

Further details of the weight-of-evidence assessment are provided in 'Annex X – Experimental and modelling data used as part of a weight-of-evidence (WoE) approach in order to conclude on the bioaccumulation potential of the congener groups of MCCP.

- C_{14} chlorinated n-alkane with 3 chlorine atoms (equivalent to 35.3% Cl wt):
    - A lipid-normalised and growth-corrected kinetic fish aquatic BCF value of ca. 11 530 L/kg was measured for C_{14} chlorinated n-alkane, 45% Cl wt. (a high weight is given to this study in the WoE approach; Unpublished, 2010h).
    - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_3$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
    - The BCF Baseline model of CATALOGIC yields a BCF prediction for $C_{14}Cl_3$ which is over the threshold of log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach). These predictions are supported by the outcome of the BCF predictions for $C_{14}Cl_2$ and $C_{14}Cl_4$ which indicate bioaccumulation potential.

  For the $C_{14}Cl_3$ group of congeners, there is one reliable fish aquatic BCF available which indicates vB for a testing material which contains $C_{14}Cl_3$ group of congeners. There is one supporting study with a BMF study which indicates B for $C_{14}Cl_3$ congeners. As supporting information, BCF predictions indicate vB for $C_{14}Cl_3$ congeners.

  ➔ Based on the weight of the evidence available, the $C_{14}Cl_3$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{14} chlorinated n-alkane with 4 chlorine atoms (equivalent to 42.3% Cl wt):
    - A lipid-normalised and growth-corrected kinetic fish aquatic BCF value of ca. 11 530 L/kg was measured for C_{14} chlorinated n-alkane, 45% Cl wt. (a high weight is given to this study in the WoE approach; Unpublished, 2010h).
    - A growth-corrected depuration rate constant of 0.018 day^{-1} for $C_{14}H_{26}Cl_4$ (42.3% Cl wt.; Fisk *et al.*, 1998b) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).

- For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al.*, 2019 and Castro, 2020).
- Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_4$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
- The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_4$ which are over the threshold of log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{14}Cl_4$ group of congeners, there is one reliable fish aquatic BCF available which indicates vB for a testing material which contains $C_{14}Cl_4$ group of congeners. There are three supporting studies: one which indicates vB in fish for $C_{14}Cl_4$ congeners, one which indicates vB in *Daphnia magna* for a testing material which contains $C_{14}Cl_4$ group of congeners (including detection of the $C_{14}Cl_4$ group of congeners in the Daphnia thus suggesting accumulation) and one BMF study which indicates B for $C_{14}Cl_4$ congeners. As supporting information, BCF predictions indicate vB for $C_{14}Cl_4$ congeners.

➔ Based on the weight of the evidence available, the $C_{14}Cl_4$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- <u>C_{14} chlorinated n-alkane with 5 chlorine atoms (equivalent to 47.9% Cl wt):</u>
  - Lipid-normalised kinetic fish dietary BCF values > 5000 were calculated for $C_{14}Cl_5$ and using a C_{14} chlorinated n-alkane, 50% Cl wt. as starting material (based on the less conservative scenario with k_g=0, see further information in Table 40; a high weight is given to this study in the WoE approach; Unpublished, 2019e).
  - A lipid-normalised and growth-corrected kinetic fish aquatic BCF value of ca. 11 530 L/kg was measured for C_{14} chlorinated n-alkane, 45% Cl wt. (a high weight is given to this study in the WoE approach; Unpublished, 2010h).
  - A growth-corrected depuration rate constant in the range of 0.013–0.015 day^{-1} for $C_{14}H_{25}Cl_5$ (47.9% Cl wt.; Fisk *et al.*, 1998b) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
  - A growth-corrected depuration rate constant in the range of 0.012–0.017 day^{-1} for $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl wt.; Fisk *et al.*, 2000) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al.*, 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_5$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_5$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{14}Cl_5$ group of congeners, there are two reliable studies: one reliable fish dietary study which concludes $C_{14}Cl_5$ group of congeners as vB and one reliable fish aquatic BCF

which indicates vB for a testing material which contains $C_{14}Cl_5$ group of congeners. There are four supporting studies: one which indicates vB in fish for $C_{14}Cl_5$ congeners; one which indicates vB in fish for a testing material which contains $C_{14}Cl_5$ group of congeners; one which indicates vB in *Daphnia magna* for a testing material which contains $C_{14}Cl_5$ group of congeners (including detection of the $C_{14}Cl_5$ group of congeners in the Daphnia thus suggesting accumulation) and one BMF study which indicates B for $C_{14}Cl_5$ congeners. As supporting information, BCF predictions indicate B/vB for $C_{14}Cl_5$ congeners.

➔ Based on the weight of the evidence available, the $C_{14}Cl_5$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{14} chlorinated n-alkane with 6 chlorine atoms (equivalent to 52.6% Cl wt):
  - Lipid-normalised and growth-corrected kinetic fish dietary BCF values > 5000 were calculated for $C_{14}Cl_6$ and using a C_{14} chlorinated n-alkane, 50% Cl wt. as starting material (see further information in Table 40; a high weight is given to this study in the WoE approach; Unpublished, 2019e).
  - A lipid-normalised and growth-corrected kinetic fish aquatic BCF value of ca. 11 530 L/kg was measured for C_{14} chlorinated n-alkane, 45% Cl wt. (a high weight is given to this study in the WoE approach; Unpublished, 2010h).
  - A growth-corrected depuration rate constant in the range of 0.016–0.024 day^{-1} for $C_{14}H_{24}Cl_6$ (52.6% Cl wt.; Fisk *et al.*, 1998b) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
  - A growth-corrected depuration rate constant in the range of 0.012–0.017 day^{-1} for $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl wt.; Fisk *et al.*, 2000) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_6$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_6$ which are over the threshold of log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  For the $C_{14}Cl_6$ group of congeners, there are two reliable studies: one reliable fish dietary study which concludes $C_{14}Cl_6$ group of congeners as vB and one reliable fish aquatic BCF which indicates vB for a testing material which contains $C_{14}Cl_6$ group of congeners. There are four supporting studies: one which indicates vB in fish for $C_{14}Cl_6$ congeners; one indicates vB in fish for a testing material which contains $C_{14}Cl_6$ group of congeners; one indicates vB in *Daphnia magna* for a testing material which contains $C_{14}Cl_6$ group of congeners (including detection of the $C_{14}Cl_6$ group of congeners in the Daphnia thus suggesting accumulation) and one BMF study which indicates B for $C_{14}Cl_6$ congeners. As supporting information, BCF predictions indicate vB for $C_{14}Cl_6$ congeners.

  ➔ Based on the weight of the evidence available, the $C_{14}Cl_6$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{14} chlorinated n-alkane with 7 chlorine atoms (equivalent to 56.5% Cl wt):

- Lipid-normalised and growth-corrected kinetic fish dietary BCF values > 5000 were calculated for $C_{14}Cl_7$ and using a C_{14} chlorinated n-alkane, 50% Cl wt. as starting material (see further information in Table 40; a high weight is given to this study in the WoE approach; Unpublished, 2019e).
- A growth-corrected depuration rate constant in the range of 0.012–0.017 day^{-1} for $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl wt.; Fisk *et al.*, 2000) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
- For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al.*, 2019 and Castro, 2020).
- Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_7$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
- The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_7$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{14}Cl_7$ group of congeners, there is one reliable fish dietary study available which concludes $C_{14}Cl_7$ group of congeners as vB. There are three supporting studies: one which indicates vB in fish for a testing material which contains $C_{14}Cl_7$ group of congeners; one indicates vB in *Daphnia magna* for a testing material which contains $C_{14}Cl_7$ group of congeners (including detection of the $C_{14}Cl_7$ group of congeners in the Daphnia thus suggesting accumulation) and one BMF study which indicates B for $C_{14}Cl_7$ congeners. As supporting information, BCF predictions indicate B/vB for $C_{14}Cl_7$ congeners.

➔ Based on the weight of the evidence available, the $C_{14}Cl_7$ group of congeners are concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{14} chlorinated n-alkane with 8 chlorine atoms (equivalent to 59.9% Cl wt):
  - Lipid-normalised kinetic fish dietary BCF values > 5000 were calculated for $C_{14}Cl_8$ and using a C_{14} chlorinated n-alkane, 50% Cl wt. as starting material (based on the less conservative scenario with $k_g=0$, see further information in Table 40; a high weight is given to this study in the WoE approach; Unpublished, 2019e).
  - A growth-corrected depuration rate constant in the range of 0.012–0.017 day^{-1} for $C_{14}H_{23.3}Cl_{6.7}$ (55.4% Cl wt.; Fisk *et al.*, 2000) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al.*, 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_8$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_8$ which are over the threshold of log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{14}Cl_8$ group of congeners, there is one reliable fish dietary study available which concludes $C_{14}Cl_8$ group of congeners as vB. There are three supporting studies: one which indicates vB in fish for a testing material which contains $C_{14}Cl_8$ group of congeners; one indicating vB in *Daphnia magna* for Cereclor S45 and detection of the $C_{14}Cl_8$ group of congeners in the Daphnia thus suggesting accumulation and one BMF study which indicates B for $C_{14}Cl_8$ congeners. As supporting information, BCF predictions indicate vB for $C_{14}Cl_8$ congeners.

➔ Based on the weight of the evidence available, the $C_{14}Cl_8$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{14} chlorinated n-alkane with 9 chlorine atoms (equivalent to 62.8% Cl wt):
  - Lipid-normalised kinetic fish dietary BCF values > 5000 were calculated for $C_{14}Cl_9$ and using a C_{14} chlorinated n-alkane, 50% Cl wt. as starting material (based on the less conservative scenario with k_g=0, see further information in Table 40; a high weight is given to this study in the WoE approach; Unpublished, 2019e).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_9$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_9$ which are over the threshold of log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  For the $C_{14}Cl_9$ group of congeners, there is one reliable fish dietary study available which concludes $C_{14}Cl_9$ group of congeners as vB. There are two supporting studies: one which indicates vB in *Daphnia magna* for Cereclor S45 and detection of the $C_{14}Cl_9$ group of congeners in the Daphnia thus suggesting accumulation and one is a BMF study which indicates B for $C_{14}Cl_9$ congeners. As supporting information, BCF predictions indicate vB for $C_{14}Cl_9$ congeners.

  ➔ Based on the weight of the evidence available, the $C_{14}Cl_9$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{14} chlorinated n-alkane with 10 chlorine atoms (equivalent to 65.4% Cl wt):
  - Lipid-normalised kinetic fish dietary BCF values > 5000 were calculated for $C_{14}Cl_{10}$ and using a C_{14} chlorinated n-alkane, 50% Cl wt. as starting material (based on the less conservative scenario with k_g=0, see further information in Table 40; a high weight is given to this study in the WoE approach; Unpublished, 2019e).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_{10}$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_{10}$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  For the $C_{14}Cl_{10}$ group of congeners, there is one reliable fish dietary study available which concludes $C_{14}Cl_{10}$ group of congeners as vB. There is one supporting BMF study which

indicates B for $C_{14}Cl_{10}$ group of congeners. As supporting information, BCF predictions indicate B for $C_{14}Cl_{10}$ congeners.

➔ Based on the weight of the evidence available, the $C_{14}Cl_{10}$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{14} chlorinated n-alkane with 11 chlorine atoms (equivalent to 67.6% Cl wt):
  - Lipid-normalised kinetic fish dietary BCF values > 5000 were calculated for $C_{14}Cl_{11}$ and using a C_{14} chlorinated n-alkane, 50% Cl wt. as starting material (based on the less conservative scenario with k_g=0, see further information in Table 40; a high weight is given to this study in the WoE approach; Unpublished, 2019e).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{14}Cl_{11}$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_{11}$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{14}Cl_{11}$ group of congeners, there is one reliable fish dietary study available which concludes $C_{14}Cl_{11}$ group of congeners as vB. There is one supporting BMF study available which indicates B for $C_{14}Cl_{11}$ group of congeners. As supporting information, BCF predictions indicate B for $C_{14}Cl_{11}$ congeners.

➔ Based on the weight of the evidence available, the $C_{14}Cl_{11}$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

Conclusion on the B-properties of the C_{15} chlorinated n-alkanes:

- C_{15} chlorinated n-alkane with 3 chlorine atoms (equivalent to 33.8% Cl wt):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_3$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_3$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{15}Cl_3$ group of congeners, there are two supporting studies: one *Daphnia magna* study which indicates vB for a testing material which contains $C_{15}Cl_3$ group of congeners (including detection of the $C_{15}Cl_3$ group of congeners in the Daphnia thus suggesting accumulation) and one BMF study which indicates B for $C_{15}Cl_3$ congeners. As supporting information, BCF predictions indicate B for $C_{15}Cl_3$ congeners. In addition, as the weight of available evidence is sufficient for the $C_{14}Cl_3$ and $C_{16}Cl_3$ groups of congeners to conclude that these are B/vB, it can be reasonably inferred that $C_{15}Cl_3$ also must be B/vB.

➔ Based on the weight of the evidence available, the $C_{15}Cl_3$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{15} chlorinated n-alkane with 4 chlorine atoms (equivalent to 40.6% Cl wt):
    - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
    - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_4$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
    - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_4$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  For the $C_{15}Cl_4$ group of congeners, there are two supporting studies: one *Daphnia magna* study which indicates vB for a testing material which contains $C_{15}Cl_4$ group of congeners (including detection of the $C_{15}Cl_4$ group of congeners in the Daphnia thus suggesting accumulation) and one BMF study which indicates B for $C_{15}Cl_4$ congeners. As supporting information, BCF predictions indicate B for $C_{15}Cl_4$ congeners. In addition, as the weight of available evidence is sufficient for the $C_{14}Cl_4$ and $C_{16}Cl_4$ groups of congeners to conclude that these are B/vB, it can be reasonably inferred that $C_{15}Cl_4$ also must be B/vB.

  ➔ Based on the weight of the evidence available, the $C_{15}Cl_4$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{15} chlorinated n-alkane with 5 chlorine atoms (equivalent to 46.2% Cl wt):
    - A growth-corrected kinetic fish aquatic BCF of around 1 833 – 2 072 L/kg was measured for a C_{15} chlorinated n-alkane, 51% Cl wt. The growth corrected depuration half-lives were 28 to 36 days (a medium weight is given to this study in the WoE approach, Thompson *et al*., 2000).
    - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
    - For *Eisenia fetida*, earthworm-soil accumulation factors (BAFs) of 2.4 for adults and 2.3 for juveniles were determined for a C_{15} chlorinated n-alkane, 51% Cl wt. (a low weight is given to this study in the WoE approach; Thompson *et al.,* 2001).
    - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_5$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
    - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_5$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach). These predictions are supported by the outcome of the BCF predictions for $C_{15}Cl_4$ and $C_{15}Cl_6$ which indicate a bioaccumulation potential.

  For the $C_{15}Cl_5$ group of congeners, there are four supporting studies: one which indicates B in fish based on a fish aquatic BCF study for a testing material which contains $C_{15}Cl_5$ congeners; one which indicates vB in *Daphnia magna* for Cereclor S45 and detection of the $C_{15}Cl_5$ group of congeners in the Daphnia thus suggesting accumulation; one which indicates B in *Eisenia fetida* for a testing material which contains $C_{15}Cl_5$ group of congeners and one which indicates B based on a BMF study for $C_{15}Cl_5$ congeners. As supporting information, BCF predictions indicate B for $C_{15}Cl_5$ congeners. In addition, as the weight of available evidence is sufficient for the $C_{14}Cl_5$ and $C_{16}Cl_5$ groups of congeners to conclude that these are B/vB, it can be reasonably inferred that $C_{15}Cl_5$ also must be B/vB.

➔ Based on the weight of the evidence available, the $C_{15}Cl_5$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{15} chlorinated n-alkane with 6 chlorine atoms (equivalent to 50.8% Cl wt):
  - A growth-corrected kinetic fish aquatic BCF of around 1 833 – 2 072 L/kg was measured for a C_{15} chlorinated n-alkane, 51% Cl wt. The growth corrected depuration half-lives were 28 to 36 days (a medium weight is given to this study in the WoE approach, Thompson *et al*., 2000).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - For *Eisenia fetida*, earthworm-soil accumulation factors (BAFs) of 2.4 for adults and 2.3 for juveniles were determined for a C_{15} chlorinated n-alkane, 51% Cl wt. (a low weight is given to this study in the WoE approach; Thompson *et al.,* 2001).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_6$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_6$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  For the $C_{15}Cl_6$ group of congeners, there are four supporting studies: one which indicates B in fish based on a fish aquatic BCF study for a testing material which contains $C_{15}Cl_6$ congeners; one which indicates vB in *Daphnia magna* for a testing material which contains $C_{15}Cl_6$ group of congeners (including detection of the $C_{15}Cl_6$ group of congeners in the Daphnia thus suggesting accumulation); one which indicates B in *Eisenia fetida* for a testing material which contains $C_{15}Cl_6$ group of congeners and one which indicates B based on a BMF study for $C_{15}Cl_6$ congeners. As supporting information, BCF predictions indicate B/vB for $C_{15}Cl_6$ congeners.

  ➔ Based on the weight of the evidence available, the $C_{15}Cl_6$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{15} chlorinated n-alkane with 7 chlorine atoms (equivalent to 54.8% Cl wt):
  - A growth-corrected kinetic fish aquatic BCF of around 1 833 – 2 072 L/kg was measured for a C_{15} chlorinated n-alkane, 51% Cl wt. The growth corrected depuration half-lives were 28 to 36 days (a medium weight is given to this study in the WoE approach, Thompson *et al*., 2000).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - For *Eisenia fetida*, earthworm-soil accumulation factors (BAFs) of 2.4 for adults and 2.3 for juveniles were determined for a C_{15} chlorinated n-alkane, 51% Cl wt. (a low weight is given to this study in the WoE approach; Thompson *et al.,* 2001).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_7$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).

- The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_7$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{15}Cl_7$ group of congeners, there are four supporting studies: one which indicates B in fish based on a fish aquatic BCF study for a testing material which contains $C_{15}Cl_7$ congeners; one which indicates vB in *Daphnia magna* for a testing material which contains $C_{15}Cl_7$ group of congeners (including detection of the $C_{15}Cl_7$ group of congeners in the Daphnia thus suggesting accumulation); one indicating B in *Eisenia fetida* for a testing material which contains $C_{15}Cl_7$ group of congeners and one which indicates B based on a BMF study for $C_{15}Cl_7$ congeners. As supporting information, BCF predictions indicate B/vB for $C_{15}Cl_7$ congeners.

➔ Based on the weight of the evidence available, the $C_{15}Cl_7$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{15} chlorinated n-alkane with 8 chlorine atoms (equivalent to 58.2% Cl wt.):
  - A growth-corrected kinetic fish aquatic BCF of around 1 833 – 2 072 L/kg was measured for a C_{15} chlorinated n-alkane, 51% Cl wt. The growth corrected depuration half-lives were 28 to 36 days (a medium weight is given to this study in the WoE approach, Thompson *et al*., 2000).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - For *Eisenia fetida*, earthworm-soil accumulation factors (BAFs) of 2.4 for adults and 2.3 for juveniles were determined for a C_{15} chlorinated n-alkane, 51% Cl wt. (a low weight is given to this study in the WoE approach; Thompson *et al.,* 2001).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_8$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_8$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{15}Cl_8$ group of congeners, there are four supporting studies: one which indicates B in fish based on a fish aquatic BCF study for a testing material which contains $C_{15}Cl_8$ congeners; one which indicates vB in *Daphnia magna* for a testing material which contains $C_{15}Cl_8$ group of congeners (including detection of the $C_{15}Cl_8$ group of congeners in the Daphnia thus suggesting accumulation); one which indicates B in *Eisenia fetida* for a testing material which contains $C_{15}Cl_8$ group of congeners and one which indicates B based on a BMF study for $C_{15}Cl_8$ congeners. As supporting information, BCF predictions indicate B for $C_{15}Cl_8$ congeners.

➔ Based on the weight of the evidence available, the $C_{15}Cl_8$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{15} chlorinated n-alkane with 9 chlorine atoms (equivalent to 61.1% Cl wt.):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).

- Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_9$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
- The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_9$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{15}Cl_9$ group of congeners, there are two supporting studies: one which indicates vB in *Daphnia magna* for Cereclor S45 and detection of the $C_{15}Cl_9$ group of congeners in the Daphnia thus suggesting accumulation and one which indicates B based on a BMF study for $C_{15}Cl_9$ congeners. As supporting information, BCF predictions indicate B for $C_{15}Cl_9$ congeners.

➔ Based on the weight of the evidence available, the $C_{15}Cl_9$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{15} chlorinated n-alkane with 10 chlorine atoms (equivalent to 63.7% Cl wt.):
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_{10}$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_{10}$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  ➔ Based on the information available for the $C_{15}Cl_{10}$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since insufficient data is available.

- C_{15} chlorinated n-alkane with 11 chlorine atoms (equivalent to 66% Cl wt.):
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{15}Cl_{11}$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{15}Cl_{11}$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  ➔ Based on the information available for the $C_{15}Cl_{11}$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since insufficient data is available.

Conclusion on the B-properties of the C_{16} chlorinated n-alkanes:

- C_{16} chlorinated n-alkane with 2 chlorine atoms (equivalent to 24.1% Cl wt.):
  - A growth-corrected depuration rate constant in the range of 0.014–0.019 day^{-1} for $C_{16}H_{31}Cl_3$ (34.1% Cl wt.; Fisk *et al.*, 1996) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - For *Mytilus edulis*, a lipid-normalised BAF value of 7 031 L/kg (steady-state value) and 7 204 L/kg (statistically determined) with confidence limits of 4 694–9 723

L/kg was measured for $C_{16}H_{30.7}Cl_{3.3}$ (34.1% Cl wt.; a medium weight is given to this study in the WoE approach; Renberg *et al.,* 1986).

- The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_2$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{16}Cl_2$ group of congeners, there are three supporting studies: one which indicates vB in fish for a testing material which contains $C_{16}Cl_2$ group of congeners; one which indicates vB in *Daphnia magna* for Cereclor S45 and detection of the $C_{16}Cl_2$ group of congeners in the Daphnia thus suggesting accumulation and one which indicates vB in *Mytilus edulis* for a testing material which contains $C_{16}Cl_2$ group of congeners. However, the BCF predictions indicate not B for $C_{16}Cl_2$ congeners. As the three supporting studies all indicate B and/or vB, all together they are considered to have a higher weight than the QSAR predictions.

➔ Based on the weight of the evidence available, the $C_{16}Cl_2$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{16} chlorinated n-alkane with 3 chlorine atoms (equivalent to 32.3% Cl wt.):
  - A growth-corrected depuration rate constant in the range of 0.014–0.019 day^{-1} for $C_{16}H_{31}Cl_3$ (34.1% Cl wt. Fisk *et al.*, 1996) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - For *Mytilus edulis*, a lipid-normalised BAF value of 7 031 L/kg (steady-state value) and 7 204 L/kg (statistically determined) with confidence limits of 4 694–9 723 L/kg was measured for $C_{16}H_{30.7}Cl_{3.3}$ (34.1% Cl wt.; a medium weight is given to this study in the WoE approach; Renberg *et al.,* 1986).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{16}Cl_3$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_3$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{16}Cl_3$ group of congeners, there are four supporting studies: one which indicates vB in fish for a testing material which contains $C_{16}Cl_3$ group of congeners; one which indicates vB in *Daphnia magna* for a testing material which contains $C_{16}Cl_3$ group of congeners (including detection of the $C_{16}Cl_3$ group of congeners in the Daphnia thus suggesting accumulation); one which indicates vB in *Mytilus edulis* for a testing material which contains $C_{16}Cl_3$ group of congeners and one which indicates B based on a BMF study for $C_{16}Cl_3$ congeners. However, the BCF predictions indicate not B for $C_{16}Cl_3$ congeners. As the four supporting studies all indicate B and/or vB, all together they are considered to have a higher weight than the QSAR predictions.

➔ Based on the weight of the evidence available, the $C_{16}Cl_3$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{16} chlorinated n-alkane with 4 chlorine atoms (equivalent to 39% Cl wt.):

- A growth-corrected depuration rate constant in the range of 0.014–0.019 day^{-1} for $C_{16}H_{31}Cl_3$ (34.1% Cl wt.; Fisk *et al.*, 1996) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
- For *Daphnia magna,* lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
- For *Mytilus edulis*, a lipid-normalised BAF value of 7 031 L/kg (steady-state value) and 7 204 L/kg (statistically determined) with confidence limits of 4 694–9 723 L/kg was measured for $C_{16}H_{30.7}Cl_{3.3}$ (34.1% Cl wt.; a medium weight is given to this study in the WoE approach; Renberg *et al.,* 1986).
- Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{16}Cl_4$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
- The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_4$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{16}Cl_4$ group of congeners, there are four supporting studies: one which indicates vB in fish for a testing material which contains $C_{16}Cl_4$ group of congeners; one which indicates vB in *Daphnia magna* for a testing material which contains $C_{16}Cl_4$ group of congeners (including detection of the $C_{16}Cl_4$ group of congeners in the Daphnia thus suggesting accumulation); one which indicates vB in *Mytilus edulis* for a testing material which contains $C_{16}Cl_4$ group of congeners and one which indicates B based on a BMF study for $C_{16}Cl_4$ congeners. However, the BCF predictions indicate not B for $C_{16}Cl_4$ congeners. As the four supporting studies all indicate B and/or vB, all together they are considered to have a higher weight than the QSAR predictions.

➔ Based on the weight of the evidence available, the $C_{16}Cl_4$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- <u>C_{16} chlorinated n-alkane with 5 chlorine atoms (equivalent to 44.5% Cl wt.):</u>
  - A growth-corrected depuration rate constant in the range of 0.014–0.019 day^{-1} for $C_{16}H_{31}Cl_3$ (34.1% Cl wt.; Fisk *et al.*, 1996) indicates a BCF above 5 000 L/kg as calculated for the purpose of this report (a medium weight is given to this study in the WoE approach).
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - For *Mytilus edulis*, a lipid-normalised BAF value of 7 031 L/kg (steady-state value) and 7 204 L/kg (statistically determined) with confidence limits of 4 694–9 723 L/kg was measured for $C_{16}H_{30.7}Cl_{3.3}$ (34.1% Cl wt.; a medium weight is given to this study in the WoE approach; Renberg *et al.,* 1986).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{16}Cl_5$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_5$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{16}Cl_5$ group of congeners, there are four supporting studies: one which indicates vB in fish for a testing material which contains $C_{16}Cl_5$ group of congeners; one which indicates vB in *Daphnia magna* for a testing material which contains $C_{16}Cl_5$ group of congeners (including detection of the $C_{16}Cl_5$ group of congeners in the Daphnia thus suggesting accumulation); one which indicates vB in *Mytilus edulis* for a testing material which contains $C_{16}Cl_5$ group of congeners and one which indicates B based on a BMF study for $C_{16}Cl_5$ congeners. As supporting information, BCF predictions indicate B for $C_{16}Cl_5$ congeners.

➔ Based on the weight of the evidence available, the $C_{16}Cl_5$ group of congeners is concluded to meet the bioaccumulation criterion (B) and the very bioaccumulative criterion (vB) of Annex XIII of the REACH Regulation.

- C_{16} chlorinated n-alkane with 6 chlorine atoms (equivalent to 49.2% Cl wt.):
    - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
    - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{16}Cl_6$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
    - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_6$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach). These predictions are supported by the outcome of the BCF predictions for $C_{16}Cl_5$ and $C_{16}Cl_7$ which are also indicating bioaccumulation potential.

For the $C_{16}Cl_6$ group of congeners, there are two supporting studies which indicate vB in *Daphnia magna* for a testing material which contains $C_{16}Cl_6$ group of congeners (including detection of the $C_{16}Cl_6$ group of congeners in the Daphnia thus suggesting accumulation) and B based on a BMF study for $C_{16}Cl_6$ congeners. As supporting information, BCF predictions indicate B for $C_{16}Cl_6$ congeners.

➔ Based on the weight of the evidence available, the $C_{16}Cl_6$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{16} chlorinated n-alkane with 7 chlorine atoms (equivalent to 53.15% Cl wt.):
    - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
    - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{16}Cl_7$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
    - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_7$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{16}Cl_7$ group of congeners, there are two supporting studies which indicate vB in *Daphnia magna* for a testing material which contains $C_{16}Cl_7$ group of congeners (including detection of the $C_{16}Cl_7$ group of congeners in the Daphnia thus suggesting accumulation) and B based on a BMF study for $C_{16}Cl_7$ congeners. As supporting information, BCF predictions indicate B for $C_{16}Cl_7$ congeners.

➔ Based on the weight of the evidence available, the $C_{16}Cl_7$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{16} chlorinated n-alkane with 8 chlorine atoms (equivalent to 56.6% Cl wt.):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45; a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{16}Cl_8$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_8$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  For the $C_{16}Cl_8$ group of congeners, there are two supporting studies which indicate vB in *Daphnia magna* for a testing material which contains $C_{16}Cl_8$ group of congeners (including detection of the $C_{16}Cl_8$ group of congeners in the Daphnia thus suggesting accumulation) and B based on a BMF study for $C_{16}Cl_8$ congeners. As supporting information, BCF predictions indicate B for $C_{16}Cl_8$ congeners.

  ➔ Based on the weight of the evidence available, the $C_{16}Cl_8$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{16} chlorinated n-alkane with 9 chlorine atoms (equivalent to 59.55% Cl wt.):
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{16}Cl_9$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_9$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  ➔ The above information is not sufficient to conclude on the $C_{16}Cl_9$ group of congeners directly. However, as the weight of available evidence is sufficient for the $C_{15}Cl_9$ and $C_{17}Cl_9$ groups of congeners to conclude that these meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation, it can be reasonably inferred that also the $C_{16}Cl_9$ group of congeners must meet (at least) the bioaccumulation criterion (B).

- C_{16} chlorinated n-alkane with 10 chlorine atoms (equivalent to 62.17% Cl wt.):
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{16}Cl_{10}$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_{10}$ which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  ➔ Based on the information available for the $C_{16}Cl_{10}$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since insufficient data is available.

- C_{16} chlorinated n-alkane with 12 chlorine atoms (equivalent to 66.6% Cl wt.):
  - A growth-corrected depuration rate constant in the range of 0.009–0.012 day^{-1} for $C_{16}H_{21}Cl_{13}$ (69% Cl wt.) indicates a BCF above 5 000 L/kg (a medium weight is given to this study in the WoE approach; Fisk *et al.*, 1996).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_{12}$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  ➔ Based on the information available for the $C_{16}Cl_{12}$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since the data available is insufficient and the results inconsistent.

- C_{16} chlorinated n-alkane with 13 chlorine atoms (equivalent to 68.4% Cl wt.):
  - A growth-corrected depuration rate constant in the range of 0.009–0.012 day^{-1} for $C_{16}H_{21}Cl_{13}$ (69% Cl wt.) indicates a BCF above 5 000 L/kg (a medium weight is given to this study in the WoE approach; Fisk *et al.*, 1996).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_{13}$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  ➔ Based on the information available for the $C_{16}Cl_{13}$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since the data available is insufficient and the results inconsistent.

- C_{16} chlorinated n-alkane with 14 chlorine atoms (equivalent to 70.1% Cl wt.):
  - A growth-corrected depuration rate constant in the range of 0.009–0.012 day^{-1} for $C_{16}H_{21}Cl_{13}$ (69% Cl wt.) indicates a BCF above 5 000 L/kg (a medium weight is given to this study in the WoE approach; Fisk *et al.*, 1996).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_{14}$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  ➔ Based on the information available for the $C_{16}Cl_{14}$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since the data available is insufficient and the results inconsistent.

- C_{16} chlorinated n-alkane with 15 chlorine atoms (equivalent to 71.6% Cl wt.):
  - A growth-corrected depuration rate constant in the range of 0.009–0.012 day^{-1} for $C_{16}H_{21}Cl_{13}$ (69% Cl wt.) indicates a BCF above 5 000 L/kg (a medium weight is given to this study in the WoE approach; Fisk *et al.*, 1996).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{16}Cl_{15}$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

  ➔ Based on the information available for the $C_{16}Cl_{15}$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since the data available is insufficient and the results inconsistent.

Conclusion on the B-properties of the C_{17} chlorinated n-alkanes:

- C_{17} chlorinated n-alkane with 2 chlorine atoms (equivalent to 23% Cl wt.):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-

C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).

- The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_2$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

➔ Based on the information available for the $C_{17}Cl_2$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since the data available is insufficient and the results inconsistent.

- C_{17} chlorinated n-alkane with 3 chlorine atoms (equivalent to 31% Cl wt.):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_3$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

➔ Based on the information available for the $C_{17}Cl_3$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since the data available is insufficient and the results inconsistent.

- C_{17} chlorinated n-alkane with 4 chlorine atoms (equivalent to 37.6% Cl wt.):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_4$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

➔ Based on the information available for the $C_{17}Cl_4$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since the data available is insufficient and the results inconsistent.

- C_{17} chlorinated n-alkane with 5 chlorine atoms (equivalent to 43% Cl wt.):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{17}Cl_5$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_5$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{17}Cl_5$ group of congeners, there are two supporting studies which indicate vB in *Daphnia magna* for a testing material which contains $C_{17}Cl_5$ group of congeners (including detection of the $C_{17}Cl_5$ group of congeners in the Daphnia thus suggesting accumulation) and B based on a BMF study for $C_{17}Cl_5$ congeners. However, the BCF predictions indicate

not B for $C_{17}Cl_5$ congeners. As the two supporting studies indicate B and/or vB, all together they are considered to have a higher weight than the QSAR predictions.

➔ Based on the weight of the evidence available, the $C_{17}Cl_5$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{17} chlorinated n-alkane with 6 chlorine atoms (equivalent to 47.65% Cl wt):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{17}Cl_6$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_6$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{17}Cl_6$ group of congeners, there are two supporting studies which indicate vB in *Daphnia magna* for a testing material which contains $C_{17}Cl_6$ group of congeners (including detection of the $C_{17}Cl_6$ group of congeners in the Daphnia thus suggesting accumulation) and B based on a BMF study for $C_{17}Cl_6$ congeners. However, the BCF predictions indicate not B for $C_{17}Cl_6$ congeners. As the two supporting studies indicate B and/or vB, all together they are considered to have a higher weight than the QSAR predictions.

➔ Based on the weight of the evidence available, the $C_{17}Cl_6$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{17} chlorinated n-alkane with 7 chlorine atoms (equivalent to 51.6% Cl wt):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{17}Cl_7$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_7$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{17}Cl_7$ group of congeners, there are two supporting studies which indicate vB in *Daphnia magna* for a testing material which contains $C_{17}Cl_7$ group of congeners (including detection of the $C_{17}Cl_7$ group of congeners in the Daphnia thus suggesting accumulation) and B based on a BMF study for $C_{17}Cl_7$ congeners. However, the BCF predictions indicate not B for $C_{17}Cl_7$ congeners. As the two supporting studies indicate B and/or vB, all together they are considered to have a higher weight than the QSAR predictions.

➔ Based on the weight of the evidence available, the $C_{17}Cl_7$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{17} chlorinated n-alkane with 8 chlorine atoms (equivalent to 55% Cl wt):

- For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
- Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{17}Cl_8$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
- The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_8$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{17}Cl_8$ group of congeners, there are two supporting studies which indicate vB in *Daphnia magna* for a testing material which contains $C_{17}Cl_8$ group of congeners (including detection of the $C_{17}Cl_8$ group of congeners in the Daphnia thus suggesting accumulation) and B based on a BMF study for $C_{17}Cl_8$ congeners. However, the BCF predictions indicate not B for $C_{17}Cl_8$ congeners. As the two supporting studies indicate B and/or vB, all together they are considered to have a higher weight than the QSAR predictions.

➔ Based on the weight of the evidence available, the $C_{17}Cl_8$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{17} chlorinated n-alkane with 9 chlorine atoms (equivalent to 58% Cl wt):
  - For *Daphnia magna*, lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww were measured for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45); (a medium weight is given to this study in the WoE approach; Castro *et al*., 2019 and Castro, 2020).
  - Lipid normalised BMFs >1 were measured in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{17}Cl_9$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_9$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

For the $C_{17}Cl_9$ group of congeners, there are two supporting studies which indicate vB in *Daphnia magna* for Cereclor S45 and detection of the $C_{17}Cl_9$ group of congeners in the Daphnia thus suggesting accumulation and B based on a BMF study for $C_{17}Cl_9$ congeners. However, the BCF predictions indicate not B for $C_{17}Cl_9$ congeners. As the two supporting studies indicate B and/or vB, all together they are considered to have a higher weight than the QSAR predictions.

➔ Based on the weight of the evidence available, the $C_{17}Cl_9$ group of congeners is concluded to meet (at least) the bioaccumulation criterion (B) of Annex XIII of the REACH Regulation.

- C_{17} chlorinated n-alkane with 10 chlorine atoms (equivalent to 60.7% Cl wt):
  - Lipid normalised BMFs >1 were found in the muscles and livers of a snake-frog predator-prey relationship for the congeners $C_{17}Cl_{10}$ (a low weight is given to this study in the WoE approach; Du *et al.*, 2020).
  - The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{17}Cl_{10}$ which are below the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and therefore indicating a lack of bioaccumulation potential (a low weight is given to QSAR predictions in the WoE approach).

➔ Based on the information available for $C_{17}Cl_{10}$ group of congeners, it is not possible to conclude on their potential for bioaccumulation since insufficient data is available.

Summary of the weight of evidence based conclusions on the bioaccumulation potential of the congener groups of MCCP:

As an overall conclusion, based on the REACH Annex XIII B/vB criteria and the above information used in a weight-of-evidence-approach, it is concluded that the congener groups $C_{14}Cl_{3–11}$ (equivalent to 35.3–67.6% Cl wt.) have B/vB properties, $C_{15}Cl_{3–9}$ (equivalent to 33.8–61.15% Cl wt.) have B and/or vB properties, $C_{16}Cl_{2–9}$ (equivalent to 24.1–59.55% Cl wt.) have B and/or vB properties and $C_{17}Cl_{5–9}$ (equivalent to 43–58% Cl wt.) have B properties (see Table 47). For other congener groups of MCCP, it is not possible to conclude on their potential for bioaccumulation due to the lack of appropriate data.

Based on the current information available, MCCP contain congener groups with B and/or vB properties at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet the 'bioaccumulation' criterion (B) and the 'very bioaccumulative' criterion (vB) in accordance with Annex XIII, points 1.1.2 and 1.2.2, of the REACH Regulation.

Table 47: Summary Table of congener groups of MCCP concluded as B and/or vB

Number chlorine atoms and Carbon chain length	Cl_2	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}
C_{14}		B / vB	B / vB	B / vB	B / vB	B / vB	B / vB	B / vB	B / vB	B / vB				
C_{15}		B / vB	B / vB	B / vB	B	B	B	B	-	-				
C_{16}	B / vB	B / vB	B / vB	B / vB	B	B	B	B	-		-	-	-	-
C_{17}	-	-	-	B	B	B	B	B	-					

Note: Symbol '-' means that not enough information is available to conclude on the B property of the congener group. Grey cells indicate when no experimental data is available on the congener group.

4. Human health hazard assessment

Mammalian toxicity data have not been reviewed except toxicokinetic information (for the purpose of B-assessment). A brief summary of relevant information from the human health risk assessment report produced under the Existing Substances Regulation EC (No.) 793/93 (HSE, 2008b) is provided for information in 'Annex XI – Brief summary of Human health hazard assessment'.

4.1 Toxicokinetics (absorption, metabolism, distribution and elimination)

All the information reported in the section is taken from EFSA's scientific opinion on the risks for animal and human health related to the presence of chlorinated paraffins in feed and food (EFSA, 2020). Data on toxicokinetics for various animal species were identified, although in several cases from studies not designed as dedicated absorption, distribution, metabolism and elimination (ADME) studies. A number of studies on the toxicokinetics of CP in rodents (rats and mice) have been retrieved in the literature search. The main outcomes of these studies are described below while a more detailed description of each individual study can be found in Appendix A of EFSA's report (EFSA, 2020).

4.1.1 Non-human information

4.1.1.1 Studies in rats

Six studies on toxicokinetics in rats are available for MCCP. Administration of CP was both via diet (repeated exposure) and gavage (repeated exposure and single dose).

In a dietary study with an MCCP (Cereclor S52, $C_{14–17}$, 52% chlorination, 10 or 625 mg/kg bw) (IRDC (1984c), unpublished study as cited in EFSA, 2020) faecal excretion was the main route of elimination (40–48% and 53–61% in low- and high-dose males, respectively; 28–31% and 62–74% in low- and high-dose females) with only a small proportion excreted in urine (0.8–3%) and expired air (0.1–0.3%). As for the SCCP, there was an indication that blood and tissue levels were proportional to the administered dose although not as clear as for the SCCP. As for the SCCP, the highest initial concentrations of radioactivity were found in the liver, ovaries and kidneys, whereas for adipose tissue, the concentration of radioactivity was highest at 7 days after the last dose and then declined more slowly than for the other tissues.

Distribution of the same MCCP ($C_{14–17}$, 52% chlorination) to the liver and adipose tissue was also reported in two other dietary studies (Birtley *et al.*, 1980 and Poon *et al.*, 1995). One study (doses from 0.4 to 400 mg/kg bw per day) reported a dose-dependent increase in the concentration of the MCCP in both liver and abdominal fat (Poon *et al.*, 1995) and the other study (doses of 0.4 and 40 mg/kg diet) reported a rapid elimination from the liver (within one week) and slow elimination from the abdominal fat (half-life of approximately 8 weeks) (Birtley *et al.*, 1980).

In addition, a dietary study (CXR Biosciences Ltd (2005a), unpublished study as cited in EFSA, 2020) with the same MCCP ($C_{14–17}$, 52% chlorination, approximately 200 mg/kg bw per day) reported that the content in the white adipose tissue increased with time until the steady-state concentration was achieved at week 13; then there was an initial rapid elimination where after the elimination rate decreased markedly. Also following a single oral dose of an MCCP (C_{15}, 52% chlorination, 525 mg/kg bw) by gavage (CXR Biosciences Ltd, 2005, as cited in EC, 2011) faecal excretion was the main route of elimination (approximately 50% excreted within the first 24 h after dosing and approximately 70% after 5 days) and only a minor proportion was excreted in the urine (approximately 5% of the administered radioactivity was eliminated in the urine after 5 days). Similarly, the initial highest concentrations of radioactivity were detected in the liver,

kidney and fat and elimination half-life was rapid for most tissues (approximately 2–5 days) and slower for white adipose tissue (about 2 weeks).

Only one study (Åhlman *et al.*, 1986) has examined metabolism, i.e. formation of sulfur-containing metabolites in female bile duct-cannulated rats given an MCCP (1-chloro-polychloro[U-^{14}C]hexadecane, 65% chlorination, 5–6 mg/kg) by injection into the portal vein. The MCCP was conjugated to mercapturic acid and glutathione and less than 3% of the total radioactivity excreted in the bile was due to the parent compound.

4.1.1.2 Studies in mice

Three studies on toxicokinetics in mice are available on MCCP with the same carbon chain length (C_{16}) but different degrees of chlorination (34% and 69%). These studies were all performed by the same Swedish group and applied the same methodology, i.e. single oral dose by gavage or by intravenous injection of radiolabelled test compounds predominantly to female mice followed by visual determination of tissue distribution by whole body autoradiography (WBA), and evaluation of tissue retention and elimination in excreta by measuring radioactivity levels of test compounds and metabolites. EFSA's CONTAM Panel noted that the WBA is a semiquantitative measure (EFSA, 2020).

Following administration of a low chlorinated MCCP (1-^{14}C-$C_{16}H_{30.7}Cl_{3.3}$, 34.1% chlorination) (Darnerud and Brandt, 1982), the WBA showed highest initial radioactivity in tissues with high cell turnover/high metabolic activity (intestinal mucosa, bone marrow, exocrine glands and brown fat), but only a low distribution to the white fat depots (oral administration); radioactivity in the brain (30 days after intravenous injection); and distribution of radioactivity in foetuses partly similar to that observed in adult females (late gestation). However, following oral administration of a higher chlorinated radiolabelled MCCP (^{14}C-labelled $C_{16}H_{20.6}Cl_{13.4}$, 69% chlorination) (Biessmann *et al.*, 1983), the WBA showed initial high levels of radioactivity in bile, liver, kidney and intestinal contents, as well as in corpora lutea up to 30 days after dosing. A long retention in fat was seen. High levels of radioactivity in adipose tissue, adrenals and in myelinated areas of the brain were seen in autoradiograms from pre-weaning (10-day-old) mice orally dosed with a highly chlorinated MCCP (C_{16}, 69% chlorination) (Eriksson and Darnerud, 1985).

In pre-weaning mice given the highly chlorinated MCCP (Eriksson and Darnerud, 1985), the level of radioactivity in the brain was approximately 3% of the dose administered in 3-day-old mice, and approximately 0.5% in 20-day-old mice (24 h after administration). At seven days the level of radioactivity was lower in both brain and liver samples.

For the low chlorinated MCCP (Darnerud and Brandt, 1982), about 33% of the administered radioactivity was exhaled as $^{14}CO_2$ within 12 h after oral administration with 6.5% of the radioactivity in the urine and 14% in the faeces. For the higher chlorinated MCCP (Biessmann et al., 1983), the elimination of radioactivity in urine was about 3% and about 66% in the faeces during 96 h; the elimination in exhaled air was about 1%.

For the low chlorinated MCCP (Darnerud and Brandt, 1982), thin-layer chromatography (TLC) of samples taken from the liver, kidney and brown fat revealed a radiolabelled substance with the same retention value as the reference parent compound suggesting that this MCCP was distributed to these tissues without further metabolism. It was stated by the authors of the article concerning the low chlorinated MCCP in mice (Darnerud and Brandt, 1982), that the results in this specific study are valid only for the MCCP studied and should not be taken as general for all CP preparations.

4.1.1.3 Farm animals, horses and companion animals

A number of studies on the toxicokinetics of CP in farm animals (poultry and fish) have been retrieved from the literature search (EFSA, 2020). The main outcomes of these studies are described below while a more detailed description of each individual study can be found in Appendix B of EFSA's report (EFSA, 2020).

4.1.1.3.1 Studies in poultry

In female laying Japanese quail orally given an SCCP (^{14}C-labelled $C_{12}H_{20.1}Cl_{5.9}$, 55.9% chlorination) or an MCCP (^{14}C-labelled $C_{16}H_{30.7}Cl_{3.3}$, 34.1% chlorination) (Biessmann *et al.*, 1982), the autoradiography distributions showed initial high radioactivity in tissues with high metabolic activity and/or high cell turnover rate, e.g. liver, intestinal mucosa, spleen, bone marrow and oviduct. High levels were also seen in the gall bladder and the kidney, as well as in lipid-rich tissues such as the outer layers of the yolk of the growing follicles, in the uropygial gland epithelium and fat. There was also a high uptake of radioactivity in the eggshells and, to a lesser extent, in the albumen. After exposure times of 4 and 8 days, the highest radioactivity was observed in fat, the yolk of the follicles and in the uropygial gland. The distribution patterns of the SCCP and the MCCP were almost identical after all exposure times: in the egg yolk and albumen the concentration of the SCCP was about half of the MCCP. However, the distribution was somewhat different following administration of a higher chlorinated MCCP (^{14}C-labelled $C_{16}H_{20.6}Cl_{13.4}$, 69% chlorination) (Biessmann *et al.*, 1983) with initial high radioactivity in bile, liver, kidney and intestinal contents; high radioactivity was also seen in the hypophysis, retina, blood and egg yolk. After 12 days, radioactivity was only observed in the lipid-rich tissues (fat, uropygial gland, egg yolk) as for the SCCP and the lower chlorinated MCCP; and in the liver. In the elimination part of the study with the SCCP and the lower chlorinated MCCP (Biessmann *et al.*, 1982), the exhalation of $^{14}CO_2$ during 8 hours following dosing with the MCCP was about twice (38.8%) that of the SCCP (21.6%); the excretion of radioactivity in urine and faeces (combined, during 8 hours) was also higher following dosing with the MCCP (13.5%) compared with SCCP (9.8%). For the higher chlorinated MCCP (Biessmann *et al.*, 1983), the elimination of radioactivity in urine and faeces (combined) was about 58% during 96 hours after administration; the elimination in exhaled air was about 1%.

4.1.1.3.2 Studies in fish

For MCCP, several studies were performed in rainbow trout, carp and bleak. Studies in which the fish were exposed via the tank water were also included, although this exposure route is not entirely relevant to dietary exposure.

In juvenile rainbow trout (*Oncorhynchus mykiss*) (Fisk *et al.,* 1996) fed diets with two different SCCP ($C_{12}H_{20}Cl_6$, 56% chlorination; $C_{12}H_{16}Cl_{10}$, 69% chlorination) and two different MCCP ($C_{16}H_{31}Cl_3$, 35% chlorination; $C_{16}H_{21}Cl_{13}$, 69% chlorination) for 40 days, followed by 160 days ($C_{12}H_{20}Cl_6$, $C_{12}H_{16}Cl_{10}$, $C_{16}H_{31}Cl_3$) or 173 days ($C_{16}H_{21}Cl_{13}$) of depuration, all four CP accumulated in the fish by day 5 of the uptake phase without reaching steady state. The depuration rate in fish exposed to $C_{16}H_{31}Cl_3$ was significantly higher than the depuration rates in fish exposed to the other three CP. The highest percentage of radioactivity was found in the carcass for all four CP (ranging from 50% to higher than 70%). Relative amounts in the liver were low (about 1.5% of the total fish weight). The metabolism of the CP was most pronounced for the lower chlorinated SCCP. According to the authors, the highly chlorinated SCCP and the lower chlorinated MCCP appear to have the greatest potential for biomagnification among the CP components. The authors also stated that reduced accumulation of the lower chlorinated SCCP should be attributed to metabolism, while uptake from the GI of the highly chlorinated MCCP may have been hindered because of its large molecular size.

In another study (Fisk *et al.,* 1998b) with juvenile rainbow trout (*Oncorhynchus mykiss*) fed diets containing 19 different CP with varying carbon chain length (C_{10}, C_{11} and C_{14}) and chlorine

content (4–8 chlorine atoms) for 40 days followed by 80 days of depuration, all of the CP were detected in the fish after 5 days of exposure. With the exception of the C_{14}–CP, most compounds reached steady state between food and fish within 30 or 40 days. Differences in bioaccumulation parameters between CP with the same molecular formula, but different chlorine positions were observed for some of the CP. The half-lives of the CP ranged from 7 to 53 days. There was a large range in the assimilation efficiencies (from 13–130%). These results showed that all of the CP were rapidly accumulated and had high assimilation efficiencies from food, that the half-lives increased with increasing carbon chain length and chlorine content, indirectly, that the CP were metabolised in the rainbow trout with the susceptibility to metabolism decreasing with greater carbon chain length and chlorine content, and that higher chlorinated C_{10}- and C_{11}-CP, and all C_{14}-CP, would biomagnify from food to fish in aquatic food chains.

In a third study (Fisk *et al.*, 2000) with juvenile rainbow trout (*Oncorhynchus mykiss*) fed diets with three different ^{14}C-CP ($C_{10}H_{15.3}Cl_{6.7}$, $C_{14}H_{23.3}Cl_{6.7}$ and $C_{18}H_{31.4}Cl_{6.6}$) at two different concentrations for 40 days followed by 160 days of depuration, all three CP accumulated readily from the food, but without reaching steady state; the uptake curves were similar for all three CP, and for the two concentrations. The assimilation efficiencies varied from 10 to 22%, except for the high-concentration SCCP group (approximately 72%). The half-lives of the LCCP (79 and 91 days) were significantly greater than those of the two shorter chain CP (26–58 days). The BMFs calculated assuming assimilation efficiencies of 50 and 90% exhibited increasing trends with increasing carbon chain length and indicate that the CP have the potential to biomagnify in aquatic food chains. These results showed that all three CP have the potential to biomagnify in aquatic food chains with increasing trends with increasing carbon chain length and greater biotransformation of the short-chain compared to the longer chain CP.

In rainbow trout (*Salmo gairdneri*) exposed during 7 days to a low chlorinated MCCP (1-chloro-polychloro-[U-^{14}C]hexadecane (PCHD-L), 23.1% chlorination) added to tank water, the initial highest radioactivity were seen in the contents of the gall bladder, pyloric caeca and intestines; a pronounced uptake was also seen in the olfactory organs and gills (Darnerud *et al.,* 1989). After 7 days in contaminated water, the uptake in the olfactory organs and gills was less marked whereas the concentration of radioactivity in fat tissue had increased. After 7 and 21 days in clean water, the distribution pattern were similar to that found after seven days in contaminated water; the olfactory organs and the gills still retained radioactivity. Following exposure to a higher chlorinated MCCP (1-chloro-polychloro-[U-^{14}C]hexadecane (PCHD-M), 51.4% chlorination), the initial distribution pattern was almost similar to that observed for PCHD-L; however, the liver was comparably more labelled after PCHD-M exposure. After seven days in contaminated water, the uptake was also generally the same as for PCHD-L; however, the uptake in fat seemed more accentuated for PCHD-M and the accumulation of radioactivity in fatty tissues was even more prominent at later time points.

In carp (*Cyprinus carpio*) given an MCCP (polychloro-1-^{14}C-hexadecane (PCHD), 34% chlorination) by injection, the cumulated excretion of $^{14}CO_2$ during 96 h amounted to 6.4% of the injected radioactivity (Darnerud *et al.,* 1983). WBA showed initial highest radioactivity in bile, intestinal contents, kidney, liver, nasal mucosa and fat; a marked uptake was also observed in gills, testis and brain. Tissue levels were generally lower 13 days after dosing. In bleak (*Alburnus alburnus*) exposed for 14 days to this MCCP added to the tank water, a marked initial uptake of radioactivity was noted in gills, nasal cavity, skin, liver and fat; a high level was also present in the brain, bile and intestinal contents. A similar distribution pattern was seen after 14 days of exposure, as well as in fish allowed to recover for 1, 7 and 35 days.

A clear relationship between the structure of CP and their uptake was seen in bleak (*Alburnus* L.) when added to tank water (Bengtsson *et al.,* 1979). A short-chain length, i.e. SCCP and a low level of chlorination showed the most effective form for uptake among the five tested CP. The CP test solutions included Witaclor 149 ($C_{10–13}$, 49% chlorination), Witaclor 159 ($C_{10–13}$, 9% chlorination), Witaclor 171P ($C_{10–13}$, 71% chlorination), Witaclor 350 ($C_{14–17}$, 50% chlorination) and Witaclor 549 ($C_{18–26}$, 49% chlorination).

[redacted]

4.1.2 Human information (including bioaccumulation in humans)

No studies on the toxicokinetics in humans were reported in EFSA (2020).

One study was identified reporting levels of SCCP and MCCP in paired samples of maternal and umbilical cord blood serum collected in China (Beijing) in 2013 (Qiao *et al.*, 2018) and several studies have reported levels in human milk (see further data in section '3.4.3.3 Mammalian and bird data'). Detection of CP in human blood and milk samples indicates that CP are absorbed to some extent in humans and detection of CP in umbilical cord blood indicates that CP can be transferred to the foetus (EFSA, 2020).

4.1.3 Physiologically based kinetic (PBK) modelling

No PBK model publications were reported in EFSA (2020).

4.1.4 Conclusion on toxicokinetics (and bioaccumulation in humans)

No studies on the toxicokinetics in humans were reported in EFSA (2020). Even if it was reported in several studies that detection of CP in human blood and milk samples indicates that CP are absorbed to some extent in humans and detection of CP in umbilical cord blood indicates that CP can be transferred to the foetus (EFSA, 2020).

Following oral administration (diet, gavage) of CP (single ^{14}C-labelled dose) to rats the major route of excretion was the faeces with only a small proportion excreted in urine and expired air. The highest initial concentrations of radioactivity were found in the liver (SCCP, MCCP, LCCP), kidneys (SCCP, MCCP) and ovaries (SCCP, MCCP, LCCP). Initial high concentrations of radioactivity were also seen in the adipose tissue following administration of SCCP whereas for MCCP the concentration of radioactivity was highest at 7 days and for LCCP the concentration of radioactivity increased up to 28 days. In general, the elimination of radioactivity from the adipose tissue was slower than for the other three tissues for all three CP groups; the elimination rate from the adipose tissue decreased with increasing carbon chain length and chlorination degree.

A similar picture regarding distribution and elimination was seen in mice administered radiolabelled SCCP or MCCP orally (gavage) and/or by intravenous injection followed by visual determination of tissue distribution by WBA and evaluation of tissue retention and elimination in excreta by measuring radioactivity levels. The studies in mice suggested that highly chlorinated SCCP and MCCP are metabolised and excreted via faeces whereas lower chlorinated SCCP and MCCP can be partly metabolised and exhaled as carbon dioxide. The studies in mice also suggested that results from one CP are valid only for the CP studied and should not be taken as general for all CP.

In broiler chickens and laying hens given diets supplemented with an SCCP the highest concentration was recovered in abdominal fat. In the laying hens, a high concentration was also found in egg yolk and liver. A similar distribution pattern was seen in laying Japanese quail given an SCCP or an MCCP orally.

According to EFSA (2020), the fish studies with rainbow trout indicated that CP were rapidly accumulated and had high assimilation efficiencies from food and that the depuration half-lives increased with increasing carbon chain length and chlorination degree. The studies also indicated that the CP have the potential to biomagnify from food to fish in aquatic food chains with increasing trends with increasing carbon chain length and greater biotransformation of the short-chain CP compared to the longer chain CP. Studies with other fish species support the potential of CP to accumulate in fish tissues.

5. Environmental hazard assessment

5.1 Aquatic compartment (including sediment)

Aquatic toxicity testing is hampered by the low water solubility, complex nature of the test substance and challenges with the analytical methods. 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 assessment.

5.1.1 Fish

5.1.1.1 Short-term toxicity to fish

No toxicity has been seen in the available acute studies with fish (EC, 2005 & 2007).

5.1.1.2 Long-term toxicity to fish

Long-term toxicity studies with fish exposed to aqueous solutions are available for *Alburnus alburnus* (bleak), *Leuciscus idus* (golden orfe), *Oncorhynchus mykiss* (rainbow trout) and *Oryzias latipes* (Japanese medaka). No toxicity was observed in these studies. Test solutions were prepared with the use of acetone as a co-solvent or with direct addition of the test material. The studies are described in detail in EC, 2005. The available studies do not meet the requirements of the current OECD TG 210, but comparison with SCCP 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 ($C_{14}H_{24.9}Cl_{5.1}$, 48% chlorination average (containing $C_{14}H_{26}Cl_4$, $C_{14}H_{25}Cl_5$, $C_{14}H_{24}Cl_6$, $C_{14}H_{23}Cl_7$); ^{14}C-$C_{14}H_{23.3}Cl_{6.7}$, 55% chlorination average (containing $C_{14}H_{26}Cl_4$, $C_{14}H_{25}Cl_5$, $C_{14}H_{24}Cl_6$, $C_{14}H_{23}Cl7$, $C_{14}H_{22}Cl_8$, $C_{14}H_{21}Cl_9$)) 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 observed at 0.78 or 29 mg/kg food, respectively, were 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. Abnormal behaviour (development of dark colouration, lack of response to tapping, spinal curvature, low activity levels and poor feeding) was observed at the highest doses, 2.9 mg/kg food and 78 mg/kg food respectively. 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.

5.1.2 Aquatic invertebrates

5.1.2.1 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 (average value; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{14} congeners having 4, 5, 6 and 7 chlorine atoms at least are expected to be present in this substance; $C_{15\text{-}16}$ congeners having 5, 6, 7 and 8 chlorine atoms at least are expected and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms at least are expected to be present in this substance (equivalent to 42.3–58.2% Cl wt.)) sometimes mixed with n-pentadecane-8-^{14}C 51% Cl wt. (average value; a Gaussian distribution has been considered by the dossier submitter to describe the composition of chlorinated congeners as follows: C_{15} congeners having 5, 6, 7 and 8 chlorine atoms at least are expected to be present in this substance (equivalent to

46.2–58.2% Cl wt.)). Results are presented in Table 48 and further details are provided in EC (2005).

Table 48: Acute aquatic toxicity of MCCP to water fleas (*Daphnia magna*)

Chlorinated n-alkane test substance	Method	Co-solvent	Analytical method	48-h EC_{50} (µg/L)	Reference
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)
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)
C_{14-17} chlorinated paraffin (52% Cl wt.)	OECD TG 202 (static)[a] GLP status unknown	Acetone	None	<100 (nominal)	Thompson and Gore (1999)
C_{14-17}, 52% Cl wt.	OECD TG 202 (static) GLP	Acetone	None	< 6.5 (nominal)	Thompson (2004)
		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); Frank and Steinhäuser (1994)

Note: a – Fewer animals and test concentrations than usual.

Thompson *et al.* (1996) reported a 48-h EC_{50} value of 5.9 µg/L, based on mean measured concentrations. Stock solutions of the test substance were made up in acetone and each test solution was prepared by adding 0.2 ml of the appropriate stock solution to 2 litres of water, under the water surface with vigorous stirring. It is considered to be well conducted and reliable without restrictions (Klimisch 1). It is noted 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.

An acute toxicity test with *D. magna* (Unpublished *et al.,* 1995) 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[21] 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 1.4). 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 MCCP concentration.

At 48 hours, around 55% immobilisation was observed at the highest concentration tested (the 100% saturated solution) but there was no immobilisation 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 MCCP into hexane). Therefore, the toxicity seen in this study may have been the result of impurities present in the saturated solutions rather than MCCP itself. The results are considered to be 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, considered in more 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 SCCP 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 1.4). 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 consistent[22] with the earlier study of Thompson *et al.* (1996) (see EC, 2005 for further details[23]).

- *Uncertain reliability of measured concentrations*: Given the adsorptive properties of MCCP it is important to measure test concentrations in aquatic tests, especially under static conditions (as used for many of the acute *Daphnia* studies). However, there can be a large degree of variation between different laboratories using the same analytical method, as well as between methods.

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

[22] 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).

[23] 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.

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

Recently, Castro *et al*. (2018) performed an acute toxicity test on *Daphnia magna* using a test solution prepared via a passive dosing system. The main aim of the study was to investigate the partitioning behaviour of five different commercial chlorinated paraffins using passive dosing.

Cereclor S45 (a C_{13-18} 45% Cl wt. commercial product) was added to medical-grade silicone at concentrations of 1, 2 and 5 mg and allowed to equilibrate in vials with M7 medium for 48h. Subsequently, 10 juvenile *Daphnia magna* (age <24h) were added to each vial. Blank vials containing silicone not dosed with the test material were also included. Five replicates were used per treatment concentration. The experiment included 10 control vials, which did not contain either silicone or test material. Test solutions were not renewed. Any immobilisation was recorded at 24 and 48 h. The test material concentration was measured using APCI-QTOF-MS. After 48h, the highest test concentration of Cereclor S45, 260 µg/L, caused immobilisation of 12 ± 8% of Daphnia. The supplementary information provides a complete congener profile of the test material, Cereclor S45. This is the same test material as used for the *Daphnia* bioaccumulation study described in Section 3.4.2 (Castro *et al*., 2019; Castro, 2020). The reliability of the study is not assignable due to missing information on the study details (Klimisch 4).

One study for the amphipod *Gammarus pulex* reported no acute effects over 96 hours up to 1 mg/L (nominal) (Thompson and Gore, 1999; cited in EC, 2005). EC (2005) also cites a study for the harpacticoid copepod *Nitocra spinipes* which gave a 96-h LC_{50} of 9 and >10 000 mg/L for a C_{14-17}, 45% Cl wt. and C_{14-17}, 52% Cl wt. substance, respectively (Tarkpea *et al.*, 1981).

5.1.2.2 Long-term toxicity to aquatic invertebrates

Thompson *et al*. (1997) reported a 21-d NOEC for *Daphnia magna* of 10 µg/L (based on mean measured concentrations). This study is considered to be well conducted and reliable without restrictions (Klimisch 1). OECD TG 202 (1984) 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. 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. In line with the current OECD TG 211, an additional endpoint has been calculated reflecting mean number of living offspring per parent animal which does not die accidentally or inadvertently during the test.

Juvenile *Daphnia magna* (<24h old) were exposed to six concentrations of MCCP for 21 days under semi-static conditions at a temperature of 20 ± 1°C. Stock solutions of MCCP were prepared in acetone. The test solutions were prepared by gradual addition of 0.05 ml of the appropriate stock solution to 2 l of the test water below the water surface with vigorous stirring. All test solutions appeared clear and colourless and were renewed three times per week. The mortality and length of the parent Daphnia was recorded as well as the number of offspring produced per parent.

The test material was Cereclor S52, C14-17, 52% Cl wt. containing 0.3% epoxy soya bean oil as stabiliser. It was mixed with radiolabelled chlorinated n-pentadecane-8-14C (51% Cl wt.) to allow radiochemical analysis of the test solutions. The testing material Cereclor S52 is expected to contain C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; C_{15-16} congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms (equivalent to 42.3–58.2% Cl wt.), based on a Gaussian distribution (as considered by the dossier submitter). The other testing material n-pentadecane-8-^{14}C 51% Cl wt. is expected to contain C_{15} congeners having 5,6,7 and 8 chlorine atoms (equivalent to 46.2–58.2% Cl wt), based on a Gaussian distribution (as considered by the dossier submitter). Test solutions were extracted with hexane and analysed with a liquid scintillation spectrometer. The extraction efficiency was 101-103%.

There was 20% parent mortality in the control samples and 0% in solvent control, as well as significantly lower number of live offspring in control samples compared to the solvent control. Therefore, the test concentration treatments were compared with the solvent control only.

The following effect concentrations are reported in the study:

- 21-day NOEC for reproduction (number of live offspring/surviving parent): 10 µg/L (mean measured concentration)
- 21-day NOEC for length of parent: 10 µg/L (mean measured concentration)
- 21-day LC_{50} for parent mortality: 25 µg/L (mean measured concentration)

Relevant data from the study are provided in Table 49.

Table 49: Summary of results of a chronic *Daphnia* toxicity test with MCCP (Thompson *et al.*, 1997)

Treatment, µg/L		Parent mortality (no. of animals out of 10)	Study endpoint: Mean number of offspring per surviving parent **	Additional 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	10.6	3.1	24
100	65	10	0	0	0	0

Note: Bold 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.
* 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.

The following issues should be noted about the study:

- 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 laboratory) 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. Indeed, significant mortality of the parent *Daphnia* was observed for the 56 µg/L nominal and 100 µg/L nominal treatment groups.

- The reproduction NOEC endpoint is reported as 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 number of offspring endpoint has been calculated reflecting parent mortality in line with the current OECD TG 211, and it is not considered that this affects the 21-day NOEC for reproduction.

- The study recorded additional observations including dead offspring (see Table 49) 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 although it may be a population-relevant effect.

- 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 available renewal period data are considered to be representative enough to allow measured concentrations to be calculated. The 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, a time-weighted mean of 0.0087 mg/L or 8.7 µg/L for the nominal 0.018 mg/L treatment has been calculated, which is the 21-day NOEC for reproduction and length. It is recommended that this value is used in preference to the reported NOEC of 0.01 mg/L or 10 µg/L.

EU (2005) included other chronic *Daphnia* results for 52% Cl wt. MCCP products (see Table 50). The testing material C_{14-17} chlorinated n-alkane 52% Cl wt. products (average value) is expected to contain C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; C_{15-16} congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms (equivalent to 42.3–58.2% Cl wt.) based on a Gaussian distribution (as considered by the dossier submitter). The other testing material n-pentadecane-8-^{14}C 51% Cl wt. (average value) is expected to contain C_{15} congeners having 5, 6, 7 and 8 chlorine atoms (equivalent to 46.2–58.2% Cl wt) based on a Gaussian distribution (as considered by the dossier submitter).

Table 50: Chronic aquatic toxicity of MCCP to water fleas (*Daphnia magna*)

Chlorinated n-alkane test substance	Method	Co-solvent	Analytical method	21-d NOEC (µg/L)	Reference
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)
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); Frank and Steinhäuser (1994)
C_{14-17}, 52% Cl wt.			Total extractable organic halogen method	ca. 4-8 (measured) [0.18 vol.%]	TNO (1993)

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.

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 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) after 3 days, 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 for 9 days, the end of the investigation. Castro *et al*. (2019) also suggest that elimination might increase when *Daphnia* are fed (see Section 0).

One additional long-term invertebrate toxicity study was summarised in EC (2005). This reported a 60-d NOEC of 0.22 mg/L for a $C_{14\text{-}17}$, 52% Cl wt. substance with Blue Mussel *Mytilus edulis* (Madeley and Thompson, 1983). No significant effects on mortality or mean shell length were observed.

5.1.3 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 liquid scintillation counting (LSC) measurements.

5.1.4 Sediment organisms

Prolonged sediment toxicity tests are available for MCCP with *Hyalella azteca, Lumbriculus variegatus* and *Chironomus riparius* and are summarised in EC (2005 & 2007). The tests were carried out using sediment spiked with a $C_{14\text{-}17}$, 52% Cl wt. substance (average value; with C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; $C_{15\text{-}16}$ congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms (equivalent to 42.3–58.2% Cl wt.) and based on a Gaussian distribution, as considered by the dossier submitter). 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).

5.1.5 Other aquatic organisms

Du *et al.* (2019) investigated the hepatosomatic index (HSI) of black-spotted frog *(Pelophylax nigromaculatus*) by calculating the ratio of the liver weight to body weight for frog individuals (further study details can be found in section '3.4.4.2 Monitoring data in biota'). According to the authors, the HSI has been used as an estimate of energy status as well as biomarkers for contaminant exposure. Since liver is an important organ mainly responsible for detoxification and energy storage, HSI could reflect, according to Du *et al.* (2019), the overall health condition of organisms. In the study, a low but significant negative correlation was found between the HSI and total CP levels (SCCP, MCCP and LCCP) in frog livers ($R = -0.620$, $p < 0.005$). The negative correlation indicated that the frog individuals with higher CP exposure tended to have downsized liver tissues. According to the authors, as elimination of contaminants need extra energy, the small hepatic tissue may be due to the reduction of hepatic glycogen deposits. This result suggests that high CP exposure may reduce the energy storage in frog liver, further leading to a lower survival rate of frogs during their hibernation.

In addition, the total CP levels in frog liver samples were negatively correlated with body weight ($R = -0.632$, $p < 0.005$) and Sex, snout-vent length (SVL) ($R = -0.679$, $p < 0.001$). These

negative correlations were low but statistically significant. Moreover, significant positive correlations were found between HSI and SVL as well as between HSI and body weight (*p < 0.005)*, indicating the negative correlations between CP levels and body weight/SVL may also be caused by the reduction of energy storage in body of frogs.

5.2 Terrestrial compartment

5.2.1 Toxicity to soil macro-organisms

Thompson *et al.* (2001) performed an earthworm (*Eisenia fetida*) reproduction test using a radiolabelled n-pentadecane-8-^{14}C, 51% wt. Cl substance (average value; with C_{15} congeners having 5, 6, 7 and 8 chlorine atoms (equivalent to 46.2–58.2% Cl wt) based on a Gaussian distribution, as considered by the dossier submitter) mixed with a commercial $C_{14\text{-}17}$, 52% Cl wt. substance (average value; with C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; $C_{15\text{-}16}$ congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms (equivalent to 42.3–58.2% Cl wt.) based on a Gaussian distribution, as considered by the dossier submitter). This study is further described in Section 3.4.3.1 and in EC, 2005. The 56-d $NOEC_{reproduction}$ from the study (based on number of offspring produced (fecundity) was 280 mg/kg dry weight soil (equivalent to 248 mg/kg wet weight) based on measured concentrations. Analyses were performed using non-specific liquid scintillation counting. This study is reported as reliable without restrictions in EC (2005).

5.2.2 Toxicity to terrestrial plants

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 $C_{14\text{-}17}$, 52% Cl wt. substance (average value; with C_{14} congeners having 4,5,6 and 7 chlorine atoms; $C_{15\text{-}16}$ congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms (equivalent to 42.3–58.2% Cl wt.) based on a Gaussian distribution, as considered by the dossier submitter) mixed with a small amount of radiolabelled n-pentadecane-8-^{14}C, 51% wt. Cl substance (average value; with C15 congeners having 5, 6, 7 and 8 chlorine atoms (equivalent to 46.2–58.2% Cl wt) based on a Gaussian distribution, as considered by the dossier submitter) is reported in EC (2005). Analyses were performed using non-specific liquid scintillation counting. The overall 28-d NOEC for each species was ≥5 000 mg/kg dry weight soil. This study is reported as reliable without restrictions in EC (2005).

5.2.3 Toxicity to soil micro-organisms

An OECD TG 216 (soil microorganisms: nitrogen transformation test) study using a $C_{14\text{-}17}$, 52% Cl wt. substance (average value; with C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; $C_{15\text{-}16}$ congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms (equivalent to 42.3–58.2% Cl wt.) based on a Gaussian distribution, as considered by the dossier submitter) is reported in EC (2005). The overall 28-d NOEC was ≥400 mg/kg dry weight soil. Analyses were performed using non-specific liquid scintillation counting. This study is reported as reliable without restrictions in EC (2005).

5.3 Microbiological activity in sewage treatment systems

The results of three tests with microorganisms are reported in EC, 2005. The lowest 24-h NOEC was 800 mg/L for a $C_{14\text{-}17}$, 41% Cl wt. substance (average value; with C_{14} congeners having 2, 3, 4 and 5 chlorine atoms; $C_{15\text{-}17}$ congeners having 3, 4, 5 and 6 chlorine atoms (equivalent to 26.6–50.8% Cl wt.) based on a Gaussian distribution, as considered by the dossier submitter) 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 toxicity of a $C_{14\text{-}17}$, 52% wt. Cl chlorinated paraffin (average value; with C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; $C_{15\text{-}16}$ congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms (equivalent to 42.3–58.2% Cl wt.) based on a Gaussian distribution, as

considered by the dossier submitter) has been tested in a 3-hour respiration inhibition test (unpublished study). The chlorinated paraffin was emulsified in water using 0.5 g/L nonylphenol ethoxylate surfactant and then incubated for 3 hours with activated sludge from a municipal sewage treatment plant. No effect on respiration was seen up to the highest concentration tested (2,000 mg/L) (Hoechst AG; as reported in BUA, 1992).

5.4 Toxicity to birds

The acute oral 1-day LD_{50} values of MCCP (Cereclor S52, $C_{14–17}$, 52% Cl wt.) were reported to be > 24,606 mg/kg bw per day for ring-necked pheasants and > 10,280 mg/kg bw per day for mallard ducks. After 5-day dietary treatment, the LC_{50} values of MCCP ($C_{14–17}$, 52% chlorination) for ring-necked pheasants and also for mallard ducks were reported to be > 24,603 mg/kg diet (Madeley and Birtley, 1980).

5.5 Summary and discussion of the environmental hazard assessment

Only limited information is available on the aquatic toxicity of individual MCCP congeners. Due to the lack of experimental studies on specific MCCP congeners, it is difficult to predict whether the aquatic toxicity of MCCP significantly varies with both chlorine content and carbon chain length. QSAR models to predict the long-term aquatic toxicity of the MCCP congeners with high degree of chlorination are expected to have issues with reliability. Many of these congeners are expected to have Log Kow >8 which is the maximum value in the log Kow range of the fish and Daphnid chronic toxicity models of ECOSAR (EPI Suite™), see Table 54 of Annex II – Modelling of log Kow and biodegradation and generation of representative structures for MCCP.

The majority of the ecotoxicity data is available for the C_{14-17}, 52% Cl wt. commercial substance.

From the available database, aquatic effects have almost exclusively been observed with the water flea *Daphnia magna*, for a C_{14-17} chlorinated n-alkane, 52% Cl wt. test material.

Due to the low water solubility of MCCP congeners, the acute studies with *Daphnia magna* may not reflect the true toxicity as it is unlikely that equilibrium was reached during such a short period of time. 48h EC_{50} results from acute *Daphnia magna* studies fall in the range < 6.5 – 2200 µg/L. The most reliable result is 48h EC_{50} 5.9 µg/L for the C_{14-17}, 52% Cl wt. substance.

For the chronic toxicity of MCCP to *Daphnia magna*, 21d NOEC (reproduction) values range from ~ 4 - 15.6 µg/L. The most reliable result is 21d NOEC 8.7 µg/L for the C_{14-17}, 52% Cl wt. substance.

The acute and chronic *Daphnia magna* studies were used for harmonised classification of MCCP as Aquatic Acute 1, Aquatic Chronic 1, H400 and H410.

The similar effect concentrations for both mortality and reproduction in *Daphnia magna* is unusual. It is assumed to be related to differences in bioavailability or elimination caused by the presence of food in the chronic study, since an investigation at the testing laboratory used for the most reliable acute and chronic studies found that fewer *Daphnia magna* died over 9 days when fed algae.

Conclusion on the T-properties of MCCP and its congener groups

Only limited experimental information is available on the aquatic toxicity of individual MCCP congeners. The majority of the ecotoxicity data is available for the commercial C_{14-17}, 52% Cl wt. substance.

48h EC50 results from acute *Daphnia magna* studies fall in the range < 6.5 – 2200 µg/L. The most reliable result is 48h EC50 5.9 µg/L for the C_{14-17}, 52% Cl wt. substance. According to the PBT guidance (REACH Chapter R.11, ECHA, 2017b), a short-term aquatic toxicity result in fish,

daphnia, or algae with EC50 or LC50 < 0.01 mg/L is sufficient to meet the T criterion. Based on this guidance, the T criterion is met.

For the chronic toxicity of MCCP to *Daphnia magna*, 21d NOEC (reproduction) values range from ~ 4 - 15.6 µg/L. The most reliable result is 21d NOEC 8.7 µg/L for the C_{14-17}, 52% Cl wt. substance which meets the toxicity criterion (T) in accordance with Annex XIII, point 1.1.3 (a), of the REACH Regulation.

For a UVCB substance like MCCP, observed toxicity may represent toxicity of one or more of its constituents. As the testing material of the acute and chronic toxicity studies available for MCCP contained several groups of congeners of MCCP and no testing and analysis was performed at the level of the congener groups, it is not possible to identify whether the congener groups present in the tested substance contributed differently to the observed toxicity.

However, the congener groups expected to be present in the test material for both these tests are C_{14} congener groups having 4, 5, 6 and 7 chlorine atoms; C_{15-16} congener groups having 5, 6, 7 and 8 chlorine atoms and C_{17} congener groups having 6, 7, 8 and 9 chlorine atoms. These same congeners have been detected in *Daphnia magna* in a bioaccumulation test reported in Section 3.4.2.3 Other supporting data (Castro *et al*., 2019; Castro, 2020 and Castro M, Personal Communication, 2020 and 2021). This indicates that these congener groups are bioavailable to *Daphnia magna* and taken up by this organism. Since these congener groups are structurally very similar (they differ only in carbon chain length and number of chlorine substituents), they can be expected to exert toxic effects by the same mode(s) of action. It is therefore reasonable to assume that all congener groups present in the C_{14-17}, 52% Cl wt. test substance contributed equivalently to the observed toxicity.

It is therefore concluded that MCCP and all the following congener groups of MCCP meet the toxicity criterion (T) in accordance with Annex XIII, point 1.1.3 (a), of the REACH Regulation: C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; C_{15} congeners having 5, 6, 7 and 8 chlorine atoms; C_{16} congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms.

6. Conclusions on the SVHC Properties

6.1 CMR assessment

Not relevant for the identification of these substances as SVHC in accordance with Article 57 points (d) to (e) REACH.

6.2 PBT and vPvB assessment

6.2.1 Assessment of PBT/vPvB properties

A weight-of-evidence determination according to the provisions of Annex XIII of REACH is used in order to conclude on the PBT/vPvB properties of MCCP at the level of the investigated congener groups ($C_{14\text{-}17}Cl_{1\text{-}(14\text{-}17)}$). All available relevant information (such as the results of standard tests, monitoring and modelling, information from the application of a trend analysis with respect to persistence among the MCCP congener groups of different carbon chain lengths and different levels of chlorination and (Q)SAR results) was considered together in a weight-of-evidence approach. All studies used have been assessed as reliable (with or without restrictions), relevant and adequate for the assessment, unless otherwise stated and specified in this document.

6.2.1.1 Persistence

Based on screening and assessment information reported in Section '3.1 Degradation' and in accordance with REACH Annex XIII, a weight-of-evidence (WoE) approach is used in order to conclude on the persistence of MCCP at the level of the investigated congener groups ($C_{14\text{-}17}Cl_{1\text{-}(14\text{-}17)}$). The weight-of-evidence approach applied for each congener group is presented below. It is important to note that all studies used in the below described weight-of-evidence approach have been assessed as reliable (with restrictions), relevant and adequate for the assessment, unless otherwise stated. The results of the OECD TG 308 simulation degradation study described in section '3.1.2.1.3 Simulation tests (water and sediments)' is given a high weight in the WoE and it is considered to provide in combination with the QSAR predictions for potential persistence of MCCP congener groups (see section '3.1.2.1.1 Estimated data') sufficient evidence to conclude that the congeners of MCCP with carbon chain lengths between C_{14} and C_{17} with a chlorination number of 3 or higher are persistent and very persistent (P/vP) in sediment. The QSAR predictions are used as supporting information to the experimental data, but are considered to be sufficient to support the conclusion drawn on the persistence of MCCP and its congener groups.

Complex composition of the MCCP and related degradation behaviour of the different congeners leads to some challenges in the persistence assessment. However, combining all the available evidence on the degradability of MCCP and its congener groups, the following can be demonstrated:

An OECD TG 308 study (Unpublished, 2019c) performed on C_{14} chlorinated n-alkane, 50% Cl. wt. indicates that the total water-sediment DT_{50} values for the $C_{14}Cl_{3\text{-}14}$ congener[24] constituting the test substance are greater than 120 days at 12°C (under aerobic conditions; see Annex XII). The fact that there was no significant measurable degradation over 120 days suggests that it is unlikely that ≥50% mineralisation or primary degradation would occur over a subsequent 60-day period. Therefore, based on this study (Unpublished, 2019c), it can be reasonably assumed that the $C_{14}Cl_{3\text{-}14}$ groups of congeners are very persistent in sediment (degradation half-lives > 180 days). The outcome of this simulation study is the kind of information that according to REACH Annex XIII shall be considered in determining whether the P criteria (Annex XIII 1.1.1

[24] The composition of the chlorinated congeners of the test substance C_{14} chlorinated n-alkane, 50% Cl. wt. was determined analytically as follows: chlorine content between 35.32–72.98% Cl wt. equivalent to 3 to 14 chlorine atoms per molecule.

(d)) or the vP criteria (Annex XIII 1.2.1 (b)) are met and therefore is given high weight in the weight-of-evidence based conclusion on the P-properties of MCCP and their congener groups.

No experimental degradation data for specific C_{15}, C_{16} or C_{17} chloroalkane substances and their congener groups is available while they are expected to be less water soluble (Glüge *et al.,* 2013) and more adsorptive (Gawor and Wania, 2013) than the C_{14} substances. QSAR predictions were used in order to investigate possible trends with respect to persistence among the MCCP congener groups of different carbon chain lengths and different levels of chlorination. Applying the screening P criteria from the PBT guidance (Chapter R.11, ECHA, 2017b), the BIOWIN model predicts that almost all of the congener groups of MCCP ($C_{14\text{-}17}$ congener groups with three or more chlorine substituents at the carbon chain) screen as potentially persistent. Furthermore, the BIOWIN model predicts decreased biodegradation with increase in number of chlorine substituents at the carbon chain, because in the model the negative coefficient for the aliphatic chloride fragment is multiplied with the number of chlorine atoms in the structure. When comparing predictions for congeners with different chain lengths but with the same number of chlorine atoms substituted at the hydrocarbon chain (e.g. $C_{15}Cl_5$ with $C_{17}Cl_5$), the predicted degradation decreases with increase in chain length. This is mainly the result of the coefficient for molecular weight decreasing. Based on the predicted and observed trends in physico-chemical properties of structures of the different MCCP congeners, which are in line with the general scientific knowledge on the expected partitioning behaviour and environmental fate of hydrophobic aliphatic chloroalkanes, it can be reasonably estimated that the $C_{15\text{-}17}$ congeners with the same or higher chlorine contents than the congeners of C_{14} chlorinated n-alkane, 50% Cl. wt. (which contains $C_{14}Cl_{3\text{-}14}$ congeners that all are P/vP) will be equally or more adsorptive to sediment, have lower water solubilities and partition stronger to octanol. They therefore will at least be equally if not more persistent in sediments.

Monitoring data on MCCP, used as supporting information in the WoE, are in line with the outcome of the simulation study and the BIOWIN predictions as they point towards persistence of MCCP in sediments.

Several ready biodegradation screening studies under conditions of enhanced bioavailability have been performed with commercial MCCP product types. Based on the results of the screening tests, it seems that the overall level of degradation appears to decline with increasing levels of chlorination (see Table 24). Overall, these screening studies are not considered appropriate for assessing and concluding on the persistence properties of UVCB substances such as MCCP and their constituents. Indeed, based on the outcome of the screening tests and in absence of information on the degree of degradation of the individual congener groups in the tests, it can be reasonably assumed that the substances tested (see Table 24) contain potentially persistent congeners. For UVCB substances, there are uncertainties related to the screening tests where the contribution of the different congeners of MCCP to the overall degradation is unknown. Therefore screening tests without further supplementary information enabling the possibility for the dossier submitter to verify the claims made with regard to the composition of the test substance, i.e. the identity of the individual congener groups and their concentration in the substance as well as on the degree of degradation of the individual congener groups in a test, are normally not sufficient to draw conclusions on the persistence of MCCP as a substance and in particular on the persistence of its individual constituents, respectively different congener groups. That is why the outcomes of the screening tests for MCCP have been given a low weight in the weight-of-evidence assessment.

It is important to highlight that the results of the higher tier degradation simulation study (OECD TG 308, Unpublished, 2019c; Annex XIII 3.2: assessment information) are to be given more weight in the weight-of-evidence assessment than the screening studies of the OECD 301 or 302 series reported in Section ‘3.1.2.1.2 Screening tests’ (Annex XIII, section 3.1: screening information). In the presence of a reliable higher tier study, which, inter alia due to consideration of the sediment compartment reflects environmental conditions wider and thus more realistically than the screening studies, it is not necessary to analyse in detail the potential reasons for potentially inconsistent outcomes of the ready biodegradation screening tests. The outcomes of

the higher tier study (Unpublished, 2019c), supersede the screening tests.

Abiotic degradation data indicate that MCCP are not expected to hydrolyse significantly. The predicted atmospheric half-life will vary for the MCCP congener groups according to degree of chlorination, with the estimated half-lives increasing with increasing number of chlorine atoms in the structure (Gawor and Wania, 2013). Based on information from Environment Canada (2008), Gawor and Wania (2013), EA (2019) and UK (2021), MCCP congeners have a range of atmospheric half-lives in the vapour phase between 0.6 to 7.1 days, thus indicating a potential for long-range transport in air for some of the MCCP congener groups. According to Howard *et al.* (1975), direct photodegradation in air for MCCP with 45% wt. Cl and 52% wt. Cl is unlikely to be a significant degradation pathway in the environment. There is no experimental data for indirect phototransformation in air. No information is available on phototransformation potential in water or soil. As a conclusion, abiotic degradation of MCCP and MCCP congeners is not considered to be a significant degradation pathway in the environment.

Monitoring data support findings from experimental and predicted data on biodegradation and abiotic degradation of MCCP congeners and MCCP, as well as on potential long-range transport. The available monitoring data, particularly from sediment core studies, suggest some dechlorination of chlorinated paraffins with high chlorine contents in sediment over time, but they also suggest that degradation in the environment may be slow and provide indirect evidence that MCCP with chlorine contents of ~ 55% by weight can persist in sediments for more than a decade. The detection and/or quantification of MCCP in marine sediments from the Arctic, in locations far away from point sources, point towards persistence of MCCP in marine sediments under aerobic conditions. Finally, concentrations of MCCP in sediment and soil seem to have increased over the last decades. Monitoring data is only used as supporting information in the weight-of-evidence approach for concluding on the degradation potential and persistence properties of MCCP.

There are no criteria in Annex XIII for half-lives in air. However, 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.

Overall weight of evidence based conclusion on the persistence properties of MCCP and their congener groups

As an overall conclusion, based on the above information used in a weight-of-evidence-approach, it is concluded that the $C_{14}Cl_{3–14}$ congener groups of MCCP (equivalent to 35.32–72.98% Cl wt.) meet the ‘persistence’ criterion (P) and the ‘very persistent’ criterion (vP) in accordance with Annex XIII, points 1.1.1 and 1.2.1, of the REACH Regulation on the basis of their persistent and very persistent (P/vP) properties in sediment (degradation half-lives > 180 days).

Based on the predicted and observed trends in physico-chemical properties it further can be reasonably estimated that also the $C_{15\text{-}17}$ congener groups of MCCP with the same or higher chlorine contents than the congeners present in C_{14} chlorinated n-alkane, 50% Cl. wt. (which contains $C_{14}Cl_{3\text{-}14}$ congener groups that all are P/vP) will at least be equally if not more persistent in sediment than the congeners of C_{14} chlorinated n-alkane, 50% Cl. wt. Consequently, it is concluded that also the $C_{15}Cl_{3\text{-}15}$, $C_{16}Cl_{3\text{-}16}$ and $C_{17}Cl_{3\text{-}17}$ congener groups of MCCP meet the ‘persistence’ (P) and ‘very persistent’ (vP) criteria of REACH Annex XIII (degradation half-life in sediment > 180 days).

Finally, since MCCP always will contain congener groups with P/vP properties at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet both the ‘persistence’ (P) and ‘very persistent’ (vP) criteria of REACH Annex XIII (degradation half-life in sediment > 180 days).

Monitoring data on MCCP support the above conclusions as they point towards persistence of MCCP in sediments.

6.2.1.2 Bioaccumulation

The congeners of MCCP have a range of log Kow values, the majority of which are equal to or exceed 6.5. They therefore meet the screening criterion set out in the PBT Guidance (REACH Chapter R.11; ECHA, 2017b) for aquatic organisms as being potentially 'bioaccumulative' (B) and/or 'very bioaccumulative' (vB) (i.e. log Kow > 4.5).

Chloroalkanes are neutral organohalogen compounds, so bioaccumulation is likely to involve simple partitioning to lipid storage tissues. The degree of bioaccumulation of the congeners will depend on their hydrophobicity (which is reflected by their octanol-water partition coefficients, log Kow ≥ 6.5) and potential to be metabolised. As described in Section 3.4.1, log Kow 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 (above 55% Cl wt.), the log Kow increases with increasing chlorine content in a non-linear fashion.

The Fisk *et al.* (1996, 1998 and 2000) studies concluded that the potential for metabolism decreases with increasing carbon chain length and chlorine content, and that it appears that the relationship of bioaccumulation and carbon chain length and chlorine content of chlorinated alkanes is complex. Gawor and Wania (2013) modelled environmental bioaccumulation potential and found that both the size of the carbon skeleton and the number of halogens influence which components will be bioaccumulative.

BCF predictions for all MCCP constituents with the BCF Baseline Model of CATALOGIC has yielded different results for isomers, reflecting that the position of the chlorine atoms appears to influence the bioaccumulation potential. The difference in predicted BCF for structural isomers of a specific congener group (e.g. $C_{14}Cl_6$) is a result of difference in the log Kow and the application of different predicted metabolic transformations by the model according to the structure. Experimental data suggest that the rate of metabolism of the chlorinated paraffins is influenced by the chain length and/or the degree of chlorination and that the proportion of unmetabolised chlorinated paraffin increased with its degree of chlorination (Unpublished, 2020).

Toxicokinetic data on mammals using radiolabelled MCCP indicate 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. Following oral administration (diet, gavage) of CP (including MCCP) to rats the major route of excretion was the faeces with only a small proportion excreted in urine and expired air. It was shown that the elimination rate from the adipose tissue decreased with increasing carbon chain length and chlorination degree (EFSA, 2020). A similar picture regarding distribution and elimination was seen in mice and Japanese quail given MCCP orally (gavage) and/or by intravenous injection. The fish studies with rainbow trout indicated that CP were rapidly accumulated and had high assimilation efficiencies from food and that the depuration half-lives increased with increasing carbon chain length and chlorination degree (EFSA, 2020). MCCP have been demonstrated to have relatively long elimination or depuration half-lives in fish and mammals (growth corrected depuration half-lives in the range of 29–80 days in rainbow trout (Fisk *et al.* (1996, 1998b and 2000) and Unpublished, 2019e) and half-life up to 8 weeks in abdominal fat of rats (Birtley *et al.*, 1980)). These long elimination half-lives mean that significant concentrations of the substance may remain within an organism for several months, possibly years, after cessation of emission.

In addition, CP (including MCCP) have been detected in human blood and milk samples which indicates that CP are absorbed to some extent in humans and detection of CP in umbilical cord blood and placenta indicates that CP can be transferred to the foetus (EFSA, 2020; Xia *et al.* 2017; Wang *et al.* 2018b).

The available (limited) field bioaccumulation studies for MCCP are equivocal: trophic magnification factors below and above 1 have been derived.

Monitoring data demonstrate widespread contamination of wildlife by MCCP at all trophic levels (including predatory species). MCCP have also been detected in samples from remote regions, including the Arctic. These data provide supporting evidence that MCCP are taken up by organisms in the environment. Only limited information is available on the actual carbon chain length distribution and chlorine contents of MCCP detected in environmental samples, although advances in analytical methodologies have meant that this has been possible in some of the more recent studies. Based on the new studies, C_{14} chain lengths are frequently the predominant congeners of MCCP found in biota (Houde *et al.,* 2008; Basconcillo *et al.,* 2015; Zeng *et al.,* 2015 and Du *et al.,* 2019), followed by C_{15} chain lengths (Du *et al.,* 2019). These findings are in line with the constituent pattern found in commercial products.

Based on screening and assessment information reported in Section 3.4, a weight-of-evidence approach is used in order to conclude on the bioaccumulation potential of MCCP and their constituents at the level of the congener groups assessed. The outcome of the weight-of-evidence approach applied for each congener group of MCCP is presented in Table 51 (for details refer to section '3.4.5 Summary and discussion of bioaccumulation').

Table 51: Congener groups of MCCP concluded as B and/or vB in accordance with REACH Annex XIII based on the data available for the different congener groups

Number chlorine atoms and Carbon chain lenght	Cl_2	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}
C_{14}		B / vB	B / vB	B / vB	B / vB	B / vB	B / vB	B / vB	B / vB	B / vB				
C_{15}		B / vB	B / vB	B / vB	B	B	B	B	-	-				
C_{16}	B / vB	B / vB	B / vB	B / vB	B	B	B	B	-		-	-	-	-
C_{17}	-	-	-	B	B	B	B	B	-					

Note: Symbol '-' means that not enough information is available to conclude on the B property of the congener group of MCCP. Grey cells indicate when no experimental data is available on the congener group of MCCP.

As an overall conclusion, it can be concluded that $C_{14}Cl_{3–11}$ congener groups of MCCP (equivalent to 35.3–67.6% Cl wt.) have B/vB properties, $C_{15}Cl_{3–9}$ congener groups of MCCP (equivalent to 33.8–61.15% Cl wt.) have B and/or vB properties, $C_{16}Cl_{2–9}$ congener groups of MCCP (equivalent to 24.1–59.55% Cl wt.) have B and/or vB properties and $C_{17}Cl_{5–9}$ congener groups of MCCP (equivalent to 43–58% Cl wt.) have B properties in accordance with REACH Annex XIII (see Table 51). For other congener groups of MCCP, it is not possible to conclude on their potential for bioaccumulation due to the lack of appropriate data.

Based on the information available, as MCCP contain congener groups with B and/or vB properties at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet the 'bioaccumulation' criterion (B) and the 'very bioaccumulative' criterion (vB) in accordance with Annex XIII, points 1.1.2 and 1.2.2, of the REACH Regulation.

6.2.1.3 Toxicity

Aquatic toxicity

Only limited information is available on the aquatic toxicity of individual MCCP congeners. Due to the lack of experimental studies on specific MCCP congeners, it is difficult to predict whether

the aquatic toxicity of MCCP significantly varies with both chlorine content and carbon chain length. QSAR models to predict the long-term aquatic toxicity of the MCCP congeners with high degree of chlorination are expected to have issues with reliability. Many of these congeners are expected to have Log Kow >8 which is the maximum value in the log Kow range of the fish and Daphnid chronic toxicity models of ECOSAR (EPI Suite™), see Table 54 of Annex II – Modelling of log Kow and biodegradation and generation of representative structures for MCCP.

The majority of the ecotoxicity data is available for the C_{14-17}, 52% Cl wt. commercial substance.

From the available database, aquatic effects have almost exclusively been observed with the water flea *Daphnia magna*, for a C_{14-17} chlorinated n-alkane, 52% Cl wt. test material.

Due to the low water solubility of MCCP congeners, the acute studies with *Daphnia magna* may not reflect the true toxicity as it is unlikely that equilibrium was reached during such a short period of time. 48h EC_{50} results from acute *Daphnia magna* studies fall in the range < 6.5 – 2200 µg/L. The most reliable result is 48h EC_{50} 5.9 µg/L for the C_{14-17}, 52% Cl wt. substance.

For the chronic toxicity of MCCP to *Daphnia magna*, 21d NOEC (reproduction) values range from ~ 4 - 15.6 µg/L. The most reliable result is 21d NOEC 8.7 µg/L for the C_{14-17}, 52% Cl wt. substance.

The acute and chronic *Daphnia magna* studies were used for harmonised classification of MCCP as Aquatic Acute 1, Aquatic Chronic 1, H400 and H410.

The similar effect concentrations for both mortality and reproduction in *Daphnia magna* is unusual. It is assumed to be related to differences in bioavailability or elimination caused by the presence of food in the chronic study, since an investigation at the testing laboratory used for the most reliable acute and chronic studies found that fewer *Daphnia magna* died over 9 days when fed algae.

Conclusion on the T-properties of MCCP and its congener groups

Only limited experimental information is available on the aquatic toxicity of individual MCCP congeners. The majority of the ecotoxicity data is available for the commercial C_{14-17}, 52% Cl wt. substance.

48h EC_{50} results from acute *Daphnia magna* studies fall in the range < 6.5 – 2200 µg/L. The most reliable result is 48h EC_{50} 5.9 µg/L for the C_{14-17}, 52% Cl wt. substance. According to the PBT guidance (REACH Chapter R.11, ECHA, 2017b), a short-term aquatic toxicity result in fish, daphnia, or algae with EC_{50} or LC_{50} < 0.01 mg/L (≈ 10 µg/L) is sufficient to meet the T criterion. Based on this guidance, the T criterion is met.

For the chronic toxicity of MCCP to *Daphnia magna*, 21d NOEC (reproduction) values range from ~ 4 - 15.6 µg/L. The most reliable result is 21d NOEC 8.7 µg/L for the C_{14-17}, 52% Cl wt. substance which meets the toxicity criterion (T) in accordance with Annex XIII, point 1.1.3 (a), of the REACH Regulation.

For a UVCB substance like MCCP, observed toxicity may represent toxicity of one or more of its constituents. As the testing material of the acute and chronic toxicity studies available for MCCP contained several groups of congeners of MCCP and no testing and analysis was performed at the level of the congener groups, it is not possible to identify whether the congener groups present in the tested substance contributed differently to the observed toxicity.

However, the congener groups expected to be present in the test material for both these tests are C_{14} congener groups having 4, 5, 6 and 7 chlorine atoms; C_{15-16} congener groups having 5, 6, 7 and 8 chlorine atoms and C_{17} congener groups having 6, 7, 8 and 9 chlorine atoms. These same congener groups have been detected in *Daphnia magna* in a bioaccumulation test reported

in Section 3.4.2.3 Other supporting data (Castro *et al*., 2019; Castro, 2020 and Castro M, Personal Communication, 2020 and 2021). This indicates that these congener groups are bioavailable to *Daphnia magna* and taken up by this organism. Since these congener groups are structurally very similar (theydiffer only in carbon chain length and number of chlorine substituents), they can be expected to exert toxic effects by the same mode(s) of action. It is therefore reasonable to assume that all congener groups present in the C_{14-17}, 52% Cl wt. test substance contributed equivalently to the observed toxicity.

It is therefore concluded that MCCP and all the following congener groups of MCCP meet the toxicity criterion (T) in accordance with Annex XIII, point 1.1.3 (a), of the REACH Regulation: C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; C_{15} congeners having 5, 6, 7 and 8 chlorine atoms; C_{16} congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms.

Mammalian toxicity

MCCP do 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 report.

6.2.2 Summary and overall conclusions on the PBT and vPvB properties

A weight-of-evidence determination according to the provisions of Annex XIII of REACH is used in order to conclude on the PBT/vPvB properties of MCCP at the level of the investigated congener groups ($C_{14-17}Cl_{1-(14-17)}$). All information (such as the results of standard tests, monitoring and modelling, information from the application of a trend analysis with respect to persistence among the MCCP congener groups of different carbon chain lengths and different levels of chlorination and (Q)SAR results) was considered together in a weight-of-evidence approach. All studies used have been assessed as reliable (with or without restrictions), relevant and adequate for the assessment, unless otherwise stated and specified in this document.

Persistence

The assessment and the conclusions on persistence are based on the following information:

- An OECD TG 308 study performed on C_{14} chlorinated n-alkane, 50% Cl. wt. indicates that the total water-sediment DT_{50} values for the $C_{14}Cl_{3-14}$ congener groups of MCCP (equivalent to 35.32–72.98% Cl wt.) are greater than 120 days at 12°C (under aerobic conditions). The fact that there was no significant measurable degradation over 120 days suggests that it is unlikely that ≥50% mineralisation or primary degradation would occur over a subsequent 60-day period. Therefore, based on this study, it can be reasonably assumed that the $C_{14}Cl_{3-14}$ groups of congeners are very persistent in sediment (degradation half-lives >180 days). The outcome of this higher tier study is given a high weight as it provides information directly comparable with the P and vP criteria set out in Annex XIII, points 1.1.1 (d) and 1.2.1 (b) of the REACH Regulation;
- Based on modelling data, almost all of the congener groups of MCCP (C_{14-17} congener groups with three or more chlorine substituents at the carbon chain) are predicted to be not readily biodegradable and hence potentially persistent. No experimental degradation data for specific C_{15}, C_{16} or C_{17} chloroalkane substances and their congener groups is available while they are expected to be less water soluble and more adsorptive than the C_{14} substances. Based on the predicted and observed trends in physico-chemical properties of structures of the different MCCP congeners, which are in line with the general scientific knowledge on the expected partitioning behaviour and environmental fate of hydrophobic aliphatic chloroalkanes, it can be reasonably estimated that the C_{15-17}

congeners with the same or higher chlorine contents than the congeners of C_{14} chlorinated n-alkane, 50% Cl. wt. (which contains $C_{14}Cl_{3-14}$ congeners that all are P/vP) will be equally or more adsorptive to sediment, have lower water solubilities and partition stronger to octanol. They therefore will at least be equally if not more persistent in sediments;

- Several ready biodegradation screening studies under conditions of enhanced bioavailability have been performed with commercial MCCP product types. Based on the results of the screening tests, it seems that the overall level of degradation appears to decline with increasing levels of chlorination and that the substances tested contain potentially persistent congeners. However, these screening studies are not considered appropriate for assessing and concluding on the persistence properties of UVCB substances such as MCCP and their constituents, as without further supplementary information enabling the possibility for the dossier submitter to verify the claims made with regard to the composition of the test substance, i.e. the identity of the individual congener groups and their concentration in the substance as well as on the degree of degradation of the individual congener groups in a test, it is not possible to draw conclusions on the persistence of the constituents of MCCP. Therefore the outcomes of the screening tests for MCCP have been assigned low weight in the WoE;
- Hydrolysis of MCCP is expected to be negligible in the environment. Photodegradation in air for MCCP congeners is unlikely to be a significant degradation pathway in the environment (estimated atmospheric half-lives in the range of 0.6–7.1 days for some of the MCCP congener groups). As a conclusion, abiotic degradation of MCCP and MCCP congeners is not considered to be a significant degradation pathway in the environment;
- Monitoring data support findings from experimental and predicted data on biodegradation and abiotic degradation of MCCP congeners and MCCP. The available monitoring data, particularly from sediment core studies, suggest some dechlorination of chlorinated paraffins with high chlorine contents in sediment over time, but they also suggest that degradation in the environment may be slow and provide indirect evidence that MCCP with chlorine contents of ~ 55% by weight can persist in sediments for more than a decade. The detection and/or quantification of MCCP in marine sediments from the Arctic, in locations far away from point sources, point towards persistence of MCCP in marine sediments under aerobic conditions.

As an overall conclusion, based on the above information used in a weight-of-evidence-approach, it is concluded that the $C_{14}Cl_{3–14}$ congener groups of MCCP (equivalent to 35.32–72.98% Cl wt.) meet the ‘persistence’ criterion (P) and the ‘very persistent’ criterion (vP) in accordance with Annex XIII, points 1.1.1 and 1.2.1, of the REACH Regulation on the basis of their persistent and very persistent (P/vP) properties in sediment (degradation half-lives > 180 days).

Based on the predicted and observed trends in physico-chemical properties it further can be reasonably estimated that also the C_{15-17} congener groups of MCCP with the same or higher chlorine contents than the congeners present in C_{14} chlorinated n-alkane, 50% Cl. wt. (which contains $C_{14}Cl_{3-14}$ congener groups that all are P/vP) will at least be equally if not more persistent in sediment than the congeners of C_{14} chlorinated n-alkane, 50% Cl. wt. Consequently, it is concluded that also the $C_{15}Cl_{3-15}$, $C_{16}Cl_{3-16}$ and $C_{17}Cl_{3-17}$ congener groups of MCCP meet the ‘persistence’ (P) and ‘very persistent’ (vP) criteria of REACH Annex XIII (degradation half-life in sediment > 180 days).

Finally, since MCCP always will contain congener groups with P/vP properties at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet both the ‘persistence’ (P) and ‘very persistent’ (vP) criteria of REACH Annex XIII (degradation half-life in sediment > 180 days).

Monitoring data on MCCP support the above conclusions as they point towards persistence of MCCP in sediments.

Bioaccumulation

The assessment and conclusions on bioaccumulation are based on the following information. The results of the studies having been given a high weight in the WoE[25] are considered to provide sufficient evidence to conclude the congeners of MCCP present in the test material used in these studies as B and/or vB. The results of the other experimental studies and the QSAR predictions are used as supplementary supporting information to conclude in the WoE approach applied.

- An OECD TG 305 study (dietary exposure) performed on C_{14} chlorinated n-alkane, 50% Cl. wt. indicates a high bioaccumulation potential with lipid-normalised kinetic fish BCF values > 5000 for $C_{14}Cl_{5-11}$ (based on the less conservative scenario with $k_g=0$, see further information in Table 40). This study is given a high weight and its results are used to conclude that the $C_{14}Cl_{5-11}$ congener groups have B/vB properties;
- An OECD TG 305 study (aqueous exposure) performed on C_{14} chlorinated n-alkane, 45% Cl wt. (which contains $C_{14}Cl_{3-6}$ congener groups) indicates a high bioaccumulation potential with a lipid-normalised and growth-corrected kinetic fish BCF value of ca. 11 530 L/kg. This study is given a high weight and its results are used to conclude that the $C_{14}Cl_{3-6}$ congener groups have B/vB properties;
- An OECD TG 305 study (aqueous exposure) performed on C_{15} chlorinated n-alkane, 51% Cl wt. (which contains $C_{15}Cl_{5-8}$ congener groups) indicates a bioaccumulation potential with a growth-corrected kinetic fish aquatic BCF of around 1 833 – 2 072 L/kg. The growth corrected depuration half-lives are between 28 to 36 days. The results of this study are used as part of the weight-of-evidence to conclude that the $C_{15}Cl_{5-8}$ congener groups have B and/or vB properties;
- Toxicokinetic data on mammals using radiolabelled MCCP indicate that absorption following oral exposure is significant. MCCP have been demonstrated to have relatively long elimination or depuration half-lives in fish and mammals (growth corrected depuration half-lives in the range of 29–80 days in rainbow trout and half-life up to 8 weeks in abdominal fat of rats). These long elimination half-lives mean that significant concentrations of the substance may remain within an organism for several months, possibly years, after cessation of emission. Based on the outcome of dietary accumulation studies equivalent to OECD TG 305, experimental depuration rate constants for MCCP congeners were used in order to predict BCF values based on the work by Brooke and Crookes, which 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 as growth-corrected depuration rate constants between 0.009–0.024 day^{-1} were found for $C_{14}H_{26}Cl_4$, $C_{14}H_{25}Cl_5$, $C_{14}H_{24}Cl_6$, $C_{14}H_{23.3}Cl_{6.7}$ (with $C_{14}Cl_{5-8}$), $C_{16}H_{31}Cl_3$ (with $C_{16}Cl_{2-5}$) and $C_{16}H_{21}Cl_{13}$ (with $C_{16}Cl_{12-15}$) congener groups. The results of these studies are used as part of the weight-of-evidence to conclude that the $C_{14}Cl_{4-8}$ and $C_{16}Cl_{2-5}$ congener groups have B/vB properties. For the remaining groups of congeners ($C_{16}H_{21}Cl_{13}$ with $C_{16}Cl_{12-15}$ as chlorination range) present in the tested substances, it is not possible to conclude on their potential for bioaccumulation since insufficient data is available;
- A bioaccumulation study (aqueous and dietary exposure) on *Daphnia magna* indicates a high bioaccumulation potential with lipid-normalised steady-state BCF of 10 000 000 L/kg lipid and steady-state wet weight BCF of ca. 50 119 L/kg ww for a C_{13}-C_{18} 45% Cl wt. product (Cereclor S45; which contains $C_{14}Cl_{4-9}$, $C_{15}Cl_{3-9}$, $C_{16}Cl_{2-8}$ and $C_{17}Cl_{2-9}$ congener groups (including congeners found in Daphnia upon exposure even if not detected in the original substance tested)). The outcome of this study is used as part of the weight-of-evidence to conclude that the $C_{14}Cl_{4-9}$, $C_{15}Cl_{3-9}$, $C_{16}Cl_{2-8}$ and $C_{17}Cl_{5-9}$ congener groups have B and/or vB properties. For the remaining groups of congeners ($C_{17}Cl_{2-4}$) present in the

[25] Details on the weight (or confidence level) given to the experimental studies/data and to the QSAR predictions used in the weight-of-evidence approach are provided in 'Annex X – Experimental and modelling data used as part of a weight-of-evidence (WoE) approach in order to conclude on the bioaccumulation potential of the congener groups of MCCP.

test substance, it is not possible to conclude on their potential for bioaccumulation since insufficient data is available;

- A bioaccumulation study (aqueous and dietary exposure) on *Mytilus edulis* indicates a high bioaccumulation potential with lipid-normalised BAF value of 7 031 L/kg (steady-state value) and 7 204 L/kg (statistically determined) with confidence limits of 4 694–9 723 L/kg for $C_{16}H_{30.7}Cl_{3.3}$ (34.1% Cl wt.; which contains $C_{16}Cl_{2-5}$). The results of this study are used as part of the weight-of-evidence to conclude that the $C_{16}Cl_{2-5}$ congener groups have B/vB properties;
- As part of an earthworm toxicity study, uptake of C_{15} chlorinated n-alkane, 51% Cl wt. by earthworms (*Eisenia fetida*) from soil was measured. Based on this study, earthworm-soil accumulation factors (BAFs) of 2.4 for adults and 2.3 for juveniles were determined for C_{15} chlorinated n-alkane, 51% Cl wt. (which contains $C_{15}Cl_{5-8}$ congener groups). The outcome of this study suggests that these group of congeners have bioaccumulative (B) properties in earthworms. The results of this study are used as part of the weight-of-evidence to conclude that the $C_{15}Cl_{5-8}$ congener groups have B and/or vB properties;
- A biomagnification study indicates a high bioaccumulation potential with lipid normalised BMFs >1 in the muscles and livers of a snake-frog predator-prey relationship for the congener groups $C_{14}Cl_{3-11}$, $C_{15}Cl_{3-11}$, $C_{16}Cl_{3-10}$ and $C_{17}Cl_{5-10}$. The results of this study are used as part of the weight-of-evidence to conclude that the $C_{14}Cl_{3-11}$, $C_{15}Cl_{3-9}$, $C_{16}Cl_{3-8}$ and $C_{17}Cl_{5-8}$ congener groups have B and/or vB properties. For other group of congeners ($C_{15}Cl_{10-11}$, $C_{16}Cl_{9-10}$ and $C_{17}Cl_{9-10}$), it is not possible to conclude on their potential for bioaccumulation since insufficient data is available;
- Modelling data are used as supporting information to the experimental data in the bioaccumulation assessment. The BCF Baseline model of CATALOGIC yields BCF predictions for $C_{14}Cl_{2-11}$, $C_{15}Cl_{3-10}$ and $C_{16}Cl_{5-10}$ congener groups which are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and/or log BCF 3.69 (BCF ~ 5000 L/kg) and therefore indicating bioaccumulation potential. Furthermore, all groups of congeners of MCCP meet the screening criterion set out in the PBT Guidance (REACH Chapter R.11; ECHA, 2017b) for aquatic organisms as being potentially 'bioaccumulative' (B) and/or 'very bioaccumulative' (vB) with a range of log Kow > 4.5.
- The available (limited) field bioaccumulation studies for MCCP are equivocal: trophic magnification factors below and above 1 have been derived.
- Monitoring data support findings from experimental and predicted data on bioaccumulation of MCCP congeners and MCCP. MCCP have been detected in human blood and milk samples which indicates that MCCP are absorbed to some extent in humans. Detection of MCCP in umbilical cord blood and placenta indicates that MCCP can be transferred to the foetus. Furthermore, monitoring data demonstrate widespread contamination of wildlife by MCCP at all trophic levels (including predatory species). MCCP have also been detected in samples from remote regions, including the Arctic. These data provide supporting evidence that MCCP are taken up by organisms in the environment.

Based on the weight of evidence of the data available, it can be concluded that the $C_{14}Cl_{3–11}$ congener groups of MCCP (equivalent to 35.3–67.6% Cl wt.) have B/vB properties, $C_{15}Cl_{3–9}$ congener groups of MCCP (equivalent to 33.8–61.15% Cl wt.) have B and/or vB properties, $C_{16}Cl_{2–9}$ congener groups of MCCP (equivalent to 24.1–59.55% Cl wt.) have B and/or vB properties and $C_{17}Cl_{5–9}$ congener groups of MCCP (equivalent to 43–58% Cl wt.) have B properties in accordance with REACH Annex XIII. For other congener groups of MCCP, it is not possible to conclude on their potential for bioaccumulation due to the lack of appropriate data.

Based on the information available, as MCCP contain congener groups with B and/or vB properties at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet the 'bioaccumulation' criterion (B) and the 'very bioaccumulative' criterion (vB) in accordance with Annex XIII, points 1.1.2 and 1.2.2, of the REACH Regulation.

Monitoring data on MCCP support the above conclusions as they point towards bioaccumulation of MCCP in biota.

Toxicity

Only limited experimental information is available on the aquatic toxicity of individual MCCP congeners. The majority of the ecotoxicity data is available for the commercial C_{14-17}, 52% Cl wt. substance.

48h EC_{50} results from acute *Daphnia magna* studies fall in the range < 6.5 – 2200 µg/L. The most reliable result is 48h EC_{50} 5.9 µg/L for the C_{14-17}, 52% Cl wt. substance. According to the PBT guidance (REACH Chapter R.11, ECHA, 2017b), a short-term aquatic toxicity result in fish, daphnia, or algae with EC_{50} or LC_{50} < 0.01 mg/L (≈ 10 µg/L) is sufficient to meet the T criterion. Based on this guidance, the T criterion is met.

For the chronic toxicity of MCCP to *Daphnia magna*, 21d NOEC (reproduction) values range from ~ 4 - 15.6 µg/L. The most reliable result is 21d NOEC 8.7 µg/L for the C_{14-17}, 52% Cl wt. substance which meets the toxicity criterion (T) in accordance with Annex XIII, point 1.1.3 (a), of the REACH Regulation.

For a UVCB substance like MCCP, observed toxicity may represent toxicity of one or more of its constituents. As the testing material of the acute and chronic toxicity studies available for MCCP contained several groups of congeners of MCCP and no testing and analysis was performed at the level of the congener groups, it is not possible to identify whether the congener groups present in the tested substance contributed differently to the observed toxicity.

However, the congener groups expected to be present in the test material for both these tests are C_{14} congener groups having 4, 5, 6 and 7 chlorine atoms; C_{15-16} congener groups having 5, 6, 7 and 8 chlorine atoms and C_{17} congener groups having 6, 7, 8 and 9 chlorine atoms. These same congener groups have been detected in *Daphnia magna* in a bioaccumulation test reported in Section 3.4.2.3 Other supporting data. This indicates that these congener groups are bioavailable to *Daphnia magna* and taken up by this organism. Since these congener groups are structurally very similar (they differ only in carbon chain length and number of chlorine substituents), they can be expected to exert toxic effects by the same mode(s) of action. It is therefore reasonable to assume that all congener groups present in the C_{14-17}, 52% Cl wt. test substance contributed equivalently to the observed toxicity.

It is therefore concluded that MCCP and all the following congener groups of MCCP meet the toxicity criterion (T) in accordance with Annex XIII, point 1.1.3 (a), of the REACH Regulation: C_{14} congeners having 4, 5, 6 and 7 chlorine atoms; C_{15} congeners having 5, 6, 7 and 8 chlorine atoms; C_{16} congeners having 5, 6, 7 and 8 chlorine atoms and C_{17} congeners having 6, 7, 8 and 9 chlorine atoms.

Conclusion on the P, B and T properties

On the basis of all the evidence available, it is concluded that the $C_{14}Cl_{3–11}$ congener groups of MCCP (equivalent to 35.3–67.6% Cl wt.) have PBT and/or vPvB properties, $C_{15}Cl_{3–8}$ congener groups of MCCP (equivalent to 33.8–58.2% Cl wt.) have PBT and/or vPvB properties, $C_{16}Cl_{3–8}$ congener groups of MCCP (equivalent to 32.3–56.6% Cl wt.) have PBT and/or vPvB properties and $C_{17}Cl_{6–9}$ congener groups of MCCP (equivalent to 47.65–58% Cl wt.) have PBT properties in accordance with Annex XIII of the REACH Regulation (see Table 52).

Based on the information available, as MCCP contain congener groups with PBT and/or vPvB properties (see Table 52) at a concentration ≥ 0.1 % (w/w), it is concluded that MCCP meet the criteria for a PBT and/or vPvB substance in accordance with Annex XIII of the REACH Regulation, and thereby they fulfil the criteria set out in REACH Articles 57(d) and/or (e).

(Note - some of the PBT and/or vPvB congener groups of MCCP listed in Table 52 have been identified in other substances than MCCP, thus suggesting that these substances also could be considered to meet the REACH Annex XIII criteria for a PBT and/or vPvB substance if these congener groups are present in a concentration ≥ 0.1 % (w/w)).

Table 52: Congener groups of MCCP concluded as PBT and/or vPvB in accordance with the criteria set out in Annex XIII of the REACH Regulation

Number chlorine atoms and Carbon chain length	Cl_1	Cl_2	Cl_3	Cl_4	Cl_5	Cl_6	Cl_7	Cl_8	Cl_9	Cl_{10}	Cl_{11}	Cl_{12}	Cl_{13}	Cl_{14}	Cl_{15}	Cl_{16}	Cl_{17}
C_{14}	-	-	vPvB	vPvB PBT	vPvB PBT	vPvB PBT	vPvB PBT	vPvB	vPvB	vPvB	vPvB	-	-	-			
C_{15}	-	-	vPvB	vPvB	vPvB PBT	PBT	PBT	PBT	-	-	-	-	-	-	-		
C_{16}	-	-	vPvB	vPvB	vPvB PBT	PBT	PBT	PBT	-	-	-	-	-	-	-	-	
C_{17}	-	-	-	-	-	PBT	PBT	PBT	PBT	-	-	-	-	-	-	-	-

Note: Symbol '-' means that not enough information is available to conclude whether the congener group has PBT and/or vPvB properties. Grey cells means congener groups not considered in the PBT/vPvB assessment.

Summary of other considerations

Based on their physical-chemical properties, some congeners of MCCP are predicted to have long-range environmental transport (estimated atmospheric half-lives in the range of 0.6–7.1 days for different MCCP congeners). Indeed, MCCP have similar physical-chemical properties to legacy persistent organic pollutants (POPs).

Monitoring data tend to confirm this prediction as it has been found that MCCP with C_{14-15} and Cl_{4-9} were found in biota from the Arctic and in air from the Antarctic. MCCP have been detected in various media in the Arctic, including in air from Svalbard, in marine sediments from the Barents Sea and the Norwegian Sea, in terrestrial, avian and marine biota samples from the Norwegian Arctic, including in top predators such as Polar Bears. MCCP were also found in air samples from the Antarctic and from the Tibetan Plateau at high altitude.

The presence of MCCP at sites remote from known point sources such as the Arctic and Antarctic therefore indicates long-range environmental transport.

Furthermore, monitoring data indicate that concentrations of MCCP have increased in biota, in sediment and in air (from the Arctic, the Tibetan Plateau and the Antarctic) during the last decades. In addition, in the Antarctic air, an increasing trend was observed in the ratio of MCCP to SCCP suggesting that the use of MCCP as substitute to SCCP had increased. Due to the PBT/vPvB properties of MCCP, the increasing trend of the concentrations of MCCP in the environment gives reason for concern.

References

Aamir M, Yin S, Zhou Y, Xu C, Liu K, Liu W (2019). Congener-specific C10-C13 and C14-C17 chlorinated paraffins in Chinese agricultural soils: Spatio-vertical distribution, homologue pattern and environmental behaviour. Environmental Pollution, 245, 789 - 798.

Abraham MH, Chadha HS, Dixon JP, Leo AJ (1994). Hydrogen bonding. 39. The partition of solutes between water and various alcohols. Journal of physical Organic chemistry, 7(12), 712–716.

ACD Percepta, ACD/Labs release 2019.2.1, Advanced Chemistry Development, Inc. (2019), http://www.acdlabs.com.

Bakke T, Boitsov S, Brevik EM, Gabrielsen GW, Green N, Helgason LB, Klungsøyr J, Leknes H, Miljeteig C, Måge A, Rolfsnes BE, Savinova T, Schlabach M, Skaare BB, Valdersnes S (2008). Mapping Selected Organic Contaminants in the Barents Sea 2007. SPFO-Report 1021/2008, TA-2400/2008, 2008.

Ballschmiter K (1994). Bestimmung von Kurtz-und Mittelkettigen Chloroparaffinen inWasser-und Sedimentproben aus Oberflächenwässern. Universität Ulm. Abt. Analytische Chemie und Umweltchemie, 10th May 1994.

Barber JL, Sweetman AJ, Thomas GO, Braekevelt E, Stern GA, Jones KC (2005). Spatial and temporal variability in air concentrations of short-chain (C_{10}-C_{13}) and medium-chain (C_{14}-C_{17}) chlorinated n-alkanes measured in the UK atmosphere. Environmental Science & Technology, 39(12), 4407 – 4415.

Barber MC (2001). Bioaccumulation and Aquatic System Simulator (BASS) User's Manual – Beta Test Version 2.1. EPA Report No. 600/R-01/035. United States Environmental Protection Agency (US - EPA), Athens, Georgia, USA.

Barber MC (2003). A review and comparison of models for predicting dynamic chemical bioconcentration in fish. Environmental Toxicology and Chemistry, 22, 1963 - 1992.

Barber MC, Suarez LA, Lassiter RR (1991). Modelling bioaccumulation of organic pollutants in fish with an application to PCBs in Lake Ontario salmonids. Canadian Journal of Fisheries and Aquatic Sciences, 48, 318 – 337.

Basconcillo LS, Backus SM, McGoldrick DJ, Zaruk D, Sverko E, Muir DCG (2015). Current status of short- and medium chain polychlorinated n-alkanes in top predatory fish across Canada. Chemosphere 127 (2015) 93–100.

Bengtsson BE, Svanberg O, Linden E, Lunde G *and* Ofstad EB, 1979. Structure related uptake of chlorinated paraffins in bleaks (*Alburnus-alburnus L*). Ambio, 8, 121–122.

Bennie DT, Sullivan CA, Maguire RJ (2000). Occurrence of chlorinated paraffins in beluga whales (*Delphinapterus leucas*) from the St. Lawrence River and rainbow trout (*Oncorhynchus mykiss*) and carp (*Cyprinus carpio*) from Lake Ontario. Water Quality Research Journal of Canada, 35, 263 - 281.

Biessmann A, Brandt I and Darnerud PO (1982). Comparitive distribution and metabolism of two 14C-labelled chlorinated paraffins in Japanese quail Coturnix coturnix japonica. Environmental Pollution Series A, Ecological and Biological, 28, 109–120. https://doi.org/10.1016/0143-1471(82)90097-6.

Biessmann A, Darnerud PO and Brandt I (1983). Chlorinated paraffins: disposition of a highly chlorinated polychlorohexadecane in mice and quail. Archives of Toxicology, 53, 79–86.

https://doi.org/10.1007/BF01460004.

Birtley RDN, Conning DM, Daniel JW, Ferguson DM, Longstaff E *and* Swan AAB (1980). Toxicological effects of chlorinated paraffins in mammals. Toxicology and Applied Pharmacology, 54, 514–525. https://doi.org/10.1016/0041-008x(80)90179-9.

Björklund K, Strömvall A-M, Malmqvist P-A (2011). Screening of organic contaminants in urban snow. Water Science & Technology, 64, 206 - 213.

Bogdal C, Alsberg T, Diefenbacher PS, Macleod M, Berger U (2015). Fast quantification of chlorinated paraffins in environmental samples by direct injection high-resolution mass spectrometry with pattern deconvolution. Anal. Chem., 87, 2852-2860.

Bogdal C, Niggeler N, Glüge J, Diefenbacher PS, Wächter D, Hungerbühler K (2017). Temporal trends of chlorinated paraffins and polychlorinated biphenyls in Swiss soils. Environmental Pollution, 220 Part B, 891 - 899.

Bohlin-Nizzetto P, Aas W, Nikiforov V (2020). Monitoring of environmental contaminants in air and precipitation, Annual report 2019. NILU report 06/2020, Norwegian Environment Agency, M-1736|2020. ISBN: 978-82-425-3003-5

Boitsov S, Klungsøyr J, Jensen HKB (2016). Pilotstudie av nye organiske miljøgifter i sedimenter fra MAREANO-området. Institute of Marine Research. Rapport: Prosjektrapport–Rapport fra Havforskningen nr. 37-2016. ISSN: 1893-4536. Dato: Desember 2016. Program: MAREANO. The Report is available in Norwegian only at: https://www.hi.no/resources/publikasjoner/rapport-fra-havforskningen/2016/rapport_pilotstudie_2016_ver_6.pdf

Boitsov S and Klungsøyr J (2018). Hydrocarbons and organic contaminants in sediments from the MAREANO area in 2017. Report series: Report from Marine Research 41-2018. ISSN: 1893-4536. Date of publication: 10.12.2018. Research group: Environmental Chemistry Project. Project: MAREANO. The Report is available in Norwegian only at: https://www.hi.no/resources/publikasjoner/Rapport-fra-Havforskningen-MAREANO-2018.2-TIL-PUBL-rett.24.10.19_.pdf

Boitsov S, Klungsøyr J, Nesje G (2019). Hydrocarbons and organic contaminants in sediments from the MAREANO area in 2018. Report series: Report from Marine Research 2019-50. ISSN: 1893-4536. Date of publication: 16.12.2019. Project no: 15312-02. Client (s): MAREANO program. Program: Marine processes and human impact. The Report is available in Norwegian only at: https://www.hi.no/hi/nettrapporter/rapport-fra-havforskningen-2019-50

Boitsov S and Sanden M (2020). Hydrocarbons and organic contaminants in sediments from the MAREANO area in 2019. Report series: Report from Marine Research 2020-47. ISSN: 1893-4536. Date of publication: 10.12.2020. Project no: 15312-02. Client (s): MAREANO program. Program: Marine processes and human impact. The Report is available in Norwegian only at: https://www.hi.no/hi/nettrapporter/rapport-fra-havforskningen-2020-47

Boitsov S (2021). Personal Communication (by e-mail) from Boitsov S to the European Chemicals Agency, January 2021.

Borgen AR, Schlabach M, Kallenborn R, Fjeld E (2001). Polychlorinated alkanes in freshwater fish. Organohalog Compd 2001;52:75–9.

Brandsma SH, van Mourik L, O'Brien JW, Eaglesham G, Leonards PEG, de Boer J, Gallen C, Mueller J, Gaus C, Bogdal C (2017). Medium-chain chlorinated paraffins (CP) dominate in Australian sewage sludge. Environmental Science & Technology, 51, 6, 3364 - 3372.
Brooke DN and Crookes MJ (2011). Case study on toxicological interactions of chlorinated

paraffins. UNEP/POPS/POPRC.7/INF/15, Stockholm Convention on Persistent Organic Pollutants.

Brooke D and Crookes M (2012). Depuration rate constant: growth correction and use as an indicator of bioaccumulation potential. Environment Agency, UK. October 2012. ISBN: 978-1-84911-283-3. Available at https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/291525/LIT_7371_44228a.pdf

Brooke DN, Crookes MJ, Merckel DAS (2012). Methods for predicting the rate constant for uptake of organic chemicals from water by fish. Environmental Toxicology and Chemistry, 31(11), 2465 - 2471.

Brown TN, Arnot JA and Wania F (2012). Iterative Fragment Selection: A Group Contribution Approach to Predicting Fish Biotransformation Half-Lives Environ. Sci. Technol., 46(15), 8253–8260.

BUA (1992). Chlorinated paraffins. GDCh - Advisory Committee on Existing Chemicals of Environmental Relevance (BUA). BUA Report 93, June 1992.

Campbell I and McConnell G (1980). Chlorinated paraffins and the environment. 1. Environmental Occurrence. Environmental Science & Technology, 9, 1209 - 1214.

Castro M, Breitholtz M, Yuan B, Athanassiadis I, Asplund L, Sobek A (2018). Partitioning of chlorinated paraffins (CPs) to *Daphnia magna* overlaps between restricted and in-use categories. Environmental Science & Technology, 52, 9713−9721.

Castro M, Sobek A, Yuan B, Breitholtz M (2019). Bioaccumulation potential of CPs in aquatic organisms: Uptake and depuration in *Daphnia magna*. Environmental Science and Technology, 53, 9533−9541.

Castro M, (2020). Chlorinated Paraffins: improved understanding of their bioaccumulation and toxicity in *Daphnia magna*. Department of Environmental Science. Stockholm University, Stockholm, ISBN 978-91-7911-072-7, ISBN 978-91-7911-073-4, http://www.diva-portal.org/smash/record.jsf?pid=diva2%3A1416211&dswid=-4440

Castro M, Personal Communication, 2020: Personal Communication (by e-mail) from Castro M to the European Chemicals Agency, December 2020.

Castro M, Personal Communication, 2021: Personal Communication (by e-mail) from Castro M to the European Chemicals Agency, January 2021.

Cefas (1999). Sampling the Levels of Short and Medium Chain Chlorinated Paraffins in the Environment. Final Report for the Department of the Environment, Transport and the Regions. The Centre for Environment, Fisheries and Aquaculture Science, Burnham-on-Crouch.

Chaemfa C, Xu Y, Li J, Chakraborty P, Syed JH, Malik RN, Wang Y, Tian C, Zhang G, Jones KC (2014). Screening of atmospheric short- and medium- chain chlorinated paraffins in India and Pakistan using polyurethane foam based passive air sampler. Environmental Science & Technology, 48, 4799 - 4808.

Chen MY, Luo XJ, Zhang XL, He MJ, Chen SJ, Mai BX (2011). Chlorinated paraffins in sediments from the Pearl River Delta, South China: Spatial and temporal distributions and implication for processes. Environmental Science & Technology, 45, 9936 - 9943.

CPIA (2000). Personal Communication from the Chlorinated Paraffins Industry Association to the Environment Agency, UK.

Coelhan M (2009). Determination of chlorinated paraffins in water samples. Organohalogen Compounds, 71, 1276 - 1280.

Coelhan M (2010). Levels of chlorinated paraffins in water. CLEAN - Soil Air Water, 38, 452 - 456.

Cooley HM, Fisk AT, Weins SC, Tomy GT, Evans RE, Muir DCG (2001). Examination of the behaviour and liver and thyroid histology of juvenile rainbow trout (*Oncorhynchus mykiss*) exposed to high dietary concentrations of C10- , C11- , C12- and C14- polychlorinated n-alkanes. Aquatic Toxicology, 54, 81 - 99.

CXR Biosciences Ltd (2003) Powrie RH. Effects of Medium Chain Chlorinated Paraffins (MCCPs) on Vitamin K Concentrations and Clotting Factors in Female Sprague Dawley Rats. *Unpublished report*.

CXR Biosciences Ltd (2004) Barton Sjand Daly PM. MCCP – Study to Assess Maternal Milk and Neonate Plasma. *Unpublished report*.

CXR Biosciences Ltd (2005a). A Dietary Study to Investigate the Toxicokinetics of Medium Chain Chlorinated Paraffins (Cerechlor S52) in Male and Female Fisher 344 Rats. CXR0282. CXR Biosciences Ltd., Dundee, UK. *Unpublished report*.

CXR Biosciences Ltd (2005b) Elcombe BM. A Dietary Study to Determine the 90 day NOAEL of Medium Chain Chlorinated Paraffins (Cereclor S52) in Male and Female Fisher 344 Rats. CXR0273. CXR Biosciences Ltd, Dundee, UK. *Unpublished report*.

CXR Biosciences Ltd (2006) Stamp SL. C_{14-17} n-Alkane, 52% Chlorinated Study of Post-natal Offspring Mortality Following Dietary Administration to CD Tats. DAR0001/062390. Huntingdon Life Sciences Ltd., Huntingdon, UK. *Unpublished report*.

Darnerud PO and Brandt I (1982). Studies on the distribution and metabolism of a ^{14}C-labeled chlorinated alkane in mice. Environmental Pollution Series a-Ecological and Biological, 27, 45–56. https://doi.org/10.1016/0143-1471(82)90062-9.

Darnerud PO, Bengtsson BE, Bergman A *and* Brandt I (1983). Chlorinated paraffins: disposition of a polychloro-[1-^{14}C]-hexadecane in carp (*Cyprinus carpio*) and bleak (*Alburnus alburnus*). Toxicology Letters, 19, 345–351. https://doi.org/10.1016/0378-4274(83)90141-8.

Darnerud PO, Bergman A, Lund BO *and* Brandt I (1989). Selective accumulation of chlorinated paraffins (C_{12} and C_{16}) in the olfactory organ of rainbow-trout. Chemosphere, 18, 1821–1827. https://doi.org/10.1016/0045-6535(89)90466-9.

de Wit CA, Bossi R, Dietz R, Dreyer A, Faxneld S, Garbus SE, Hellström P, Koschorreck J, Lohmann N, Roos A, Sellström U, Sonne C, Treu G, Vorkamp K, Yuan B, Eulaers I (2020). Organohalogen compounds of emerging concern in Baltic Sea biota: Levels, biomagnification potential and comparisons with legacy contaminants. Environment International, 144, 106037.

Diem K and Lentner C (1971). Scientific Tables, 7th Ed. Ciba Geigy, Basel.

Dimitrov S, Georgieva DG, Pavlov TS, Karakolev YH, Karamertzanis PG, Rasenberg M and Mekenyan OG (2015). UVCB substances: methodology for structural description and application to fate and hazard assessment. Environmental Toxicology and Chemistry, 34, 2450-62.

Drouillard KG, Tomy GT, Muir DCG, Friesen KJ (1998). Volatility of chlorinated n-alkanes (C_{10-12}): vapour pressures and Henry's Law constants. Environmental Toxicology and Chemistry, 17, 1252 - 1260.

Du X, Yuan B, Zhou Y, Benskin JP, Qiu Y, Yin G, Zhao J (2018). Short-, medium-, and long-chain chlorinated paraffins in wildlife from paddy fields in the Yangtze River delta. Environmental Science & Technology, 52, 1072−1080.

Du X, Yuan B, Zhou Y, de Wit C A, Zheng Z, Yin G (2020). Chlorinated Paraffins in Two Snake Species from the Yangtze River Delta: Tissue Distribution and Biomagnification. Environmental Science & Technology, 54(5), 2753-2762.

Du X, Yuan B, Zhou Y, Zheng Z, Wu Y, Qiu Y, Zhao J, Yin G (2019). Tissue-specific accumulation, sexual difference, and maternal transfer of chlorinated paraffins in Black-Spotted Frogs. Environmental Science and Technology, 53, 4739–4746.

EA [The UK Environment Agency] (2009). Environmental risk assessment: long-chain chlorinated paraffins. Science report. January 2009. Available at: https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/290855/scho0109bpgr-e-e.pdf

EA (2010). Conclusion of Substance Evaluation for Transitional Dossiers for Medium-chain Chlorinated Paraffins. Available at: https://echa.europa.eu/documents/10162/13628/alkanes_MCCP_pbtsheet_en.pdf/d503f71c-f7fa-4db8-bdf2-7497d372e2c9

EA (2011). Estimation of fish bioconcentration factor (BCF) from depuration data. Environment Agency Science Report, SCHO0811BUCE-E-E, Bristol, UK. Accessed at: https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/291527/scho0811buce-e-e.pdf

EA (2012a). Depuration Rate Constant as an Indicator of Bioaccumulation Potential. Environment Agency, Bristol, UK. Available from https://www.gov.uk/government/uploads/system/uploads/attachment_data/file/291525/LIT_7371_44228a.pdf

EA (2019). Substance evaluation conclusion and evaluation report for Medium-chain chlorinated paraffins /Alkanes, C_{14-17}, chloro EC No 287-477-0, Environment Agency, December 2019 available at: https://echa.europa.eu/information-on-chemicals/evaluation/community-rolling-action-plan/corap-table/-/dislist/details/0b0236e1807e3841

EC [European Communities] (2000). European Union Risk Assessment Report: Alkanes, C_{10-13}, chloro-. 1st Priority List, Volume 4. European Commission Joint Research Centre, EUR 19101 EN. Accessed at: https://echa.europa.eu/documents/10162/f343cb93-2c44-4f19-91e8-4c0730edf604

EC (2005). European Union Risk Assessment Report: Alkanes, C_{14-17}, Chloro- . 3rd Priority List, Volume 58. European Commission Joint Research Centre, EUR 21640 EN. Accessed at: https://echa.europa.eu/documents/10162/584faee8-d13a-41dd-8b33-959ad1a81171

EC (2007). Updated Risk Assessment of Alkanes, C_{14-17}, Chloro- (Medium-chain Chlorinated Paraffins). Draft Enviropnment Addendum of August 2007. Available at: https://echa.europa.eu/documents/10162/d317126f-75bc-4ba6-a8be-7ecaa2a96656.

ECHA (2008). Member State Committee Support document for identification of Alkanes, C_{10-13}, Chloro (EC Number: 287-476-5; CAS Number: 85535-84-8) as a substance of very high concern. Adopted on 8 October 2008. Available at: https://echa.europa.eu/documents/10162/2edcfedb-ec53-4754-8598-e787a8ff7a58

EC (2011). European Union Risk Assessment Report. Alkanes, C_{14-17}, chloro (MCCP). Part II – human health. CAS No: 85535-85-9. EINECS No: 287-477-0. European Chemicals Bureau.

Institute for Health and Consumer Protection. Available online: http://publications.jrc.ec.europa.eu/repository/

ECHA (2012a). Member State Committee Support document for identification of Tricosafluorododecanoic acid (EC Number: 206-203-2; CAS Number: 307-55-1) as a substance of very high concern because of its vPvB properties. Adopted on 13 December 2012. Available at: https://echa.europa.eu/documents/10162/44fd0731-2211-0216-b984-e3cd0f32d5ca

ECHA (2012b). Member State Committee Support document for identification of Heptacosafluorotetradecanoic acid (EC Number: 206-803-4; CAS Number: 376-06-7) as a substance of very high concern because of its vPvB properties. Adopted on 13 December 2012. Available at: https://echa.europa.eu/documents/10162/08046ee8-0933-a564-0df2-da48cda2bc6b

ECHA (2012c). Member State Committee Support document for identification of Henicosafluoroundecanoic acid (EC Number: 218-165-4; CAS Number: 2058-94-8) as a substance of very high concern because of its vPvB properties. Adopted on 13 December 2012. Available at: https://echa.europa.eu/documents/10162/9bcff514-6625-baa9-edd9-80ee9e82c86a

ECHA (2014). Decision on substance evaluation pursuant to article 46(1) of regulation (EC) NO 1907/2006 for alkanes, C14-17, chloro (MCCP, Medium-chain, chlorinated paraffins), CAS No 85535-85-9 (EC No 287-477-0). Accessed at: https://echa.europa.eu/documents/10162/d489cc70-7b49-46d8-b208-56e5b738a35e

ECHA (2015). Decision of the Board of Appeal of the European Chemicals Agency, 09 September 2015. Case number: A-004-2014. Accessed at https://echa.europa.eu/documents/10162/bcc34f8d-ce53-48cd-9f17-605ad512853a

ECHA (2015a). Member State Committee (MSC) Opinion on persistency and bioaccumulation of Octamethylcyclotetrasiloxane (D4) EC Number: 209-136-7; CAS Number: 556-67-2 and Decamethylcyclopentasiloxane (D5) EC Number: 208-764-9; CAS Number: 541-02-6 according to a MSC mandate. Adopted on 22 April 2015. Available at: https://echa.europa.eu/documents/10162/13641/art77-3c_msc_opinion_on_d4_and_d5_20150422_en.pdf

ECHA (2017a). Guidance on Information Requirements and Chemical Safety Assessment Chapter R.7b: Endpoint specific guidance Version 4.0. June 2017.

ECHA (2017b). Guidance on Information Requirements and Chemical Safety Assessment Chapter R.11: PBT/vPvB assessment Version 3.0. June 2017.

ECHA (2017c). Guidance on Information Requirements and Chemical Safety Assessment Chapter R.7c: Endpoint specific guidance Version 3.0. June 2017.

ECHA (2017d). Member State Committee Support document for identification of Benz[a]anthracene (EC Number: 200-280-6; CAS Number: 56-55-3) as a substance of very high concern because of its carcinogenic (Article 57(a)), PBT (Article 57(d)) and vPvB (Article 57 (e)) properties. Adopted on 30 November 2017. Available at: https://echa.europa.eu/documents/10162/75ad552f-1e59-2599-e379-55ecec998d3f

ECHA (2017e). Member State Committee Support document for identification of Dechlorane plus as a substance of very high concern because of its vPvB properties (Article 57 (e)). Adopted on 30 November 2017. Available at: https://echa.europa.eu/documents/10162/97b3c3bf-f38a-f3e2-6b53-45654bcc02dc

ECHA (2018a). Member State Committee Support document for identification of

dodecamethylcyclohexasiloxane (D6) (EC Number: 208-762-8CAS Number: 540-97-6) (as a substance of very high concern because of its PBT and vPvB properties (Article 57 (d) and (e)). Adopted on 13 June 2018. Available at: https://echa.europa.eu/documents/10162/a9682f4b-fc3e-cd99-3db9-b0f9f383c3c5

ECHA (2018b). Member State Committee Support document for identification of terphenyl, hydrogenated (EC number: 262-967-7; CAS number: 61788-32-7) as a substance of very high concern because of its vPvB properties (Article 57 (e)). Adopted on 1 June 2018. Available at: https://echa.europa.eu/documents/10162/fb7a9167-7d65-dd4c-2aa2-b8182d4a8e37

EFSA [European Food Safety Authority] (2020). Scientific opinion on the Risk assessment of chlorinated paraffins in feed and food. EFSA Panel on Contaminants in the Food Chain (CONTAM): Schrenk D, Bignami M, Bodin L, Chipman JK, del Mazo J, Grasl-Kraupp B, Hogstrand C, Hoogenboom LR, Leblanc JC, Nebbia CS, Ntzani E, Petersen A, Sand S, Schwerdtle T, Vleminckx C, Wallace H, Brüschweiler B, Leonards P, Rose M, Binaglia M, Horváth Z, Ramos Bordajandi L and Nielsen E. EFSA Journal 2020; 18(3): 5991, 220 pp. doi: 10.2903/j.efsa.2020.5991. Accessed (23 December 2020) at: https://efsa.onlinelibrary.wiley.com/doi/full/10.2903/j.efsa.2020.5991

Environment Agency Japan (1991). Chemicals in the Environment. Report on Environmental Survey and Wildlife Monitoring of Chemicals in F.Y. 1988 and 1989. Office of Health Studies, Department of Environmental Health, Environment Agency Japan, 1991.

Environment Canada (2008). Follow-up Report on a PSL1 Assessment for Which Data Were Insufficient to Conclude Whether the Substances Were “Toxic” to the Environment and to the Human Health. Chlorinated Paraffins. Accessed at https://www.canada.ca/content/dam/eccc/migration/main/Lcpe-cepa/documents/substances/pc-cp/CP_followup-eng.pdf

Eriksson P *and* Darnerud PO (1985). Distribution and retention of some chlorinated hydrocarbons and a phthalate in the mouse brain during the pre-weaning period. Toxicology, 37, 185–203. https://doi.org/10.1016/0300-483X(85)90082-4.

Erickson RJ and McKim JM (1990a). A model for exchange of organic chemicals at fish gills: Flow and diffusion limitations. Aquatic Toxicology, 18, 175 - 197.

Erickson RJ and McKim JM (1990b). A simple flow-limited model for exchange of organic chemicals at fish gills. Environmental Toxicology and Chemistry, 9, 159 - 165.

Euro Chlor (1999). Chlorinated Paraffins Sector Group. Letter dated 03/10/99 and E-mail dated 29 October 1999 as cited in EC, 2005.

Euro Chlor (2009). Comments from the Chlorinated Paraffins Sector Group of Euro Chlor on: Growth correction of the BCF from medium-chain chlorinated paraffins determined in the OECD 305 method, February 2009.

Evenset A, Christensen GN, Kallenborn R (2005). Selected chlorobornanes, polychlorinated naphthalenes and brominated flame retardants in Bjørnøya (Bear Island) freshwater biota. Environ Pollut 2005; 136:419–30.

Fisk AT, Cymbalisty CD, Bergman A, Muir DCG (1996). Dietary accumulation of C12- and C16- chlorinated alkanes by juvenile rainbow trout (*Oncorhynchus mykiss*). Environmental Toxicology and Chemistry, 15, 1775 - 1782.

Fisk AT, Wiens SC, Webster GRB, Bergman A, Muir DCG (1998a). Accumulation and depuration of sediment-sorbed C12- and C16- polychlorinated alkanes by oligochaetes (*Lumbriculus variegatus*). Environmental Toxicology and Chemistry, 17, 2019 - 2026.

Fisk AT, Cymbalisty CD, Tomy GT, Muir DCG (1998b). Dietary accumulation and depuration of individual C10- , C11- and C14- polychlorinated alkanes by juvenile rainbow trout (*Oncorhynchus mykiss*). Aquatic Toxicology, 43, 209 - 221.

Fisk AT, Tomy GT, Cymbalisty CD, Muir DCG (2000). Dietary accumulation and quantitative structure-activity relationships for depuration and biotransformation of short (C10), medium (C14) and long (C18) carbon-chain polychlorinated alkanes by juvenile rainbow trout (*Oncorhynchus mykiss*). Environmental Toxicology and Chemistry, 19, 1508 - 1516.

Fjeld E, Schlabach M, Berge JA, Green N, Eggen T, Snilsberg P, Vogelsang C, Rognerud, Kjellberg G, Enge EK, Dye C and Gundersen H (2005). Survey of Select New Organic Pollutants in 2004. Brominated Flame Retardants, Perfluoroalkyl Substances, Irgarol, Diuron, BHT and Dicofol. SFT TA-2096/2005.

FOCUS (2014). Generic guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration. Report of the FOCUS Work Group on Degradation Kinetics.18 December 2014. Version 1.1, 440 pp. Available at: http://eusoils.jrc.ec.europa.eu/public_path/projects_data/focus/dk/docs/FOCUSkineticsvc1.1Dec2014.pdf

Fridén UE, McLachlan MS, Berger U (2011). Chlorinated paraffins in indoor air and dust: concentrations, congener patterns, and human exposure. Environ. Int., 37, 1169 - 1174.

Frank U (1993). Ökotoxizität von Chloroparaffinen. Institut für Wasser- Boden und Lufthygiene, 23 November, 1993. *Unpublished report*.

Frank U and Steinhäuser FG (1994). Ökotoxizität schwerlöslicher stoffgemische am biespiel der daphnientoxizität von chlorparaffinen. Vom Wasser, 83, 203 - 211.

Gao W, Cao DD, Wang YJ, Wu J, Wang Y, Wang YW, Jiang GB (2018). External exposure to short- and medium-chain chlorinated paraffins for the general population in Beijing, China. Environ. Sci. Technol. 52, 32−39.

Gawor A and Wania F (2013). Using quantitative structural property relationships, chemical fate models, and the chemical partitioning space to investigate the potential for long range transport and bioaccumulation of complex halogenated chemical mixtures, Environ. Sci.: Process. Impacts, 15, 1671−1684.

Glüge J, Bogdal C, Scheringer M, Buser AM, Hungerbühler K (2013). Calculation of physicochemical properties for short- and medium-chain chlorinated paraffins. Journal of Physical and Chemical Reference Data, 42, 023103.

Glüge J, Schinkel L, Hungerbuehler K, Cariou R and Bogdal C (2018). Environmental risks of medium-chain chlorinated paraffins (MCCP) - A review. Environmental Science & Technology, 52(12), 6743 - 6760.

Green NW, Schøyen M, Hjermann DØ, Øxnevad S, Ruus A, Lusher A, Beylich B, Lund E, Tveiten L, Håvardstun J, Jenssen MTS, Ribeiro AL, Bæk K (2018). Contaminants in Coastal Waters of Norway 2017. The Norwegian Environment Agency. ISBN 978-82-577-7037-2.

Green NW, Schøyen M, Hjermann DØ, Øxnevad S, Ruus A, Lusher A, Beylich B, Lund E, Tveiten L, Jenssen MTS, Håvardstun J, , Ribeiro AL, Doyer I, Rundberget JT, Bæk K (2019). Contaminants in Coastal Waters of Norway 2018. The Norwegian Environment Agency. ISBN 978-82-577-7147-8.

Greenpeace (1995). Greenpeace Zur Sache: Chloroparaffine, May 1995.

Harju M, Herzke D, Kaasa H (2013). Perfluorinated alkylated substances, brominated flame retardants and chlorinated paraffins in the Norwegian Environment – Screening 2013. NILU-report OR 31/2013: 105. Available at: https://www.nilu.com/wp-content/uploads/dnn/31-2013-dhe-pfas-screening-mildir-versjon.pdf

Hayton WL and Barron MG (1990). Rate-limiting barriers to xenobiotic uptake by the gill. Environmental Toxicology and Chemistry, 9, 151 - 157.

Heeb NV, Schalles S, Lehner S, Schinkel L, Schilling I, Lienemann P, Bogdal C, Kohler HPE (2019). Biotransformation of short-chain chlorinated paraffins (SCCPs) with LinA2: A HCH and HBCD converting bacterial dehydrohalogenase. Chemosphere, 226, 744 - 754.

Heimstad ES, Nygård T, Herzke D, Bohlin-Nizzetto P (2018) Environmental Pollutants in the Terrestrial and Urban environment. NILU - Norwegian Institute for Air Research. NILU OR 20/2018. NILU project no. O-117065.

Hendriks AJ, van der Linde A, Cornelissen G, Sijm DTHM (2001). The power of size. 1. Rate constants and equilibrium ratios for accumulation of organic substances related to octanol-water partition ratio and species weight. Environmental Toxicology and Chemistry, 20, 1399 - 1420.

Herzke D, Kaasa H, Gravem F, Gregersen H, Jensen JGB, Hveding ØP, Horn JE, Sagerup K, Christensen GN, Gabrielsen GW, Hansen SA, Harju M, Katsoyiannis A, Borgen AR, Enge EK, Warner N, Heimstad ES (2013). Perfluorinated alkylated substances, brominated flame retardants and chlorinated paraffins in the Norwegian Environment - Screening 2013. M-40-2013. June 2013.

Herzke D, RostKowski P, Harju M, Borgen AR, Christensen-Dalsgaard S (2019). Assessment of additives used in plastic in seabirds. NILU - Norwegian Institute for Air Research. NILU report 1/2019. ISBN: 978-82-425-2962-6.

Hilger B, Fromme H, Völkel W, Coelhan M (2011a). Effects of chain length, chlorination degree, and structure on the octanol-water partition coefficients of polychlorinated n-alkanes. Environmental Science Technology, 45, 7, 2842 - 2849.

Hilger B, Coelhan M, Völkel W (2011b). Determination of chlorinated paraffins in human breast milk by HRGC-ECNI-LRMS. Organohalogen Compounds, 73, 1611 - 1613.

Hoechst AG (1987). Unveröffenlichte Messungen in der Umbebung des Werkes Gersthofen der Hoechst AG. Unveröffentlichte Meßmethode der ICI, modifiziert. Hoechst AG, Frankfurt/Main (as reported in BUA, 1992).

Houde M, Muir DCG, Tomy GT, Whittle DM, Teixeira C, Moore S (2008). Bioaccumulation and trophic magnification of short- and medium- chain chlorinated paraffins in food webs from Lake Ontario and Lake Michigan. Environmental Science & Technology, 42, 3893 - 3899.

HSE [Health & Safety Executive] (2008a). Annex XV Restriction Report: Medium chain chlorinated paraffins (MCCPs). Submitted by: United Kingdom, 30 November 2008. Available at: https://echa.europa.eu/documents/10162/13630/trd_uk_MCCP_en.pdf/99f3adcd-6481-46f7-a3de-3961158fcf94.

HSE (2008b). Risk Assessment of Alkanes, C_{14-17}, chloro (Medium-Chained Chlorinated Paraffins). Draft of February 2008. Available at: https://echa.europa.eu/documents/10162/13630/trd_rar_uk_MCCP_en.pdf/b879f97d-9cea-49e1-9a84-4b3c6a4eb447.

Huang H, Gao L, Qiao L (2017). Bioaccumulation and biomagnification of short and medium-chain polychlorinated paraffins in different species of fish from Liaodong Bay, North China.

Scientific Reports, 7, Article number: 10749.

Huber S, Warner NA, Nygård T, Remberger M, Harju M, Uggerud HT, Kaj L, Hanssen L (2015). A broad cocktail of environmental pollutants found in eggs of three seabird species from remote colonies in Norway. Environmental Toxicology and Chemistry, 34 (6): 1296–1308.

Hussy I, Webster L, Russell M, Moffat C (2012). Determination of chlorinated paraffins in sediments from the Firth of Clyde by gas chromatography with electron capture negative ionisation mass spectrometry and carbon skeleton analysis by gas chromatography with flame ionisation detection. Chemosphere, 88, 292 – 299.

Hüttig J and Oehme M (2005). Presence of chlorinated paraffins in sediments from the North and Baltic Seas. Archives of Environmental Contamination and Toxicology, 49, 449 - 456.

Hüttig J and Oehme M (2006). Congener group patterns of chloroparaffins in marine sediments obtained by chloride attachment chemical ionization and electron capture negative ionization. Chemosphere, 64, 1573 - 1581.

ICI (1992). Personal Communication, as reported in Willis *et al.* (1994).

Iozza S, Müller C E, Schmid P, Bogdal C, Oehme M (2008). Historical profiles of chlorinated paraffins and polychlorinated biphenyls in a dated sediment core from Lake Thun (Switzerland). Environmental Science & Technology, 42, 1045 - 1050.

Iozza S, Schmid P, Oehme M (2009a). Development of a comprehensive analytical method for the determination of chlorinated paraffins in spruce needles applied in passive air sampling. Environmental Pollution, 157, 3218 - 3224.

Iozza S, Schmid P, Oehme M, Bassan R, Belis C, Jakobi G, Kirchner M, Schramm K-W, Kräuchi N, Moche W, Offenthaler I, Weiss P, Simončič P, Knoth W (2009b). Altitude profiles of total chlorinated paraffins in humus and spruce needles from the Alps (MONARPOP). Environmental Pollution, 157, 3225 - 3231.

IRDC (International Research and Development Corporation) (1984c). 13-Week Dietary Toxicity Study in Rats with Combined Excretion, Tissue Level and Elimination Studies/Determination of Excretion, Tissue Level and Elimination after Single Oral (Gavage) Administration to Rats. Chlorinated Paraffin: 52% Chlorination of Intermediate Chain Length n-Paraffins, ^{14}C labeled CP. Sponsor: Chlorinated Paraffin Program. Report No. 438-026/438-023.

IRDC (1985). Chlorinated Paraffin: Reproduction Range-finding Study in Rats. IRDC Report No. 438/049. International Research and Development Corporation, Mattawan, Michigan, USA 49071. *Unpublished report*.

Ismail N, Gewurtz SB, Pleskach K, Whittle FM, Helm PA, Marvin CH and Tomy GT (2009). Brominated and chlorinated flame retardants in Lake Ontario, Canada, lake trout (*Salvelinus namaycush*) between 1979 and 2004 and possible influences of food-web changes. Environmental Toxicology and Chemistry, 28, 910 - 920.

Jansson B, Andersson R, Asplund L, Litzén N, Nylund K, Sellström U, Uvemo U B, Wahlberg C, Wideqvist U, Odsjö T, Olsson M (1993). Chlorinated and brominated persistent organic compounds in biological samples from the environment. Environmental Toxicology and Chemistry, 12, 1163 - 1174.

Jartun M, Fjeld E, Bæk K, Løken KB, Rundberget T, Grung M, Schlabach M, Warner NA, Johansen I, Lyche JL, Berg V, Nøstbakken OJ (2018). Monitoring of environmental contaminants in freshwater ecosystems', The Norwegian Environment Agency M-1106-2018: 136.

Jiang L, Gao W, Ma X, Wang Y, Wang C, Li Y, Yang R, Fu J, Shi J, Zhang Q, Wang Y, Jiang G (2021). Long-term investigation of the temporal trends and gas/particle partitioning of short- and medium-chain chlorinated paraffins in ambient air of king George Island, Antarctica. Environmental Science & Technology 2021, 55, 230–239. Available at: https://doi.org/10.1021/acs.est.0c05964

Kemmlein S, Hermeneit A, Rotard W (2002). Carbon skeleton analysis of chloroparaffins in sediment, mussels and crabs. Organohalogen Compounds, 59, 279 - 282.

Kirk-Othmer (1993). Chlorocarbons, -Hydrocarbons (paraffins). Encyclopedia of Chemical Technology. Volume 6. Fourth Edition. John Wiley and Sons, Inc.

Klečka G, Persoon C, Currie R (2010). Chemicals of emerging concern in the Great Lakes Basin: An analysis of environmental exposures. Reviews of Environmental Contamination and Toxicology, 207, 1 - 93.

Koh I-O and Thiemann W (2001). Study of photochemical oxidation of standard chlorinated paraffins and identification of degradation products. Journal of Photochemistry and Photobiology A: Chemistry, 139, 2–3, 205 - 215.

Krätschmer K, Schächtele A, Malisch R, Vetter W (2019). Chlorinated paraffins (CP) in salmon sold in southern Germany: Concentrations, homologue patterns and relation to other persistent organic pollutants. Chemosphere, 227, 630 – 637.

Labadie P, Blasi C, Le Menach K, Geneste E, Babut M, Perceval O, Budzinski H (2019). Evidence for the widespread occurrence of short- and medium- chain chlorinated paraffins in fish collected from the Rhône River basin (France). Chemosphere, 223, 232 - 239.

LMC (2018). OASIS Catalogic v. 5.13.1.156. Laboratory of Mathematical Chemistry (LMC), Burgas, Bulgaria.

Li Q, Cheng X, Cui Y, Sun J, Li J, Zhang G (2018). Short- and medium- chain chlorinated paraffins in the Henan section of the Yellow River: Occurrences, fates, and fluxes. Science of the Total Environment, 640–641, 1312 - 1319.

Li T, Wan Y, Gao S, Wang B, Hu J (2017). High-throughput determination and characterization of short- , medium- , and long- chain chlorinated paraffins in human blood. Environmental Science and Technology, 2017, 51 (6), 3346 – 3354.

Li T, Gao S, Ben Y, Zhang H, Kang Q and Wan Y (2018). Screening of chlorinated paraffins and unsaturated analogues in commercial mixtures: Confirmation of their occurrences in the atmosphere. Environmental Science & Technology, 52(4), 1862 - 1870.

Ma X, Wang Y, Gao W, Wang Y, Wang Z, Yao Z, Jiang G (2018). Air–Seawater Gas Exchange and Dry Deposition of Chlorinated Paraffins in a Typical Inner Sea (Liaodong Bay), North China. Environmental Science & Technology 2018 52 (14), 7729-7735.

Ma X, Zhang H, Zhou H, Na G, Wan Z, Chen C, Chen J, Chen J (2014). Occurrence and gas/particle partitioning of short- and medium- chain chlorinated paraffins in the atmosphere of Fildes Peninsula of Antarctica. Atmospheric Environment, 90, 10 - 15.

Madeley JR and Birtley RDN (1980). Chlorinated paraffins and the environment. 2. Aquatic and avian toxicology. Environmental Science and Technology, 14, 1215-1221.

Madeley JR and Thompson RS (1983). Toxicity of Chlorinated Paraffin to Mussels (*Mytilus edulis*) - 52% Chlorination of Intermediate Chain Length n-Paraffin. ICI Confidential Report BL/B/2289. *Unpublished report*.

Miljødirektoratet. Grenseverdier for klassifisering av vann, sediment og biota. M-608 2016.

Moore S, Vromet L, Rondeau B (2004). Comparison of metastable atom bombardment and electron capture negative ionization for the analysis of polychloroalkanes. Chemosphere 54(4): 453-459

Muir D, Braekevelt E, Tomy G, Whittle M (2002). Analysis of Medium Chain Chlorinated Paraffins in Great Lake Food Webs and in a Dated Sediment Core for Lake St. Francis in the St. Lawrence River System. Preliminary Report August 2002. National Water Research Institute, Burlington, ON.

Murray T, Frankenberry M, Steele DH, Heath RG (1987a). Chlorinated Paraffins: A Report on the Findings from Two Field Studies, Sugar Creek, Ohio, Tinkers Creek, Ohio. Volume 1, Technical Report. United States Environmental Protection Agency Report EPA 560/5-87-012, 1987.

Murray T, Frankenberry M, Steele DH, Heath RG (1987b). Chlorinated Paraffins: A Report on the Findings from Two Field Studies, Sugar Creek, Ohio, Tinkers Creek, Ohio. Volume 2, Appendix D. The Quality Assurance Project Plan. United States Environmental Protection Agency Report EPA 560/5/87-012, 1987.

Nicholls CR, Allchin CR, Law RJ (2001). Levels of short and medium chain length polychlorinated n-alkanes in environmental samples from selected industrial areas in England and Wales. Environmental Pollution, 114, 415 – 430.

Nilsson M-L, Bengtsson S, Kylin H (2012). Identification and determination of chlorinated paraffins using multivariate evaluation of gas chromatographic data. Environmental Pollution, 163, 142 - 148.

Norsk Vann (2018) Organic Pollutants in Norwegian Wastewater Sludge – Results from the Survey in 2017/18. Report 248.

OECD (2006). OECD Guidelines for the Testing of Chemicals, Revised Introduction To The OECD Guidelines For Testing Of Chemicals, Section 3 Part I: Principles And Strategies Related To The Testing Of Degradation Of Organic Chemicals. Adopted 23 March 2006.

OECD (2013). Validation Report of a Ring Test for the OECD 305 Dietary Eexposure Bioaccumulation Fish Test. Additional Report Including Results Using a Lower Feeding Rate. Series on Testing and Assessment. No. 191. ENV/JM/MONO(2013)15.

OECD (2017). Guidance Document on Aspects of OECD TG 305 on Fish Bioaccumulation. Series on Testing & Assessment. No. 264. ENV/JM/MONO(2017)16.

Pan X, Tang J, Tian C, Li J, Zhang G (2018). Short- and medium- chain chlorinated paraffins in sediments from the Laizhou Bay area, North China: Implications for transportation from rivers to marine environment. Environmental Pollution, 243, 1460 - 1468.

Petersen M, Bussmann P, Grümping R, Like G (2006). Analysis of short-chain (C10-13) and medium-chain chlorinated paraffins (C_{14-17}) in Norwegian sediment and water samples by GC/ECNI-MS. Organohalogen Compounds, 68, 2101 - 2104.

Poon R, Lecavalier P, Chan P, Viau C, Hakansson H, Chu I, Valli VE (1995). Subchronic toxicity of a medium-chain chlorinated paraffin in the rat. Journal of Applied Toxicology, 15, 455–463. https://doi.org/10.1002/jat.2550150607

Post DM (2002). Using stable isotopes to estimate trophic position: models, methods, and assumptions. Ecology, 83 (3), 703 – 718.

Pribylová P, Klánová J, Holoubek I (2006). Screening of short- and medium- chain chlorinated paraffins in selected riverine sediments and sludge from the Czech Republic. Environmental pollution, 144, 248 - 254.

Qiao L, Gao L, Xia D, Huang H, Zheng M (2017). Short- and medium- chain chlorinated paraffins in sediments from the middle reaches of the Yangtze River: Spatial distributions, source apportionment and risk assessment. Science of the Total Environment, 575, 1177 - 1182.

Qiao L, Gao L, Zheng M, Xia D, Li J, Zhang L, Wu Y, Wang R, Cui L, Xu C (2018). Mass Fractions, Congener Group Patterns, and Placental Transfer of Short- and Medium-Chain Chlorinated Paraffins in Paired Maternal and Cord Serum. Environmental Science and Technology, 52, 10097–10103. https://doi.org/10.1021/acs.est.8b02839

Qiao L, Xia D, Gao L, Huang H, Zheng M (2016). Occurrences, sources and risk assessment of short- and medium- chain chlorinated paraffins in sediments from the middle reaches of the Yellow River, China. Environmental Pollution, 219, 483 - 489.

Renberg L, Tarkpea M, Sundstrom G (1986). The use of the bivalve *Mytilus Edulis* as a test organism for bioconcentration studies: II. The bioconcentration of two ^{14}C-labeled chlorinated paraffins. Ecotoxicology and Environmental Safety, 11, 361 - 372

Renberg L, Sundström G, Sundh-Nygård K (1980). Partition coefficients of organic chemicals derived from reverse phase thin layer chromatography. Evaluation of methods and application on phosphate esters, polychlorinated paraffins and some PCB-substitutes. Chemosphere, 9, 683-691.

Reth M, Ciric A, Christensen G N, Heimstad E S, Oehme M (2006). Short- and medium- chain chlorinated paraffins in biota from the European Arctic – differences in homologue group patterns. Science of the Total Environment, 367, 252 - 260.

Reth M and Oehme M (2004). Limitations of low resolution mass spectrometry in the electron capture negative ionization mode for the analysis of short- and medium-chain chlorinated paraffins, Anal. Bioanal. Chem. 378 (2004) 1741–1747.

Reth M, Zencak Z, Oehme M (2005a). First study of congener group patterns and concentrations of short- and medium- chain chlorinated paraffins in fish from the North and Baltic Sea. Chemosphere, 58, 847 - 854.

Reth M, Zencak Z, Oehme M, (2005b). New quantification procedure for the analysis of chlorinated paraffins using electron capture negative ionization mass spectrometry. Journal of Chromatography A 1081, 225–231.

Rieger R and Ballschmiter K (1995). Semivolatile organic compounds – polychlorinated dibenzo-*p*-dioxins (PCDD), dibenzofurans (PCDF), biphenyls (PCB), hexachlorobenzene (HCB), 4 4'-DDE and chlorinated paraffins (CP) – as markers in sewer films. Fresenius Journal of Analytical Chemistry, 352, 715 - 724.

Ruus A, Bæk K, Petersen K, Allan I, Beylich B, Schlabach M, Warner N, Borgå K, Helberg M (2018). Environmental Contaminants in an Urban Fjord, 2017. The Norwegian Environment Agency. NIVA Report no. 7368-2019. ISBN: 978-82-577-7103-4.

Ruus A, Bæk K, Rundberget T, Allan I, Beylich B, Schlabach M, Warner N, Borgå K, Helberg M (2019). Environmental Contaminants in an Urban Fjord, 2018', NIVA-report 7410-2019: 99.

Schinkel L, Bogdal C, Canonica E, Cariou R, Bleiner D, McNeill K, Heeb NV (2018). Analysis of medium-chain and long-chain chlorinated paraffins: the urgent need for more specific analytical standards. Environmental Science and Technology Letters, 5, 12, 708 – 717.

Schlabach M, van Bavel B, Baz Lomba JA, Borgen A, Wing Gabrielsen G, Götsch A, Halse AK, Hanssen L, Sunde Krogseth I, Nikiforov V, Nygård T, Bohlin Nizzetto P, Reid M, Rostkowski P, Samanipour S (2018). Screening Programme 2017. AMAP assessment compounds. Environmental monitoring, M-1080|2018. ISBN: 978-82-425-2940-4.

Schmid PP and Müller MD (1985). Trace level detection of chlorinated paraffins in biological and environmental samples using gas chromatography/mass spectrometry with negative-ion chemical ionization. Journal-Association of Official Analytical Chemists, 68, 427 - 430.

Shojania S (1999). The enumeration of isomeric structures for polychlorinated n-alkanes. Chemosphere, 3 (9), 2125 - 2141.

Sijm DTHM, Sinnige T L (1995). Experimental octanol/water partition coefficients of chlorinated paraffins. Chemosphere, 31, 4427 - 4435.

Smith SR (2009). Organic contaminants in sewage sludge (biosolids) and their significance for agricultural recycling. Phil. Trans. R. Soc. A., 367, 4005 - 4041.

Spacie A and Hamelink JL (1982). Alternative models for describing the bioconcentration of organics in fish. Environmental Toxicology and Chemistry, 1, 309 - 320.

Steinberg SM and Emerson DW (2012). On-line dechlorination-hydrogenation of chlorinated paraffin mixtures using GC and GC/MS. Environmental Monitoring and Assessment, 184, 2119 - 2131.

Streit B and Sire EO (1993). On the role of blood proteins for uptake, distribution, and clearance of waterborne lipophilic xenobiotics by fish: A linear system analysis. Chemosphere, 26, 1031 - 1039.

Sun YZ, Wang XT, Zhang Y, Sun YF, Li M, Ma Z (2013). Level, composition and sources of medium-chain chlorinated paraffins in soils from Chongming Island. Huan Jing Ke Xue, 34(11), 4420 - 4426.

Swedish Environmental Protection Agency (1998). Persistent Organic Pollutants. A Swedish View of an International Problem. Monitor No. 16.

Tarkpea M, Lindén E, Bengtsson BE, Larsson Å, Svanberg O (1981). Product Control Studies at the Brackish Water Toxicology Laboratory 1979-1980. Nyköping, Swedish Environmental Protection Agency, NBL Report 1981-03-23 (in Swedish; as reported in WHO, 1996). *Unpublished report*.

Thomann RV (1989). Bioaccumulation model of organic chemical distribution in aquatic food chains. Environmental Science & Technology, 23, 699 - 707.

Thomas GO and Jones KC (2002). Chlorinated Paraffins in Human and Bovine Milk-fat. A Report on a Research Project Funded by the Eurochlor Chlorinated Paraffin Sector Group. Department of Environmental Sciences, Lancaster University, UK. *Unpublished report*.

Thomas GO, Braekevelt E, Stern G, Martin FL and Jones KC (2003). Further Work on Chlorinated Paraffins in Human Milk-fat. A Report on a Research Project Funded by the Eurochlor Chlorinated Paraffin Sector Group. Department of Environmental Sciences, Lancaster University, UK. *Unpublished report*.

Thomas KV, Langford KH, Muthanna T, Schlabach M, Enge E J, Borgen A, Ghebremeskel M, Gundersen H, Leknes H, Uggerud H, Haglund P, Liao Z, Liltved H (2011). Occurrence of Selected Organic Micropollutants and Silver at Wastewater Treatment Plants in Norway. Klima-og forurensningsdirektoratet, TA 2784, 2011.

Thompson RS, Williams NJ and Gillings E (1996). Chlorinated Paraffin (52% Chlorinated, C_{14-17}): Acute Toxicity to *Daphnia magna*. Zeneca Unpublished Report, BL5871/B. *Unpublished report*.

Thompson RS, Williams NJ and Gillings E (1997). Chlorinated Paraffin (52% Chlorinated, C_{14-17}): Chronic Toxicity to *Daphnia magna.* Zeneca Unpublished Report, BL5875/B. *Unpublished report*.

Thompson RS, Gillings E and Cumming RI (1998). Short-chain chlorinated paraffin (55% chlorinated): Determination of organic carbon partition coefficient (K_{OC}). Zeneca Unpublished Report BL6426/B.

Thompson RS and Gore NR (1999). Chlorinated Paraffin (52% Chlorinated, C_{14-17}): Acute Toxicity to Two Freshwater Crustaceans, *Gammarus pulex* and *Daphnia magna*. Zeneca, BLS2643/B. *Unpublished report*.

Thompson RS, Caunter JE and Gillings E (2000). Medium-chain Chlorinated Paraffin (51% Chlorinated n-Pentadecane-8-14C): Bioconcentration and Elimination by Rainbow Trout (Oncorhynchus mykiss). AstraZeneca Unpublished Report BL6869/B. Unpublished report.

Thompson RS, Hutchings MJ and Gillings E (2001). Medium-chain chlorinated paraffin (52% chlorinated, C14-17): Effects in soil on the survival, growth and reproduction of the earthworm, Eisenia fetida. AstraZeneca Unpublished Report BL7115/B.

Thompson RS (2004). Medium-chain Chlorinated Paraffin (C_{14-17}, 52% Chlorinated): A Comparison of Acute Toxicity to *Daphnia magna* Using Two Different Carrier Solvents and Water-accommodated Fractions. AstraZeneca Unpublished Report, BLS3192/B.

TNO (1993). Semi-static Reproduction Test with Chlorparaffin Hoechst 52 flüssig and *Daphnia* magna (OECD Guideline no 202). TNO Environmental and Energy Research. TNO report IMW-R-93/020. *Unpublished report*.

Tolls J, Sijm DTHM. (1995). A preliminary evaluation of the relationship between bioconcentration and hydrophobicity for solubilising agents. Environmental Toxicology and Chemistry, 14, 1675 - 1685.

Tomy GT, Fisk AT, Westmore JB, Muir DCG (1998). Environmental chemistry and toxicology of polychlorinated n-alkanes. Reviews of Environmental Contamination and Toxicology, 158, 53 - 128.

UK (2021). Draft proposal to list “Chlorinated paraffins with carbon chain lengths in the range C_{14-17} and chlorination levels ≥45% chlorine by weight” in Annex A, B or C to the Stockholm Convention on Persistent Organic Pollutants. Available at: https://www.gov.uk/government/publications/chlorinated-paraffins-with-carbon-chain-lengths-in-the-range-c14-17

Unpublished (2010a). Biodegradability of polychlorinated tetradecane (45%) in the closed bottle test

Unpublished (2010b). Biodegradability of C_{14-17} chlorinated paraffin (45.6% Cl) in the closed bottle test

Unpublished (2010c). Biodegradability of a C_{14-17} medium chain chlorinated paraffin (63.2% Cl w/w) in the closed bottle test

Unpublished (2010d). Biodegradability of Medium-Chain Chlorinated Paraffin (51.7% Cl w/w) in the Closed Bottle Test

Unpublished (2010e). Biodegradability of Chlorinated Tetradecanes in Closed Bottle Tests Inoculated with Activated Sludge and River Water.

Unpublished (2010f). Evaluation of the Ultimate Biodegradability of Chlorinated Tetradecanes using in Sequence Batch Reactors.

Unpublished (2010g). Biodegradability of Chlorinated n-alkanes C_{10-13} (50%; SCCP); Closed Bottle Test Method.

Unpublished (2010h). [^{14}C]-Chlorinated n-Tetradecane: Determination of the Bioconcentration in Rainbow Trout (*Oncorhynchus mykiss*).

Unpublished (2010i). Analysis of ^{14}C-labeled Polychlorinated C_{14} Exposed Fish. Report R-10/06-1, IVM Institute for Environmental Studies.

Unpublished (2013). Comments on Preliminary Bioaccumulation Assessment of Medium Chain Chlorinated Paraffins (MCCPs). REACH Registrants.

Unpublished (2014a). Biodegradability of C15 Chlorinated n-Alkane, 51% Cl (wt.) in the Closed Bottle Test (OECD TG 301D).

Unpublished (2014b). Biodegradability of C15 Chlorinated n-Alkane, 51% Cl (wt.) in the Closed Bottle Test (OECD TG 301).

Unpublished (2014c). Bioaccumulation Assessment of Medium-Chain Chlorinated Paraffins (MCCP). REACH Registrants.

Unpublished (2018a). Biodegradability of C_{14} Chlorinated n-Alkane, 50% Cl (wt.) in the Closed Bottle Test (OECD TG 301D).

Unpublished (2018b). Biodegradability of C_{14} Chlorinated n-Alkane, 55% Cl (wt.) in the Closed Bottle Test (OECD TG 301D).

Unpublished (2018c). Biodegradability of C_{14} Chlorinated n-Alkane, 60% Cl (wt.) in the Closed Bottle Test (OECD TG 301D).

Unpublished (2018d). Biodegradability of C_{15} Chlorinated n-Alkane, 51% Cl (wt.) in the Closed Bottle Test (OECD TG 301D).

Unpublished (2019a). Water Solubility Determination of C_{14} Polychlorinated n-Alkane with 50% Cl by Weight.

Unpublished (2019b). 1-Octanol/Water Partition Coefficient Determination of C_{14} Polychlorinated n-Alkane with 50% Cl by Weight.

Unpublished (2019c). C_{14} Chlorinated Paraffin: Aerobic Transformation in Aquatic Sediment Systems (simulation study).

Unpublished (2019d). Determination of C_{14} polychlorinated n-alkane with 50% Cl by weight in sediments from OECD 308 biodegradation tests (specific analysis).

Unpublished (2019e) C_{14} Chlorinated Paraffin: A Dietary Exposure Bioaccumulation Test with the Rainbow Trout (*Oncorhynchus mykiss*).

Unpublished (2019f) Determination of C_{14} Polychlorinated n-alkane with 50% Cl by weight in fish tissue and fish diet from OECD 305 bioaccumulation tests.

Unpublished (2020). Metabolism of chlorinated paraffins. Laboratory of Mathematical Chemistry (LMC), Burgas, Bulgaria.

US EPA (2012). Estimation Programs Interface (EPI) Suite™, v 4.1. United States Environmental Protection Agency, Washington, DC, USA.

Vander Zanden MJ and Fetzer WW (2007). Global patterns of aquatic food chain length. Oikos 116: 1378–1388. ISSN 0030-1299.

van Zeijl H (1997). Report of the Results of the One-off DIFFCHEM-project. Oslo and Paris Convention for the Prevention of Marine Pollution. Environmental Assessment and Monitoring Committee (ASMO), Copenhagen, 7 - 11 April 1997.

Wang Y, Cai Y, Jiang G (2010). Research processes of persistent organic pollutants (POPs) newly listed and candidate POPs in Stockholm Convention. Sci. Sin. Chem. 2010, 40, 99−123.

Wang R, Gao L, Zheng M, Tian Y, Li J, Zhang L, Wu Y, Huang H, Qiao L, Liu W, Su G, Liu G, Liu Y (2018a). Short- and medium- chain chlorinated paraffins in aquatic foods from 18 Chinese provinces: Occurrence, spatial distributions, and risk assessment. Science of the Total Environment, 615, 1199–1206.

Wang Y, Gao W, Wang Y, Jiang G (2018b). Distribution and pattern profiles of chlorinated paraffins in human placenta of Henan Province, China. Environmental Science & Technology Letters, 5, 9 - 13.

Wang R, Gao L, Zheng M, Li J, Zhang L, Wu Y, Wang G, Xiong L, Ding D, Lu D, Qiao L, Cui L, Xu C (2019) Characterization of short- and medium- chain chlorinated paraffins in cereals and legumes from 19 Chinese provinces. Chemosphere, 226, 282 – 289.

Wang XT, Wang XK, Zhang Y, Chen L, Sun YF, Li M, Wu MH (2014). Short- and medium- chain chlorinated paraffins in urban soils of Shanghai: Spatial distribution, homologue group patterns and ecological risk assessment. Science of the Total Environment, 490, 144 - 152.

Wang XT, Zhou J, Lei BL, Zhou JM, Xu SY, Hu BP, Wang DQ, Zhang DP, Wu MH (2016). Atmospheric occurrence, homologue patterns and source apportionment of short- and medium- chain chlorinated paraffins in Shanghai, China: Biomonitoring with Masson pine *(Pinus massoniana L.)* needles. Science of the Total Environment, 560–561, 92 - 100.

Wang XT, Xu SY, Wang XK, Hu BP, Jia HH (2017). Occurrence, homologue patterns and source apportionment of short- and medium- chain chlorinated paraffins in suburban soils of Shanghai, China. Chemosphere, 180, 302 - 311.

Wang Y, Li J, Cheng Z, Li Q, Pan X, Zhang R, Liu D, Luo C, Liu X, Katsoyiannis A, Zhang G (2013). Short- and medium- chain chlorinated paraffins in air and soil of subtropical terrestrial environment in the Pearl River Delta, South China: Distribution, composition, atmospheric deposition fluxes, and environmental fate. Environmental Science & Technology, 47, 2679 - 2687.

Wegmann F, Cavin L, MacLeod M, Scheringer M and Hungerbühler K (2009): The OECD software tool for screening chemicals for persistence and long-range transport potential. Environmental Modeling and Software, 24, 228-237.

Wicker J, Lorsbach T, Gütlein M, Schmid E, Latino D, Kramer S, Fenner K (2016). EnviPath – The environmental contaminant biotransformation pathway resource. Nucleic Acids Research, 44, D502–D508.

Willis B, Crookes MJ, Diment J, Dobson SD (1994). TSD/19, Environmental hazard assessment: Chlorinated paraffins. Toxic Substances Division, Directorate for Air, Climate and Toxic Substances, Department of the Environment. ISBN 0 85125 627 9.

Wu J, Cao D, Gao W, Lv K, Liang Y, Fu J, Gao Y, Wang Y, Jiang G (2019). The atmospheric

transport and pattern of Medium chain chlorinated paraffins at Shergyla Mountain on the Tibetan Plateau of China. Environmental Pollution, 245, 46 – 52.

Wu J, Gao W, Liang Y, Fu JJ, Gao Y, Wang YW, Jiang GB (2017). Spatio-temporal distribution and alpine behavior of short chain chlorinated paraffins in air at Shergyla Mountain and Lhasa on the Tibetan plateau of China. Environ. Sci. Technol. 51, 11136–11144.

Xia D, Gao L, Zhu S, Zheng M (2014). Separation and screening of short-chain chlorinated paraffins in environmental samples using comprehensive two-dimensional gas chromatography with micro electron capture detection. Analytical and Bioanalytical Chemistry, 406, 7561–7570. https://doi.org/10.1007/s00216-014-8209-6

Xia D, Gao L, Zheng M, Li J, Zhang L, Wu Y, Tian Q, Huang H, Qiao L (2017). Human exposure to short- and medium- chain chlorinated paraffins via mothers' milk in Chinese urban population. Environmental Science & Technology, 51, 608-615.

Xia D, Gao L, Zheng M, Tian Q, Huang H, and Qiao L (2016). A novel method for profiling and quantifying short- and medium- chain chlorinated paraffins in environmental samples using comprehensive Two-Dimensional Gas Chromatography–Electron Capture Negative Ionization High-Resolution Time-of-Flight Mass Spectrometry. Environmental Science & Technology, 50, 14, 7601 - 7609.

Xu C, Zhang Q, Gao L, Zheng M, Qiao L, Cui L, Wang R, Cheng J (2019). Spatial distributions and transport implications of short- and medium- chain chlorinated paraffins in soils and sediments from an e-waste dismantling area in China. Science of the Total Environment, 649, 821 - 828.

Xu J, Gao Y, Zhang H, Zhan F, Chen J (2016). Dispersion of short- and medium- chain chlorinated paraffins (CPs) from a CP production plant to the surrounding surface soils and coniferous leaves. Environmental Science & Technology, 50, 12759 - 12766.

Yuan B and de Wit CA (2018). Screening chlorinated paraffins in Swedish terrestrial birds and mammals (2012-2017). Report: Dnr 2219-17-011, ärendenr NV-04762-17.

Yuan B, Bogdal C, Berger U, MacLeod M, Gebbink WA, Alsberg T, de Wit CA (2017a). Quantifying short-chain chlorinated paraffin congener groups. Environmental Science & Technology, 51, 10633-10641. Available at: https://pubs.acs.org/doi/pdf/10.1021/acs.est.7b02269

Yuan B, Brüchert V, Sobek A and de Wit CA (2017b). Temporal trends of C_8–C_{36} chlorinated paraffins in Swedish coastal sediment cores over the past 80 years. Environmental Science & Technology, 51, 14199-14208.

Yuan B, Vorkamp K, Roos AM, Faxneld S, Sonne C, Garbus SE, Lind Y, Eulaers I, Hellström P, Dietz R, Persson S, Bossi R, de Wit CA (2019). Accumulation of short- , medium- , and long-chain chlorinated paraffins in marine and terrestrial animals from Scandinavia. Environmental Science and Technology, 53, 3526 – 3537.

Yuan B, Lysak DH, Soong R, Haddad A, Hisatsune A, Moser A, Golotvin S, Aryropoulos D, Simpson AJ, Muir CG (2020). Chlorines are not evenly substituted in chlorinated paraffins: A predicted NMR pattern matching framework for isomeric discrimination in complex contaminant mixtures. Environmental Science and Technology Letters, 7, 496–503. Available at: https://pubs.acs.org/doi/pdf/10.1021/acs.estlett.0c00244

Zeng L, Lam JCW, Horii Y, Li X, Chen W, Qiu J-W, Leung KMY, Yamazaki E, Yamashita N, Lam PKS (2017). Spatial and temporal trends of short- and medium- chain chlorinated paraffins in sediments off the urbanized coastal zones in China and Japan: A comparison study. Environmental Pollution 224, 357 - 367.

Zeng L, Lam JCW, Wang Y, Jiang G, Lam PKS (2015). Temporal trends and pattern changes of short- and medium- chain chlorinated paraffins in marine mammals from the South China Sea over the past decade. Environmental Science & Technology, 49, 11348 - 11355.

Zeng L, Wang T, Han W, Yuan B, Liu Q, Wang Y, Jiang G (2011). Spatial and Vertical Distribution of Short Chain Chlorinated Paraffins in Soils from Wastewater Irrigated Farmlands. Environ. Sci. Technol. 2011, 45 (6), 2100–2106.

Åhlman M, Bergman A, Darnerud PO, Egestad B, Sjovall J (1986). Chlorinated paraffins: formation of sulphur-containing metabolites of polychlorohexadecane in rats. Xenobiotica, 16, 225–232. https://doi.org/10.3109/00498258609043525

Annex I – Theoritical % weight chlorine content of congeners of MCCP

Chlorination formula	C	H	Cl	Molecular Weight (g/mol)	% Chlorination by weight
C14H30Cl0	14	30	0	198	0.00
C14H29Cl	14	29	1	232.5	15.27
C14H28Cl2	14	28	2	267	26.59
C14H27Cl3	14	27	3	301.5	35.32
C14H26Cl4	14	26	4	336	42.26
C14H25Cl5	14	25	5	370.5	47.91
C14H24Cl6	14	24	6	405	52.59
C14H23Cl7	14	23	7	439.5	56.54
C14H22Cl8	14	22	8	474	59.92
C14H21Cl9	14	21	9	508.5	62.83
C14H20Cl10	14	20	10	543	65.38
C14H19Cl11	14	19	11	577.5	67.62
C14H18Cl12	14	18	12	612	69.61
C14H17Cl13	14	17	13	646.5	71.38
C14H16Cl14	14	16	14	681	72.98
C15H32	15	32	0	212	0.00
C15H31Cl	15	31	1	246.5	14.40
C15H30Cl2	15	30	2	281	25.27
C15H29Cl3	15	29	3	315.5	33.76
C15H28Cl4	15	28	4	350	40.57
C15H27Cl5	15	27	5	384.5	46.16
C15H26Cl6	15	26	6	419	50.84
C15H25Cl7	15	25	7	453.5	54.80
C15H24Cl8	15	24	8	488	58.20
C15H23Cl9	15	23	9	522.5	61.15
C15H22Cl10	15	22	10	557	63.73
C15H21Cl11	15	21	11	591.5	66.02
C15H20Cl12	15	20	12	626	68.05
C15H19Cl13	15	19	13	660.5	69.87
C15H18Cl14	15	18	14	695	71.51
C15H17Cl15	15	17	15	729.5	73.00
C16H34	16	34	0	226	0.00
C16H33Cl	16	33	1	260.5	13.63
C16H32Cl2	16	32	2	295	24.07
C16H31Cl3	16	31	3	329.5	32.32
C16H30Cl4	16	30	4	364	39.01
C16H29Cl5	16	29	5	398.5	44.54
C16H28Cl6	16	28	6	433	49.19
C16H27Cl7	16	27	7	467.5	53.16

Chlorination formula	C	H	Cl	Molecular Weight (g/mol)	% Chlorination by weight
C16H26Cl8	16	26	8	502	56.57
C16H25Cl9	16	25	9	536.5	59.55
C16H24Cl10	16	24	10	571	62.17
C16H23Cl11	16	23	11	605.5	64.49
C16H22Cl12	16	22	12	640	66.56
C16H21Cl13	16	21	13	674.5	68.42
C16H20Cl14	16	20	14	709	70.10
C16H19Cl15	16	19	15	743.5	71.62
C16H18Cl16	16	18	16	778	73.01
C17H36Cl0	17	36	0	240	0.00
C17H35Cl	17	35	1	274.5	12.93
C17H34Cl2	17	34	2	309	22.98
C17H33Cl3	17	33	3	343.5	31.00
C17H32Cl4	17	32	4	378	37.57
C17H31Cl5	17	31	5	412.5	43.03
C17H30Cl6	17	30	6	447	47.65
C17H29Cl7	17	29	7	481.5	51.61
C17H28Cl8	17	28	8	516	55.04
C17H27Cl9	17	27	9	550.5	58.04
C17H26Cl10	17	26	10	585	60.68
C17H25Cl11	17	25	11	619.5	63.03
C17H24Cl12	17	24	12	654	65.14
C17H23Cl13	17	23	13	688.5	67.03
C17H22Cl14	17	22	14	723	68.74
C17H21Cl15	17	21	15	757.5	70.30
C17H20Cl16	17	20	16	792	71.72
C17H19Cl17	17	19	17	826.5	73.02

Annex II – Modelling of log Kow and biodegradation and generation of representative structures for MCCP

Structures used in the QSAR predictions to represent MCCP

For the QSAR predictions a selection of structures representing congener- groups of MCCP and their structural isomers was enumerated with the software UVCB G Graph v. 1.8.0 (Dimitrov *et al.*, 2015). The software generated the SMILES for the enumerated structures.

60 structures were enumerated for the congeners of each carbon chain length (C14-C17) representing the more typical chlorination degree of commercial mixtures with 40–65% chlorination by weight. This selection formed group 1. For congeners outside of this chlorination range (<40 % or >65% chlor content) a smaller number of structures (20–28) was chosen per carbon chain length, forming group 2 (see Table 53). The structures are presented in Figures 3-6.

The software was programmed to enumerate linear structures and not allowing for a second chlorine substitution on the same carbon (even though MCCP may contain structures with branching and germinal position of the chlorine atoms). Structures with chlorine atom(s) on the terminal carbon(s) were not excluded from the selection. Although such congeners are less likely to be present in the commercial mixtures, there is currently no evidence to indicate that they could not form in the chlorination reaction and that they would not be present in the commercial mixtures. Attempts to describe the isomeric distribution of chlorinated paraffins samples by means of NMR spectroscopy have been described in the literature. These indicate that chlorine atoms may be found on adjacent carbon atoms as well as terminal carbon atoms, especially for substances having higher chlorination degrees. (Yuan *et al.*, 2020).

The software first calculated all possible combinations of the structure per specific carbon chain length and specific number of chlorine atoms according to the predefined boundaries described above. Then a selection based on log Kow was made, so that twenty fractions based on difference in log Kow were defined. From each of the fractions three structures were chosen at random. For group 1 this resulted in 60 structures per chain length. For Group 2, the selection yielded less structures because there were fractions in the log Kow range that did not contain any structures. It was indeed the intention to have less structures for the lower and higher ends of the chlorination content. The selection yielded a relatively even number of structural isomers per congener group, in most cases six or seven for the congener groups in group 1 (range 6 – 9) (see Table 55 (BIOWIN predictions) for number of generated structures per congener group).

Table 53: Number of input structures used in the QSAR predictions

Congener groups	Chlorination content (approximately)	Number of structures
Group 1		
C14 Cl3-11	> 40 ≥ 65% Cl wt.	60
C15 Cl4-11	> 40 ≥ 65% Cl wt.	60
C16 Cl4-12	> 40 ≥ 65% Cl wt.	60
C17 Cl4-12	> 40 ≥ 65% Cl wt.	59
Group 2		
C14 Cl 1-2 and 12-14	< 40% and > 65% wt.	20
C15 Cl 1-3 and 12-15	< 40% and > 65% wt.	28
C16 Cl 1-3 and 13-16	< 40% and > 65% wt.	25
C17 Cl 1-3 and 13-17	< 40% and > 65% wt.	28

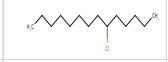
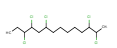
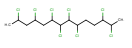
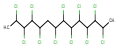
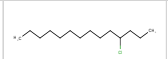
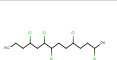
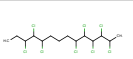
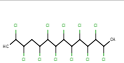
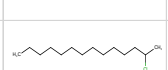
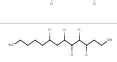
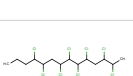
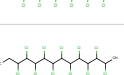
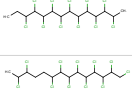
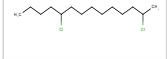
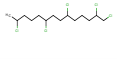
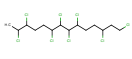
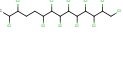
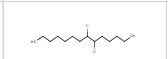
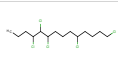
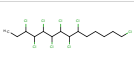
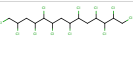
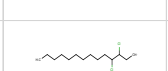
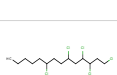
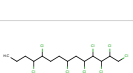
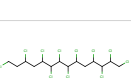
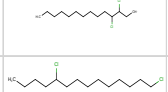
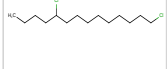
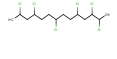
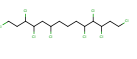
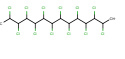
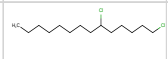
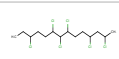
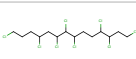
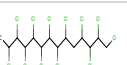
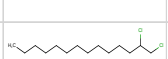
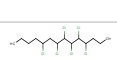
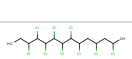
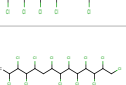
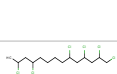
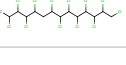
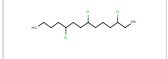
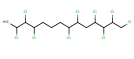
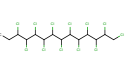
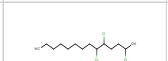
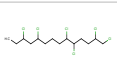
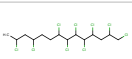
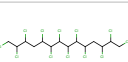
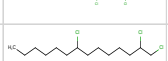
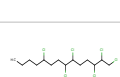
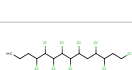
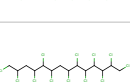
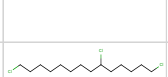
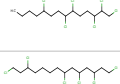
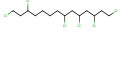
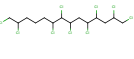
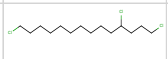
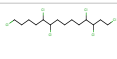
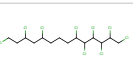
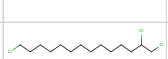
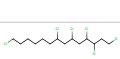
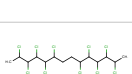
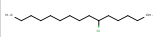
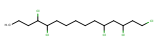
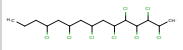
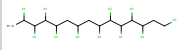
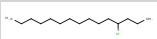
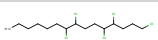
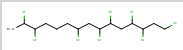
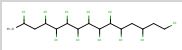
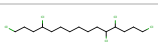
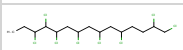
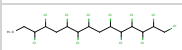
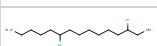
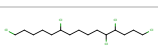
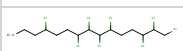
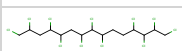
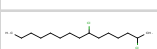
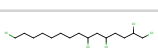
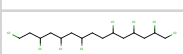
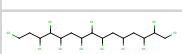
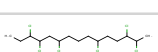
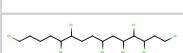
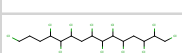
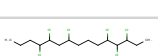
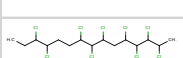
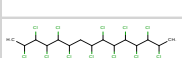
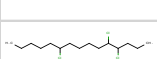
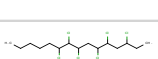
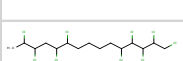
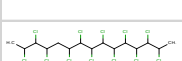
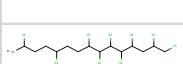
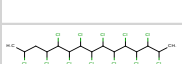
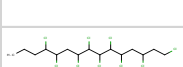
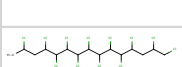
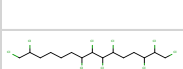
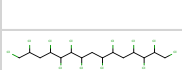
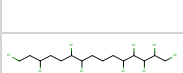
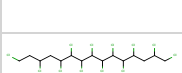
Con-gener	Input structure	Con-gener	Input structure	Con-gener	Input structure	Con-gener	Input structure
C14Cl1		C14Cl5		C14Cl8		C14Cl11	
C14Cl1		C14Cl5		C14Cl8		C14Cl11	
C14Cl1		C14Cl5		C14Cl8		C14Cl11	
C14Cl2		C14Cl5		C14Cl8		C14Cl11	
C14Cl2		C14Cl5		C14Cl8		C14Cl11	
C14Cl2		C14Cl5		C14Cl8		C14Cl11	
C14Cl2		C14Cl6		C14Cl8		C14Cl12	
C14Cl2		C14Cl6		C14Cl8		C14Cl12	
C14Cl2		C14Cl6		C14Cl9		C14Cl12	
C14Cl3		C14Cl6		C14Cl9		C14Cl12	
C14Cl3		C14Cl6		C14Cl9		C14Cl12	
C14Cl3		C14Cl6		C14Cl9		C14Cl12	
C14Cl3		C14Cl6		C14Cl9		C14Cl13	
C14Cl3		C14Cl6		C14Cl10		C14Cl13	
C14Cl4		C14Cl7		C14Cl10		C14Cl13	
C14Cl4		C14Cl7		C14Cl10		C14Cl14	
C14Cl4		C14Cl7		C14Cl10			
C14Cl4		C14Cl7		C14Cl10			
C14Cl4		C14Cl7		C14Cl10			
C14Cl4		C14Cl7		C14Cl10			

Figure 3: Input structures for the congener groups $C_{14}Cl_{1-14}$

Con-gener	Input structure	Con-gener	Input structure	Con-gener	Input structure	Con-gener	Input structure
C15Cl1		C15Cl5		C15Cl8		C15Cl11	
C15Cl1		C15Cl5		C15Cl8		C15Cl11	
C15Cl1		C15Cl5		C15Cl8		C15Cl11	
C15Cl2		C15Cl5		C15Cl8		C15Cl11	
C15Cl2		C15Cl5		C15Cl8		C15Cl11	
C15Cl2		C15Cl6		C15Cl8		C15Cl11	
C15Cl3		C15Cl6		C15Cl9		C15Cl12	
C15Cl3		C15Cl6		C15Cl9		C15Cl12	
C15Cl3		C15Cl6		C15Cl9		C15Cl12	
C15Cl3		C15Cl6		C15Cl9		C15Cl12	
C15Cl3		C15Cl6		C15Cl9		C15Cl12	
C15Cl4		C15Cl7		C15Cl9		C15Cl13	
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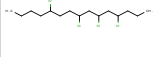
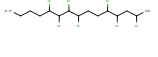
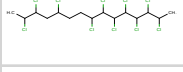
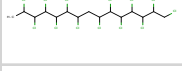
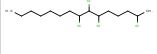
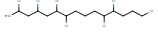
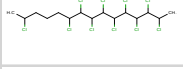
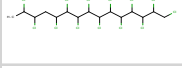
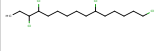
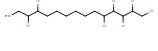
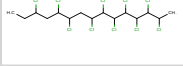
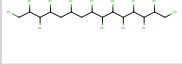
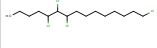
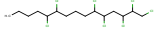
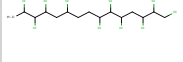
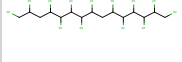
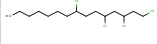
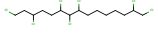
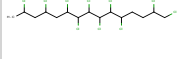
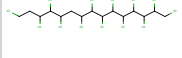
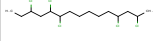
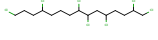
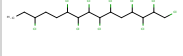
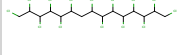
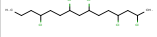
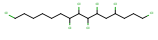
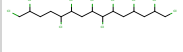
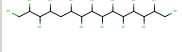
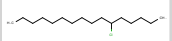
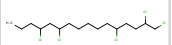
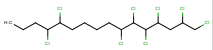
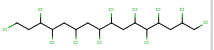
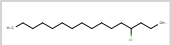
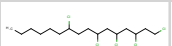
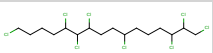
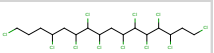
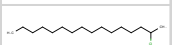
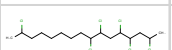
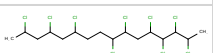
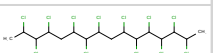
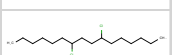
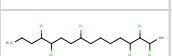
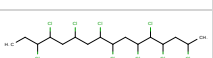
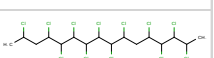
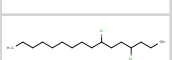
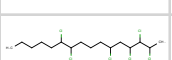
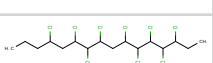
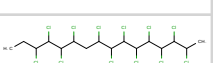
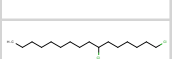
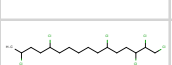
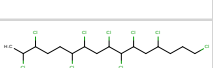
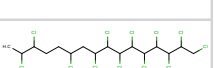
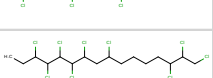
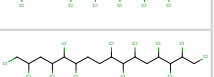
C15Cl4		C15Cl7		C15Cl10		C15Cl13	
C15Cl4		C15Cl7		C15Cl10		C15Cl13	
C15Cl4		C15Cl7		C15Cl10		C15Cl13	
C15Cl5		C15Cl7		C15Cl10		C15Cl14	
C15Cl5		C15Cl7		C15Cl10		C15Cl14	
C15Cl5		C15Cl8		C15Cl10		C15Cl14	
C15Cl5		C15Cl8		C15Cl10		C15Cl15	

Figure 4: Input structures for the congener groups $C_{15}Cl_{1\text{-}15}$

Con-gener	Input structure	Con-gener	Input structure	Con-gener	Input structure	Con-gener	Input structure
C16Cl1		C16Cl5		C16Cl8		C16Cl11	
C16Cl1		C16Cl5		C16Cl8		C16Cl11	
C16Cl1		C16Cl6		C16Cl9		C16Cl12	
C16Cl2		C16Cl6		C16Cl9		C16Cl12	
C16Cl2		C16Cl6		C16Cl9		C16Cl12	
C16Cl2		C16Cl6		C16Cl9		C16Cl12	
C16Cl3		C16Cl6		C16Cl9		C16Cl12	
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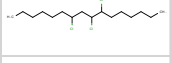
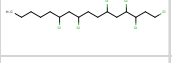
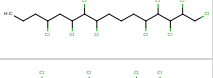
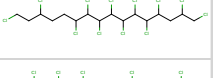
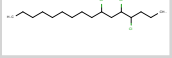
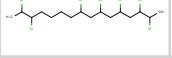
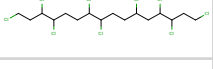
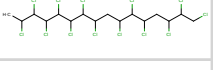
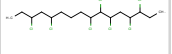
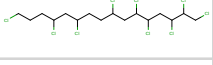
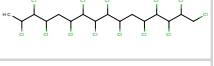
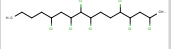
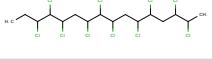
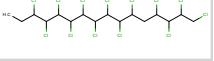
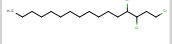
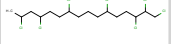
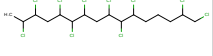
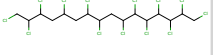
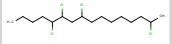
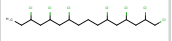
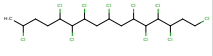
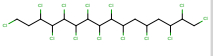
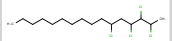
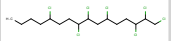
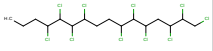
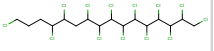
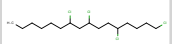
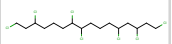
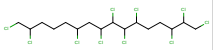
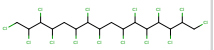
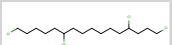
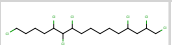
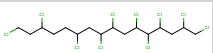
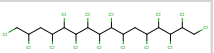
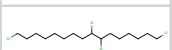
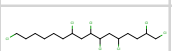
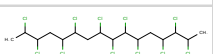
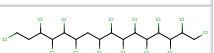
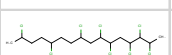
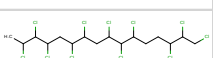
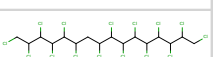
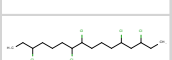
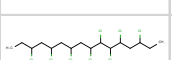
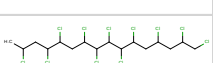
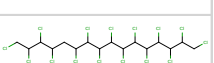
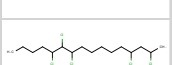
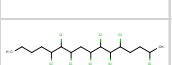
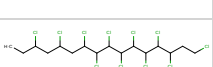
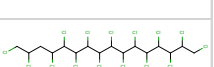
C16Cl3		C16Cl7		C16Cl9		C16Cl13	
C16Cl3		C16Cl7		C16Cl9		C16Cl13	
C16Cl3		C16Cl7		C16Cl10		C16Cl13	
C16Cl3		C16Cl7		C16Cl10		C16Cl13	
C16Cl4		C16Cl7		C16Cl10		C16Cl13	
C16Cl4		C16Cl7		C16Cl10		C16Cl13	
C16Cl4		C16Cl7		C16Cl10		C16Cl14	
C16Cl4		C16Cl7		C16Cl10		C16Cl14	
C16Cl4		C16Cl7		C16Cl11		C16Cl14	
C16Cl4		C16Cl8		C16Cl11		C16Cl15	
C16Cl5		C16Cl8		C16Cl11		C16Cl15	
C16Cl5		C16Cl8		C16Cl11		C16Cl15	
C16Cl5		C16Cl8		C16Cl11		C16Cl16	
C16Cl5							

Figure 5: Input structures for the congener groups $C_{16}Cl_{1-16}$

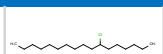
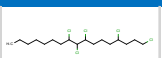
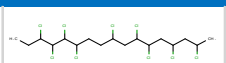
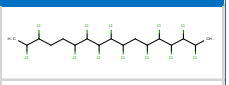
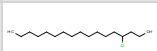
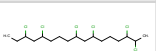
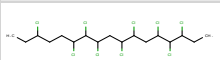
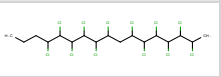
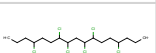
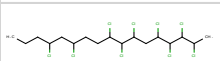
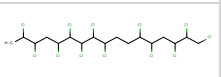
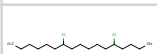
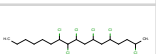
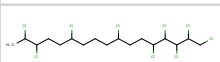
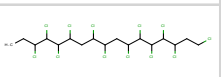
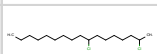
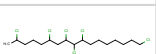
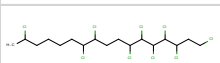
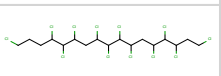
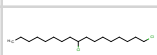
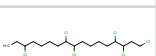
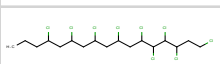
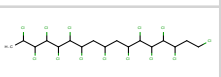
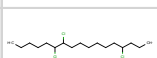
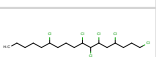
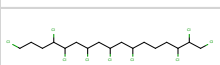
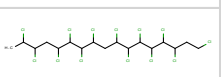
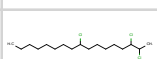
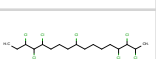
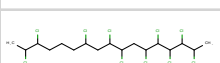
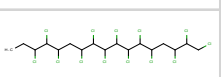
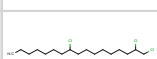
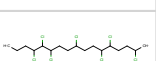
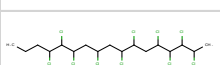
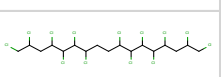
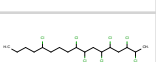
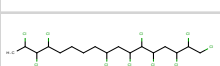
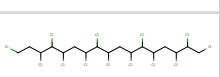
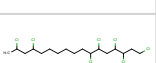
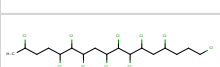
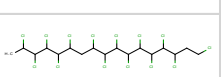
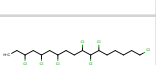
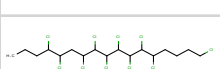
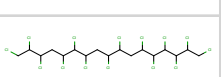
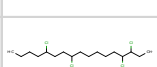
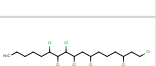
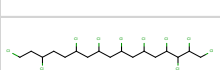
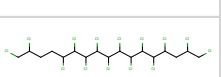
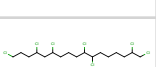
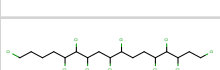
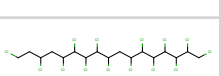
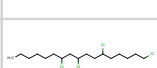
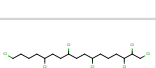
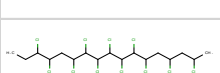
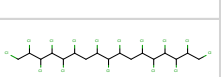
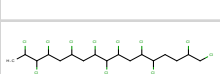
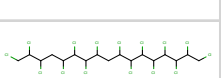
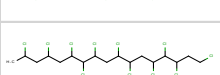
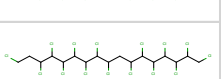
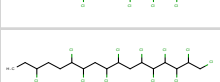
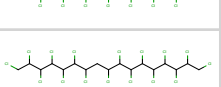
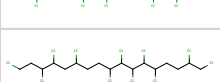
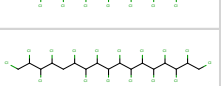
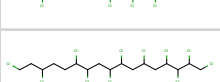
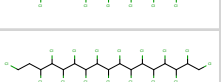
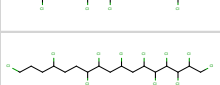
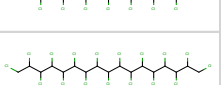
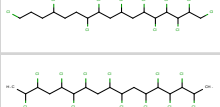
Con-gener	Input structure	Con-gener	Input structure	Con-gener	Input structure	Con-gener	Input structure
C17Cl1		C17Cl5		C17Cl9		C17Cl12	
C17Cl1		C17Cl6		C17Cl9		C17Cl12	
C17Cl1		C17Cl6		C17Cl9		C17Cl12	
C17Cl2		C17Cl6		C17Cl9		C17Cl12	
C17Cl2		C17Cl6		C17Cl9		C17Cl12	
C17Cl2		C17Cl6		C17Cl9		C17Cl13	
C17Cl3		C17Cl6		C17Cl9		C17Cl13	
C17Cl3		C17Cl7		C17Cl10		C17Cl13	
C17Cl3		C17Cl7		C17Cl10		C17Cl13	
C17Cl3		C17Cl7		C17Cl10		C17Cl13	
C17Cl3		C17Cl7		C17Cl10		C17Cl14	
C17Cl3		C17Cl7		C17Cl10		C17Cl14	
C17Cl4		C17Cl7		C17Cl10		C17Cl14	
C17Cl4		C17Cl7		C17Cl10		C17Cl14	
C17Cl4		C17Cl7		C17Cl11		C17Cl15	
C17Cl4		C17Cl7		C17Cl11		C17Cl15	
C17Cl4		C17Cl8		C17Cl11		C17Cl15	
C17Cl5		C17Cl8		C17Cl11		C17Cl16	
C17Cl5		C17Cl8		C17Cl11		C17Cl16	
C17Cl5		C17Cl8		C17Cl11		C17Cl16	
C17Cl5		C17Cl8		C17Cl11		C17Cl17	
C17Cl5		C17Cl8		C17Cl12			

Figure 6: Input structures for the congener groups $C_{17}Cl_{1-17}$

Predictions of log Kow and biodegradation potential for a series of generated MCCP structures.

- The predictions for log Kow were carried out with the log P models contained within the ACD Percepta program, ACD/Labs release 2019.2.1 (Advanced Chemistry Development, Inc., 2019) for the following MCCP congener groups $C_{14}Cl_{1-14}$, $C_{15}Cl_{1-15}$, $C_{16}Cl_{1-16}$ and $C_{17}Cl_{1-17}$ and their structural isomers. ACD Percepta has three methods for predicting log P, the Log P GALAS method, the Log P Classic method and the Log P Consensus method. The predicted log Kow were compared against the recommended log Kow values by Glüge *et al.,* 2013. The Log P Consensus method was the preferred method unless the predicted log Kow was outside of the lower range of log Kow values that has been recommended by Glüge *et al.,* 2013. If that was the case, then the higher log Kow prediction from the Log P Classic or from the Log P GALAS method was chosen given that the reliability of the Log P GALAS prediction was > 0.5. See Table 57 for the predictions, choice of method unless log P Consensus method was used and recommended log Kow values by Glüge *et al.,* 2013.

- The biodegradation predictions were carried out using the BIOWIN 2 (non-linear probability model), BIOWIN 3 (ultimate biodegradation model) and BIOWIN 6 (MITI nonlinear model) of the BIOWIN v4.10 program (EPI Suite™ v 4.1) (US EPA, 2012). The summary of persistence is based on the combination of BIOWIN 2 or BIOWIN 6 and the BIOWIN 3 prediction as follows; BIOWIN 2 <0.5 and BIOWIN 3 <2.25, or BIOWIN 6 <0.5 and BIOWIN 3 <2.25: potentially persistent or very persistent (P/vP). BIOWIN 2 <0.5 and BIOWIN 3 between 2.25 and 2.75, or BIOWIN 6 <0.5 and BIOWIN 3 between 2.25 and 2.75: potentially persistent or very persistent (P/vP), more information needed. This is in accordance to the to the PBT guidance (Chapter R.11, ECHA, 2017b). See table 58 for the predictions and screening conclusion.

The main text of the report should be consulted for further discussion of results.

Table 54: Estimated log Kow (ACD Percepta log P methods) for a series of hypothetical chlorinated paraffin structures

	Congener group	Input structure									Recommended range (Glüge *et al.*, 2013).
		1	2	3	4	5	6	7	8	9	
Log Kow other method used*	C14Cl1	7.7	7.69 Classic	7.69 Classic							7.66 - 7.76
Log Kow other method used	C14Cl2	7.19 Classic	7.8	7.95	7.38 Classic	7.63	8.16				
Log Kow other method used	C14Cl3	6.68 Classic	7.68	7.24	7.06 Classic	7.05 Classic	6.89				6.77 - 7.80
Log Kow other method used	C14Cl4	6.76 Classic	6.65 Classic	7.21	7.12 Classic	6.65 Classic	7.94				
Log Kow other method used	C14Cl5	6.43 Classic	6.2 Galas	7.45	6.23 Galas	6.62 Classic	7.35				6.88 - 7.89
Log Kow other method used	C14Cl6	6.4 Galas	6.36 Galas	6.76	6.45 Classic	6.7 Galas	7.01 Galas	6.7 Classic	6.71	6.63 Classic	
Log Kow other method used	C14Cl7	6.6 Galas	6.26 Galas	6.58	6.64	6.59	6.89 Galas				6.57 - 7.97
Log Kow other method used	C14Cl8	6.55 Galas	6.67	6.59	6.62	7.15	6.93	6.78	6.66		
Log Kow other method used	C14Cl9	6.92	6.83	6.75	7	6.99	7.1				6.21 - 7.99
Log Kow other method used	C14Cl10	7.04	7.18	7.05	7.23	7.04	7.23	7.05			
Log Kow other method used	C14Cl11	7.3	7.29	7.46	7.35	7.25	7.41				6.87 - 8.09
Log Kow other method used	C14Cl12	7.63	7.6	7.6	7.78	7.57	7.57	7.66			6.94 - 8.03
Log Kow other method used	C14Cl13	7.91	7.91	8							

	Congener group	Input structure									Recommended range (Glüge *et al.*, 2013).
		1	2	3	4	5	6	7	8	9	
Log Kow other method used	C14Cl14	8.25									
Log Kow other method used	C15Cl1	8.22 Classic	8.25	8.25							8.22 - 8.29
Log Kow other method used	C15Cl2	7.31	7.84	7.98							
Log Kow other method used	C15Cl3	7.22 Classic	7.42	8	7.69 Classic	7.59	8.92				7.37 - 8.30
Log Kow other method used	C15Cl4	7.47 Classic	7.29 Classic	8.15	7.13 Classic	7.65 Classic	8.15				
Log Kow other method used	C15Cl5	7.01 Classic	6.78 Classic	7.58	6.55	7.2 Classic	7.59	6.8 Classic	6.81 Classic	7.1 Classic	7.14 - 8.41
Log Kow other method used	C15Cl6	6.63 Galas	6.97 Classic	7.71	6.57 Galas	6.64 Classic	7.71	7.08			
Log Kow other method used	C15Cl7	6.81 Galas	6.98 Classic	7.05 Galas	7.58	7.36	7.21	7.15	7.14		6.99 - 8.48
Log Kow other method used	C15Cl8	6.81 Galas	6.99 Classic	7.33 Classic	7.23 Galas	7.18 Galas	7.28	7.02 Galas	7.03		
Log Kow other method used	C15Cl9	7.19 Galas	7.35 Galas	7.19 Galas	7.23 Classic	7.97 Galas	7.68 Galas	7.68 Galas			7.61 - 8.55
Log Kow other method used	C15Cl10	7.25	7.43	7.35	7.22	7.28	7.41	7.19	7.26	7.47	
Log Kow other method used	C15Cl11	7.57	7.65	7.62	7.49	7.54	7.56				6.88 - 8.54
Log Kow other method used	C15Cl12	7.81	7.81	7.87	7.84	7.73	7.92				
Log Kow other method used	C15Cl13	8.1	8.1	8.1	8.16	8.07	8.16				7.53 - 8.62

	Congener group	Input structure									Recommended range (Glüge *et al.*, 2013).
		1	2	3	4	5	6	7	8	9	
Log Kow other method used	C15Cl14	8.4	8.4	8.4							
Log Kow other method used	C15Cl15	8.76									
Log Kow other method used	C16Cl1	8.76 Classic	8.76 Classic	8.76 Classic							8.73 - 8.84
Log Kow other method used	C16Cl2	7.9	8.79	8.95							
Log Kow other method used	C16Cl3	7.98 Classic	8.15	8.98	8.17 Classic	8.22 Classic	9.19				7.86 - 8.87
Log Kow other method used	C16Cl4	7.76 Classic	9.1	7.79	7.61 Classic	7.85 Classic	8.19 Classic				
Log Kow other method used	C16Cl5	7.27 Classic	7.78 Classic	7.79	7.68 Classic	7.44 Classic	7.93				7.61 - 8.98
Log Kow other method used	C16Cl6	7.26 Classic	7.22 Classic	7.9	7.17 Classic	7.04 Galas	8.08				
Log Kow other method used	C16Cl7	7.07	7.28 Classic	7.28 Classic	7.22 Galas	7.3 Classic	7.3 Galas	7.2 Galas	7.62	7.4 Galas	7.34 - 9.00
Log Kow other method used	C16Cl8	7.14 Galas	7.46	7.52 Classic	7.36	7.7	7.64				
Log Kow other method used	C16Cl9	7.27 Galas	7.3 Galas	7.52	7.61 Galas	7.65	7.65	7.34	7.47		7.27 - 9.06
Log Kow other method used	C16Cl10	7.46	7.5	7.53	7.7	7.74	7.52				
Log Kow other method used	C16Cl11	7.63	7.66	7.72	7.99	7.74	7.66	7.83			7.20 - 9.09
Log Kow other method used	C16Cl12	7.98	8.03	8.16	8.1	7.98	8.16				

	Congener group	Input structure									Recommended range (Glüge *et al.*, 2013).
		1	2	3	4	5	6	7	8	9	
Log Kow other method used	C16Cl13	8.26	8.26	8.45	8.31	8.42	8.4				7.45 - 9.12
Log Kow other method used	C16Cl14	8.57	8.57	8.66							
Log Kow other method used	C16Cl15	8.9	8.9	8.9							
Log Kow other method used	C16Cl16	9.28									
Log Kow other method used	C17Cl1	9.29 Classic	9.29 Classic	9.47 Classic							9.28 - 9.37
Log Kow other method used	C17Cl2	8.79 Classic	9.09	8.65							
Log Kow other method used	C17Cl3	8.51 Classic	8.63	8.77	8.65 Classic	8.65 Classic	8.94 Classic				8.41 - 9.43
Log Kow other method used	C17Cl4	8.01 Classic	8.25 Classic	8.16	8.14 Classic	8.14 Classic					
Log Kow other method used	C17Cl5	7.8 Classic	7.79 Classic	8.06	8.03 Classic	7.98 Classic	8.88				8.04 - 9.52
Log Kow other method used	C17Cl6	7.58 Classic	7.5 Classic	8.3	7.99 Classic	7.7 Classic	8.44				
Log Kow other method used	C17Cl7	7.59	7.33	7.52 Classic	7.76 Classic	7.77 Classic	8.67	7.64 Classic	7.58 Classic	7.88	7.59 - 9.53
Log Kow other method used	C17Cl8	7.58	7.73	7.71	7.53	7.79	7.73				
Log Kow other method used	C17Cl9	7.56	7.6	7.66	7.76	7.9	8.02	7.8			7.35 - 9.58
Log Kow other method used	C17Cl10	7.76	7.87	7.93	7.78	8.13	8.01	7.97			

	Congener group	Input structure									Recommended range (Glüge *et al.*, 2013).
		1	2	3	4	5	6	7	8	9	
Log Kow other method used	C17Cl11	8.14	7.88	7.94	8.08	8.01	8	8.1			7.57 - 9.72
Log Kow other method used	C17C12	8.14	8.22	8.52	8.17	8.36	8.29				
Log Kow other method used	C17Cl13	8.6	8.5	8.62	8.45	8.47					7.87 - 9.69
Log Kow other method used	C17Cl14	8.86	8.71	8.81	8.93						
Log Kow other method used	C17Cl15	9.07	9.07	9.17							8.74 - 9.85
Log Kow other method used	C17Cl16	9.41	9.41	9.52							
Log Kow other method used	C17Cl17	9.8									

*In case any of the other two methods of ACD Percepta than the log P Consensus method was chosen for the prediction, it is stated in the table (see section 3.4.1.1 for further details).

Table 55: Estimated biodegradation (BIOWIN 2, 3 and 6) for a series of generated MCCP structures

Congener group	No. of input structures	EPI Suite™ Predictions			Summary of persistence
		BIOWIN 2	BIOWIN 6	BIOWIN 3	
C14Cl1	3	0.4239 - 0.823	0.4572	2.8098 - 3.1081	Does not screen as P/vP
C14Cl2	6	0.0661 - 0.309	0.0883 - 0.1986	2.5605 - 2.8588	Potentially P/vP, more information needed
C14Cl3	6	0.0011 - 0068	0.011 - 0.0679	2.0128 - 2.3112	Potentially P/vP
C14Cl4	6	0.0001 -0.0007	0.0013 - 0.0033	1.7635 - 2.0619	Potentially P/vP
C14Cl5	6	0 - 0.0001	0.0001 - 0.0004	1.5142 - 1.8126	Potentially P/vP
C14Cl6	9	0	0 - 0.0001	1.2649 - 1.5633	Potentially P/vP
C14Cl7	6	0	0	1.0157 - 1.314	Potentially P/vP
C14Cl8	8	0	0	0.7664	Potentially P/vP
C14Cl9	6	0	0	0.5171	Potentially P/vP
C14Cl10	7	0	0	0.2678	Potentially P/vP
C14Cl11	6	0	0	0.0185	Potentially P/vP
C14Cl12	7	0	0	-0.2308	Potentially P/vP
C14Cl13	3	0	0	-0.4801	Potentially P/vP
C14Cl14	1	0	0	-0.7294	Potentially P/vP
C15Cl1	3	0.3762 - 0.7921	0.4633	2.7788-3.0771	Does not screen as P/vP (borderline)
C15Cl2	3	0.0548	0.0903 - 0.2025	2.5295	Potentially P/vP more information needed
C15Cl3	6	0.0009 - 0.0055	0.0113 - 0.0284	1.9818 - 2.2802	Potentially P/vP
C15Cl4	6	0.0001 - 0.0005	0.0013 - 0.0033	1.7325 - 2.0309	Potentially P/vP
C15Cl5	9	0.0001 - 0	0.001 - 0.0004	1.4832 - 1.7816	Potentially P/vP
C15Cl6	7	0	0.0001 – 0	1.234 - 1.5323	Potentially P/vP
C15Cl7	8	0	0	0.9847 - 1.283	Potentially P/vP
C15Cl8	8	0	0	0.7354	Potentially P/vP
C15Cl9	7	0	0	0.4861	Potentially P/vP
C15Cl10	9	0	0	0.2368	Potentially P/vP
C15Cl11	6	0	0	-0.0125	Potentially P/vP
C15C12	6	0	0	-0.2618	Potentially P/vP

Congener group	No. of input structures	EPI Suite™ Predictions			Summary of persistence
		BIOWIN 2	BIOWIN 6	BIOWIN 3	
C15C13	6	0	0	-0.5111	Potentially P/vP
C15Cl14	3	0	0	-0.7604	Potentially P/vP
C15Cl15	1	0	0	-1.0097	Potentially P/vP
C16Cl1	3	0.3307 - 0.7574	0.4694	2.7478 - 3.0461	Does not screen as P/vP (borderline)
C16Cl2	3	0.0453 - 0.2309	0.0923 -0.2065	2.4985 - 2.7968	Potentially P/vP, more information needed
C16Cl3	6	0.0007 - 0.0281	0.0291 - 0.0116	1.9508 - 2.5475	Potentially P/vP
C16Cl4	6	0.0001 - 0.0004	0.0013 - 0.0087	1.706 - 1.9999	Potentially P/vP
C16Cl5	6	0	0.0002 - 0.0004	1.4523 - 1.7506	Potentially P/vP
C16Cl6	6	0	0	1.203 - 1.5013	Potentially P/vP
C16Cl7	9	0	0	0.9537 - 1.252	Potentially P/vP
C16Cl8	6	0	0	0.7044 - 1.0027	Potentially P/vP
C16Cl9	8	0	0	0.4551	Potentially P/vP
C16Cl10	6	0	0	0.2058	Potentially P/vP
C16Cl11	7	0	0	-0.0435	Potentially P/vP
C16Cl12	6	0	0	-0.2928	Potentially P/vP
C16Cl13	6	0	0	-0.5421	Potentially P/vP
C16Cl14	3	0	0	-0.7914	Potentially P/vP
C16Cl15	3	0	0	-1.0407	Potentially P/vP
C16Cl16	1	0	0	-1.29	Potentially P/vP
C17Cl1	3	0.2882 - 0.719	0.4755 - 0.6987	2.7168 - 3.0151	Potentially P/vP, more information needed
C17Cl2	3	0.0375 - 0.1987	0.0944 - 0.2106	2.4675 - 2.7658	Potentially P/vP, more information needed
C17Cl3	6	0.0006 - 0.0037	0.0118 - 0.0728	1.9199 -2.2182	Potentially P/vP
C17Cl4	5	0.0001 - 0.0004	0.0014 - 0.0089	1.6706 - 1.9689	Potentially P/vP
C17Cl5	6	0	0.0002 - 0.0004	1.4213 - 1.7196	Potentially P/vP
C17Cl6	6	0	0	1.172 - 1.4703	Potentially P/vP
C17Cl7	9	0	0	0.9227 - 1.221	Potentially P/vP
C17Cl8	6	0	0	0.6734 - 0.9717	Potentially P/vP

Congener group	No. of input structures	EPI Suite™ Predictions			Summary of persistence
		BIOWIN 2	BIOWIN 6	BIOWIN 3	
C17Cl9	7	0	0	0.4241	Potentially P/vP
C17Cl10	7	0	0	0.1748	Potentially P/vP
C17Cl11	7	0	0	-0.0745	Potentially P/vP
C17Cl12	6	0	0	-0.3238	Potentially P/vP
C17Cl13	5	0	0	-0.5731	Potentially P/vP
C17Cl14	4	0	0	-0.8224	Potentially P/vP
C17Cl15	3	0	0	-1.0717	Potentially P/vP
C17Cl16	3	0	0	-1.321	Potentially P/vP
C17C17	1	0	0	-1.5703	Potentially P/vP

*Potentially persistent or very persistent, more information needed due to the BIOWIN 3 predictions being between 2.25 and 2.75 according to PBT guidance, Chapter R.11 (ECHA, 2017b).

Annex III – Summary of environmental monitoring data

The following tables outline the available environmental monitoring data for MCCP in surface water, sludge, sediment, soil, biota and air.

Table 56: Summary of levels of MCCP in surface water and sludge

SUMMARY OF LEVELS OF MCCP 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)
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)

SUMMARY OF LEVELS OF MCCP IN SURFACE WATER AND SLUDGE				
Location	Year/Comment	Units	Concentration	Reference
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: N55º 5.7' W1º 9.3'	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
North Sea: N57º 26.2' W1º 17.0'	Relates to C_{10-20}	µg/L	not detected	Campbell and McConnell (1980)
North Sea: N57º 56.5' W1º 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)
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)

SUMMARY OF LEVELS OF MCCP IN SURFACE WATER AND SLUDGE				
Location	Year/Comment	Units	Concentration	Reference
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)
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)

SUMMARY OF LEVELS OF MCCP IN SURFACE WATER AND SLUDGE				
Location	Year/Comment	Units	Concentration	Reference
Downstream of a chlorinated paraffin manufacturing plant, Canada		µg/L	<1	Tomy *et al.* (1998)
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. MCCP 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). MCCP 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). MCCP 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. MCCP detectable in 2 samples (the concentrations may relate to SCCP + MCCP 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 57: Summary of levels of MCCP in sediment and soil
Note: soil samples are reported at the end of the Table

SUMMARY OF LEVELS OF MCCP IN SEDIMENT AND SOIL				
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)
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)

SUMMARY OF LEVELS OF MCCP IN SEDIMENT AND SOIL				
Location	Year/ Comment	Units	Concentration	Reference
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: N55º 5.7' W1º 9.3'	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
North Sea: N57º 26.2' W1º 17.0'	Relates to C_{10-20}	µg/kg	not detected	Campbell and McConnell (1980)
North Sea: N57º 56.5' W1º 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)
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)

SUMMARY OF LEVELS OF MCCP IN SEDIMENT AND SOIL				
Location	Year/ Comment	Units	Concentration	Reference
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)
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 LCCP (only traces of MCCP present)	µg/kg dry wt.	10.5	van Zeijl (1997)
Schelde estuary	Mean levels of total chlorinated paraffins - predominantly LCCP (only traces of MCCP present)	µg/kg dry wt.	5.5	van Zeijl (1997)

SUMMARY OF LEVELS OF MCCP IN SEDIMENT AND SOIL				
Location	Year/ Comment	Units	Concentration	Reference
Liffey River estuary	Mean levels of total chlorinated paraffins - predominantly LCCP (only traces of MCCP present)	µg/kg dry wt.	4.8	van Zeijl (1997)
Forth estuary	Mean levels of total chlorinated paraffins - predominantly LCCP (only traces of MCCP present)	µg/kg dry wt.	3.3	van Zeijl (1997)
Humber estuary	Mean levels of total chlorinated paraffins - predominantly LCCP (only traces of MCCP 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)
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)

SUMMARY OF LEVELS OF MCCP IN SEDIMENT AND SOIL				
Location	Year/ Comment	Units	Concentration	Reference
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)
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	MCCP 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)

SUMMARY OF LEVELS OF MCCP IN SEDIMENT AND SOIL				
Location	Year/ Comment	Units	Concentration	Reference
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	44.8	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)
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)

SUMMARY OF LEVELS OF MCCP IN SEDIMENT AND SOIL				
Location	Year/ Comment	Units	Concentration	Reference
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 58: Summary of levels of MCCP in biota (and some foodstuffs)

SUMMARY OF LEVELS OF MCCP 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 MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
	United Kingdom, remote from industry			not detected in liver, brain kidney, mesenteric fat	
Domestic Sheep *Ovis aries*	United Kingdom, close to chlorinated paraffin production site	Relates to C_{10-20}	µg/kg	200 (liver); 50 (mesenteric fat); 50 (kidney); not detected in heart, lung or perinephritic fat	Campbell and McConnell (1980)
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)
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)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
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)
Blue mussel	Baltic sea (Darsser Ort, Arkona Basin)	2015, Mean concentration of MCCP in soft body; n=100	ng/g lw	210	de Wit *et al.* (2020)
Viviparous eelpout	Baltic sea (Darsser Ort, Arkona Basin)	2015, Mean concentration of MCCP in the muscle; females and males 2 years; n=47	ng/g lw	130	de Wit *et al.* (2020)
Atlantic herring	Baltic sea (Byxelkrok, Western Gotland Basin)	2014 and 2016, Mean concentration of MCCP in muscle; females and males 7–13 years, n=40; females and males 6–12 years, n=38	ng/g lw	130	de Wit *et al.* (2020)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
Atlantic herring	Baltic sea (Byxelkrok, Western Gotland Basin)	2014 and 2016, Mean concentration of MCCP in liver; females and males 7–13 years, n=40; females and males 6–12 years, n=38	ng/g lw	160	de Wit *et al.* (2020)
Grey seal	Baltic sea (Western Gotland Basin, Åland Sea, Northern Baltic Proper)	2006–2009 and 2009–2010, Mean concentration of MCCP in muscle; 2 females and 3 males juveniles 0–1 year, n=5; adult males 8–11 years, n=4	ng/g lw	n.a.	de Wit *et al.* (2020)
Grey seal	Baltic sea (Western Gotland Basin, Åland Sea, Northern Baltic Proper)	2006–2009 and 2009–2010, Mean concentration of MCCP in blubber; 2 females and 3 males juveniles 0–1 year, n=5; adult males 8–11 years, n=4	ng/g lw	57	de Wit *et al.* (2020)
Grey seal	Baltic sea (Western Gotland Basin, Åland Sea, Northern Baltic Proper)	2006–2009 and 2009–2010, Mean concentration of MCCP in liver; 2 females and 3 males (juveniles 0–1 year), n=5; adult males 8–11 years, n=4	ng/g lw	220	de Wit *et al.* (2020)
Harbor seal	Baltic sea (Western Gotland Basin, Eastern Gotland Basin)	2014–2015 and 2012–2016, Mean concentration of MCCP in muscle; juvenile males, n=5; adults, n=4	ng/g lw	n.a.	de Wit *et al.* (2020)
Harbor seal	Baltic sea (Western Gotland Basin, Eastern Gotland Basin)	2014–2015 and 2012–2016, Mean concentration of MCCP in blubber; juvenile males, n=5; adults, n=4	ng/g lw	82	de Wit *et al.* (2020)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
Harbor seal	Baltic sea (Western Gotland Basin, Eastern Gotland Basin)	2014–2015 and 2012–2016, Mean concentration of MCCP in liver; juvenile males, n=5; adults, n=4	ng/g lw	390	de Wit *et al.* (2020)
Harbor porpoise	Baltic sea (Eastern Gotland Basin)	2008 and 2006–2012, Mean concentration of MCCP in muscle; 1 female and 1 male (juveniles), n=2; 3 females and 1 male (adults), n=4	ng/g lw	n.a.	de Wit *et al.* (2020)
Harbor porpoise	Baltic sea (Eastern Gotland Basin)	2008 and 2006–2012, Mean concentration of MCCP in blubber; 1 female and 1 male (juveniles), n=2; 3 females and 1 male (adults), n=4	ng/g lw	48	de Wit *et al.* (2020)
Harbor porpoise	Baltic sea (Eastern Gotland Basin)	2008 and 2006–2012, Mean concentration of MCCP in liver; 1 female and 1 male (juveniles), n=2; 3 females and 1 male (adults), n=4	ng/g lw	290	de Wit *et al.* (2020)
Common eider	Baltic sea (Christiansø, Bornholm Basin)	2015, Mean concentration of MCCP in eggs; female adults, n=5/5	ng/g lw	170	de Wit *et al.* (2020)
Common eider	Baltic sea (Christiansø, Bornholm Basin)	2015, Mean concentration of MCCP in liver; female adults, n=5/5	ng/g lw	370	de Wit *et al.* (2020)
Common guillemot	Baltic sea (St. Karlsö, Western Gotland Basin)	2016, Mean concentration of MCCP in eggs; n=4/5	ng/g lw	62	de Wit *et al.* (2020)
White-tailed eagle	Baltic sea (Kalmar/Blekinge Counties, Stockholm/Uppsala Counties)	2015, Mean concentration of MCCP in eggs; n=4/5	ng/g lw	200	de Wit *et al.* (2020)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
Fish	Industrial areas of the United Kingdom 1998	Highest concentration - tentatively identified as MCCP	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 al.* (2003)
Human milk	Bavaria	60 Samples. MCCP 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.)	
		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)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
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 Archived samples from 2004	µg/kg	25 8	Ismail *et al.* (2009)
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 Lake Michigan	Mean concentration, 1999 - 2004	µg/kg	not detected not detected	Houde *et al.* (2008)
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	Mean concentration,	µg/kg	109	Houde *et al.* (2008)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
	Lake Michigan	1999 - 2004		not detected	
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.* (2005a)
Spruce needles	The Alps	Eight samples collected in October 2004. Concentrations refer to MCCP.	µg/kg	5.2 - 95	Iozza *et al.* (2009a)
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)
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)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
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)
Cod	Liaodong Bay, North China	2017	µg/kg lipid weight	22.37 ± 9.17	Huang *et al.* (2017)
Common Barbel *Barbus barbus*	Chéran River (mean)	2019	µg/kg lipid weight	7 123	Labadie *et al.* (2019)
	Usses River (mean)	2019	µg/kg lipid weight	4 615	
	Combeauté River (mean)	2019	µg/kg lipid weight	5 423	
	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)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
Rat *Rattus norvegicus*	Oslo, Norway	2017, liver	µg/kg ww	Mean: 183 Median: 177 Minimum: 81.0 Maximum: 327	Heimstad *et al.* (2017)
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	2018	µg/kg ww	Median±SD:2.81 ±4 Min.: 2.76 Max.:9.52	Green *et al.* (2019)
	Tjøme, Outer Oslofjord, Norway	2018	µg/kg ww	Median±SD: 34.4±10 Min.: 30.2 Max.:49.7	
	Singlekalven, Hvaler, Norway	2018	µg/kg ww	Median±SD: 7.21±12 Min.: 7.16 Max.:27.6	
	Sylterøya, Langesundfjord, Norway	2018	µg/kg ww	Median±SD: 42.4±1119 Min.: 3.27 Max.:1960	
	Nordnes, Bergen harbour, Norway	2018	µg/kg ww	Median±SD: 87.1±13 Min.: 67.3 Max.:91.4	
	Vågsvåg, Outer Nordfjord, Norway	2018	µg/kg ww	Median±SD: 11.5±3 Min.: 10.9 Max.:16.1	
	Ålesund harbour area, Norway	2018	µg/kg ww	Median±SD: 21.7±4 Min.: 19.7 Max.:26.8	
	Ørland area, Outer Trondheimsfjord, Norway	2018	µg/kg ww	Median±SD: 28.1±4 Min.: 23.5 Max.:31.5	

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
Atlantic Cod *Gadus morhua*	Bodø harbour, Norway	2018	µg/kg ww	Median±SD: 170±644 Min.: 33.3 Max.:1210	Green *et al.* (2019)
	Mjelle, Bodø area, Norway	2018	µg/kg ww	Median±SD: 7.61±1 Min.: 6.04 Max.:7.9	
	Svolvær airport area, Norway	2018	µg/kg ww	Median±SD: 53.1±30 Min.: 48.2 Max.:103	
	Inner Oslofjord, Norway	2018, liver	µg/kg ww	Median±SD: 105.5±25 Min.: 66.8 Max.:146	
	Tjøme, Outer Oslofjord, Norway	2018, liver	µg/kg ww	Median±SD: 65.9±117.7 Min.: 50.5 Max.:474	
	Kirkøy, Hvaler, Norway	2018, liver	µg/kg ww	Median±SD: 60.95±82 Min.: 57.3 Max.:224	
	Stathelle area, Langesundfjord, Norway	2018, liver	µg/kg ww	Median±SD: 108±66 Min.: 70.2 Max.:266	
	Kristiansand harbour area, Norway	2018, liver	µg/kg ww	Median±SD: 77.8±35 Min.: 65.6 Max.:171	
	Inner Sørfjord, Norway	2018, liver	µg/kg ww	Median±SD: 99.6±79 Min.: 52.7 Max.:331	
	Bømlo, Outer Selbjørnfjord, Norway	2018, liver	µg/kg ww	Median±SD: 69.5±28 Min.: 49.5 Max.:131	
	Bergen harbour area, Norway	2018, liver	µg/kg ww	Median±SD: 80.8±516 Min.: 58.5 Max.:1830	

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
	Ålesund harbour area, Norway	2018, liver	µg/kg ww	Median±SD: 114±225 Min.: 50 Max.:957	
	Trondheim harbour, Norway	2018, liver	µg/kg ww	Median±SD: 107±62 Min.: 62.3 Max.:288	
	Austnesfjord, Lofoten, Norway	2018, liver	µg/kg ww	Median±SD: 124.5±72 Min.: 68.4 Max.:320	
	Tromsø harbour area, Norway	2018, liver	µg/kg ww	Median±SD: 77±1373 Min.: 50 Max.:5390	
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 *Gadus morhua*	Inner Oslofjord, Norway	2017, liver	µg/kg ww	Median: 498.0	Green *et al.* (2018)
	Tjøme, Outer Oslofjord, Norway	2017, liver	µg/kg ww	Median: 35.15	

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
	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	
Mink *Neovison vison*	Islands of Sommarøy and Hillerøy, in Troms County, Norway	2013 and 2014, liver; n=10 samples; detection frequency = 100%	ng/g ww	Average: 13 Min. – Max.: 1.1–32	Schlabach *et al.* (2018)
Common gull *Larus canus*	Tromsøya island, Tromsø, Norway	June 2017, eggs; n=5 eggs; detection frequency = 100%	ng/g ww	Average: 40 Min. – Max.: 9.4–87	Schlabach *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	
		2014, female and male 7 – 13 years, liver	µg/kg lipid	140	
		2014 female and male, 7–13 years, muscle	µg/kg lipid	120	

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
Common Eider *Somateria mollissima*	Scandinavia	2016 female and male, 6 – 12 years, liver	µg/kg lipid	170	Yuan *et al.* (2019)
		2016, female and male 6 – 12 years, muscle	µg/kg lipid	140	
		2015, female adults, liver	µg/kg lipid	440	
		2015, egg	µg/kg lipid	140-200	
		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 *Phocoena phocoena*	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)	
		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)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
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)
Red-backed Rat Snake *Elaphe rufodorsata*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in liver; October 2011, N=9; Relates to MCCP with 53.1±0.4 Cl wt (mean value).	ng/g lw	1 500±970 (<LOQ–3 500)	Du *et al.* (2020)
Red-backed Rat Snake *Elaphe rufodorsata*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in muscle; October 2011, N=9; Relates to MCCP with 52.3±0.4 Cl wt (mean value).	ng/g lw	5 500±3 500 (2 100 – 11 000)	Du *et al.* (2020)
Red-backed Rat Snake *Elaphe rufodorsata*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in adipose tissues; October 2011, N=9; Relates to MCCP with 54.4±1.4 Cl wt (mean value).	ng/g lw	230±420 (<LOQ – 1 300)	Du *et al.* (2020)
Short-tailed Mamushi *Gloydius brevicaudus*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in liver; October 2011, N=7; Relates to MCCP with 54.0±0.7 Cl wt (mean value).	ng/g lw	1 800±1 800 (<LOQ–5 100)	Du *et al.* (2020)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
Short-tailed Mamushi *Gloydius brevicaudus*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in muscle; October 2011, N=7; Relates to MCCP with 57.0±0.2 Cl wt (mean value).	ng/g lw	14 000±5 700 (7 400–22 000)	Du *et al.* (2020)
Short-tailed Mamushi *Gloydius brevicaudus*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in adipose tissues; October 2011, N=7; Relates to MCCP with 54.7±0.9 Cl wt (mean value).	ng/g lw	170±110 (44–290)	Du *et al.* (2020)
Black-spotted Frogs *Pelophylax nigromaculatus*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in liver; 2011; females N=12; Relates to MCCP with 53.5±0.2 Cl wt	ng/g ww	69±47 (31–190)	Du *et al.* (2019)
Black-spotted Frogs *Pelophylax nigromaculatus*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in liver; 2011; males N=12; Relates to MCCP with 53.6±0.4 Cl wt	ng/g ww	68±59 (5.5–180)	Du *et al.* (2019)
Black-spotted Frogs *Pelophylax nigromaculatus*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in eggs; 2011; N=12; Relates to MCCP with 53.9±0.6 Cl wt	ng/g ww	16±14 (<LOQ–52)	Du *et al.* (2019)
Black-spotted Frogs *Pelophylax nigromaculatus*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in muscle; 2011; females N=3 pool samples; Relates to MCCP with 52.8±0.6 Cl wt	ng/g ww	5±3	Du *et al.* (2019)
Black-spotted Frogs *Pelophylax nigromaculatus*	Paddy fields in the Yangtze River Delta, China	mean±SD (min-max) values in muscle; 2011; males N=2 pool samples; Relates to MCCP with 52.2–52.4 Cl wt	ng/g ww	25±50	Du *et al.* (2019)
Pond Loach *Misgurnus anguillicaudatus*	Paddy fields in the Yangtze River Delta, China	Median (min-max); 2011	µg/kg lw µg/kg dw	2 500 (1 400 – 2 600) 270 (170 – 430)	Du *et al.* (2018)
Rice Field Eel *Monopterus albus*	Paddy fields in the Yangtze River Delta, China	Median (min-max); 2011	µg/kg lw	2 600 (820 – 3 700)	Du *et al.* (2018)

SUMMARY OF LEVELS OF MCCP 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); 2011	µg/kg dw µg/kg lw µg/kg dw	140 (50 – 270) 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); 2011	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); 2011	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); 2011	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); 2011	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); 2011	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); 2011	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)
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)
Herring Gull *Larus argentatus*	Inner Oslofjord	Blood (detected in all 15 samples)	µg/kg ww	Arithmetic mean 28.23 (range: 8.2-76)	Ruus *et al.* (2018)

SUMMARY OF LEVELS OF MCCP IN BIOTA (and some foodstuffs)					
Sample	Location	Comment	Units	Level	Reference
	Outer Oslofjord	Blood (detected in all 15 samples)	µg/kg ww	Arithmetic mean 38.87 (range: 5.8-200)	Ruus *et al.* (2018)
	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 59: Summary of levels of MCCP in air

SUMMARY OF LEVELS OF MCCP IN AIR				
Location	Comment	Units	Concentration	Reference
Birkenes, Norway	Air samples (bulk concentrations: sum gas- and particle phase), 2019, monthly and annual mean concentrations	pg/m^3	267 (January) <190 (Feb.) <190 (March) <190 (April) <190 (May) 287 (June) 1507 (July) 336 (August) <190 (Sept.) 414 (October) 460 (Nov.) <190 (Dec.) 327 (mean in 2019)	Bohlin-Nizzetto *et al.*, 2020
Dongjiang River, China	Air samples Atmospheric depositions (wet and dry) at 11 sites	µg/sampler µg/(m^{2}d)	4.1 5.3	Wang *et al.* (2013)
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)

Annex IV – Modelling of bioaccumulation potential (BCF)

The BCF Baseline model (v. 03.10) of CATALOGIC (v.5.13.1.156)(LMC, 2018) has been used to predict BCF of congener groups $C_{14}Cl_{1-14}$, $C_{15}Cl_{1-15}$, $C_{16}Cl_{1-16}$ and $C_{17}Cl_{1-17}$ and their structural isomers. The selection and generation of structures to represent MCCP is explained in 'Annex II – Modelling of log Kow and biodegradation and generation of representative structures for MCCP'. In addition to the general selection, some additional structures were further selected for some congener groups in order to gain a better understanding of the spread of BCF predictions within the congener group. For the following congener groups additional structures were generated; $C_{14}Cl_{9}$, $C_{14}Cl_{10}$, $C_{15}Cl_{3}$, $C_{15}Cl_{9}$, $C_{15}Cl_{10}$, $C_{16}Cl_{4}$, $C_{16}Cl_{5}$, $C_{16}Cl_{10}$ and $C_{16}Cl_{11}$. In total 420 structures were used for the BCF predictions (see Table 60 below).

Table 60: Evaluation of applicability domain for the MCCP congeners

	Total no structures	In AD*	Out AD*	Structural domain out	Metabolic domain out
C14	102	69	33	21	12
C15	110	70	40	22	18
C16	121	72	49	26	23
C17	87	53	34	19	15
Total	420	264	156	88	68
%		63%	37%	21%	16%

*AD =Applicability domain

Table 61: BCF predictions, input log Kow and B conclusions for MCCP congeners and their structural isomers

	Congener group	Input structure										Overall conclusion
		1	2	3	4	5	6	7	8	9	10	
Log BCF	C14Cl1	2.93	2.62	2.25								
B potential		not B	not B	not B								not B
Log Kow input		7.7	7.69	7.69								
Log BCF	C14Cl2	3.58	3.36	2.88	2.76	2.18	1.74					
B potential		B	B	not B	not B	not B	not B					B
Log Kow input		7.19	7.8	7.95	7.38	7.63	8.16					
Log BCF	C14Cl3	3.85	3.19	3.02	1.63	1.45	1.84					
B potential		vB	not B	not B	not B	not B	not B					vB
Log Kow input		6.68	7.68	7.24	7.06	7.05	6.89					

	Congener group	Input structure										Overall conclusion
		1	2	3	4	5	6	7	8	9	10	
Log BCF	C14Cl4	2.33	3.79	3.77	2.73	1.89	2.61					
B potential		not B	vB	vB	not B	not B	not B					vB
Log Kow input		6.76	6.65	7.21	7.12	6.65	7.94					
Log BCF	C14Cl5	3.82	3.74	3.58	3.04	3.12	2.96					
B potential		vB	vB	B	not B	not B	not B					B/vB
Log Kow input		6.43	6.2	7.45	6.23	6.62	7.35					
Log BCF	C14Cl6	3.82	3.81	3.81	3.12	3.14	3.18	1.06	2.42	2.53		
B potential		vB	vB	vB	not B	not B	not B	not B	not B	not B		vB
Log Kow input		6.4	6.36	6.76	6.45	6.7	7.01	6.7	6.71	6.63		
Log BCF	C14Cl7	3.8	3.65	3.85	3.17	3.22	2.56					
B potential		vB	B	vB	not B	not B	not B					B/vB
Log Kow input		6.6	6.26	6.58	6.64	6.59	6.89					
Log BCF	C14Cl8	3.89	3.87	3.81	3.2	3.1	3.12	2.55	2.66			
B potential		vB	vB	vB	not B	not B	not B	not B	not B			vB
Log Kow input		6.55	6.67	6.59	6.62	7.15	6.93	6.78	6.66			
Log BCF	C14Cl9	3.76	3.17	3.17	3.09	2.52	2.44	3.8	3.14	2.6	3.16	
B potential		vB	not B	not B	not B	not B	not B	vB	not B	not B	not B	vB
Log Kow input		6.92	6.83	6.75	7	6.99	7.1	6.95	6.9	6.79	6.85	
Log BCF	C14Cl10	3.63	3.02	3.09	3	2.51	2.42	2.49	3.64	2.37	3.1	
B potential		B	not B	not B	not B	not B	not B	not B	B	not B	not B	B
Log Kow input		7.04	7.18	7.05	7.23	7.04	7.23	7.05	7.3	7.17	6.99	
Log BCF	C14Cl11	3.59	3.58	3.57	2.99	2.25	2.31					
B potential		B	B	B	not B	not B	not B					B
Log Kow input		7.3	7.29	7.46	7.35	7.25	7.41					
Log BCF	C14C12	3.39	2.87	2.8	2.69	2.23	2.17	2.16				
B potential		B	not B	not B	not B	not B	not B	not B				not B
Log Kow input		7.63	7.6	7.6	7.78	7.57	7.57	7.66				
Log BCF	C14C13	2.01	2.05	2.02	1.64							
B potential		not B	not B	not B	not B							not B

	Congener group	Input structure										Overall conclusion
		1	2	3	4	5	6	7	8	9	10	
Log Kow input		7.91	7.91	8	8.25							
Log BCF	C14Cl14	1.58	1.61	1.59								
B potential		not B	not B	not B								not B
Log Kow input		8.4	8.4	8.4								
Log BCF	C15Cl1	2.33	2.09	1.72								
B potential		not B	not B	not B								not B
Log Kow input		8.22	8.25	8.25								
Log BCF	C15Cl2	2.91	2.39	1.94								
B potential		not B	not B	not B								not B
Log Kow input		7.31	7.84	7.92								
Log BCF	C15Cl3	2.46	3.57	3.05	1.46	2.69	1.29	2	3.53	1.94	3.54	
B potential		not B	B	not B	not B	not B	not B	not B	B	not B	B	B
Log Kow input		7.22	7.42	8	7.69	7.59	8.92	7.5	7.42	7.5	7.45	
Log BCF	C15Cl4	3.34	3.61	3	2.97	2.64	1.24					
B potential		B	B	not B	not B	not B	not B					B
Log Kow input		7.47	7.29	8.15	7.13	7.65	8.15					
Log BCF	C15Cl5	3.67	1.93	3.53	3.07	2.89	2.9	2.45	2.44	2.2		
B potential		B	not B	B	not B	not B	not B	not B	not B	not B		B
Log Kow input		7.01	6.78	7.58	6.55	7.2	7.59	6.8	6.81	7.1		
Log BCF	C15Cl6	3.63	3.71	3.34	1.27	3.11	2.77	2.42				
B potential		B	vB	B	not B	not B	not B	not B				B/vB
Log Kow input		6.63	6.97	7.71	6.57	6.64	7.71	7.08				
Log BCF	C15Cl7	3.75	3.65	2.96	2.8	2.91	2.31	2.4	2.47			
B potential		vB	B	not B	not B	not B	not B	not B	not B			B/vB
Log Kow input		6.81	6.98	7.05	7.58	7.36	7.21	7.15	7.14			
Log BCF	C15Cl8	3.68	3.55	3.58	2.96	2.94	2.99	2.41	2.39			
B potential		B	B	B	not B	not B	not B	not B	not B			B
Log Kow input		6.99	7.33	7.23	7.18	7.28	7.02	7.03	7.03			
Log BCF	C15Cl9	3.53	2.83	3.05	3	1.87	1.98	2.03	3.62			

	Congener group	Input structure										Overall conclusion
		1	2	3	4	5	6	7	8	9	10	
B potential		B	not B	not B	not B	not B	not B	not B	B			B
Log Kow input		7.19	7.35	7.19	7.23	7.97	7.68	7.68	7.19			
Log BCF	C15Cl10	3.52	3.44	3.58	2.87	2.9	2.76	2.4	2.22	2.25	3.48	
B potential		B	B	B	not B	not B	not B	not B	not B	not B	B	B
Log Kow input		7.25	7.43	7.35	7.22	7.28	7.41	7.19	7.26	7.47	7.48	
Log BCF	C15Cl11	2.64	2.75	2.73	2.24	2.13	2.12					
B potential		not B	not B	not B	not B	not B	not B					not B
Log Kow input		7.57	7.65	7.62	7.49	7.54	7.56					
Log BCF	C15Cl12	3.22	3.27	3.2	2.54	2.15	2.04					
B potential		not B	not B	not B	not B	not B	not B					not B
Log Kow input		7.81	7.81	7.87	7.84	7.73	7.92					
Log BCF	C15Cl13	2.44	2.46	2.36	1.76	1.8	1.81					
B potential		not B	not B	not B	not B	not B	not B					not B
Log Kow input		8.1	8.1	8.1	8.16	8.07	8.16					
Log BCF	C15Cl14	1.58	1.61	1.59								
B potential		not B	not B	not B								not B
Log Kow input		8.4	8.4	8.4								
Log BCF	C15Cl15	1.32										
B potential		not B										not B
Log Kow input		8.76										
Log BCF	C16Cl1	1.9	1.55	1.33								
B potential		not B	not B	not B								not B
Log Kow input		8.76	8.76	8.76								
Log BCF	C16Cl2	2.42	1.63	1.24								
B potential		not B	not B	not B								not B
Log Kow input		7.9	8.79	8.95								
Log BCF	C16Cl3											
B potential		2.59 not B	2.97 not B	2.16 not B	1.67 not B	1.47 not B	1.1 not B					not B
Log Kow input		7.98	8.15	8.98	8.17	8.22	9.19					

	Congener group	Input structure										Overall conclusion
		1	2	3	4	5	6	7	8	9	10	
Log BCF	C16Cl4	3.34	1.9	1.46	1.22	1.89	0.92	2.65	1.35	2.38	2.6	
B potential		B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B
Log Kow input		7.76	9.1	7.79	7.61	7.85	8.19	7.76	7.42	7.67	8.48	
Log BCF	C16Cl5	3.53	3.19	3.19	2.66	2.67	1.11	3.38	2.86	3.43	2.36	
B potential		B	not B	not B	not B	not B	not B	B	not B	B	not B	B
Log Kow input		7.27	7.78	7.79	7.68	7.44	7.93	7.55	7.73	7.49	8.12	
Log BCF	C16Cl6	3.51	3.49	3.16	2.83	2.99	2.34					
B potential		B	B	not B	not B	not B	not B					B
Log Kow input		7.26	7.22	7.9	7.17	7.04	8.08					
Log BCF	C16Cl7	3.45	3.41	3.52	2.82	2.9	2.79	2.15	2.05	2.18		
B potential		B	B	B	not B	not B	not B	not B	not B	not B		B
Log Kow input		7.07	7.28	7.28	7.22	7.3	7.3	7.2	7.62	7.4		
Log BCF	C16Cl8	3.51	3.41	3.33	2.86	2.62	2.06					
B potential		B	B	B	not B	not B	not B					B
Log Kow input		7.14	7.46	7.52	7.36	7.7	7.64					
Log BCF	C16Cl9	3.41	3.47	3.26	2.54	2.59	2.71	2.23	2.13			
B potential		B	B	not B	not B	not B	not B	not B	not B			B
Log Kow input		7.27	7.3	7.52	7.61	7.65	7.65	7.34	7.47			
Log BCF	C16Cl10	3.34	2.61	2.68	2.54	1.91	2.14	2.65	2.77	3.34	3.41	
B potential		B	not B	not B	not B	not B	not B	not B	not B	B	B	B
Log Kow input		7.46	7.5	7.53	7.7	7.74	7.52	7.53	7.43	7.65	7.46	
Log BCF	C16Cl11	3.19	2.63	2.57	2.32	2	1.99	1.92	2.97	3.16	2.98	
B potential		not B	not B	not B	not B	not B	not B	not B	not B	not B	not B	not B
Log Kow input		7.63	7.66	7.72	7.99	7.74	7.66	7.83	8.06	7.87	8.06	
Log BCF	C16Cl12	3.01	2.99	2.88	2.27	1.76	1.75					
B potential		not B	not B	not B	not B	not B	not B					not B
Log Kow input		7.98	8.03	8.16	8.1	7.98	8.16					
Log BCF	C16Cl13	2.19	2.25	2.13	1.57	1.43	1.58					
B potential		not B	not B	not B	not B	not B	not B					not B

	Congener group	Input structure										Overall conclusion
		1	2	3	4	5	6	7	8	9	10	
Log Kow input		8.26	8.26	8.45	8.31	8.42	8.4					
Log BCF	C16Cl14	1.47	1.54	1.38								
B potential		not B	not B	not B								not B
Log Kow input		8.57	8.57	8.66								
Log BCF	C16Cl15	1.28	1.32	1.26								
B potential		not B	not B	not B								not B
Log Kow input		8.9	8.9	8.9								
Log BCF	C16Cl16	1.12										
B potential		not B										not B
Log Kow input		9.28										
Log BCF	C17Cl1	1.48	1.17	0.9								
B potential		not B	not B	not B								not B
Log Kow input		9.29	9.29	9.47								
Log BCF	C17Cl2	2.55	1.35	1.33								
B potential		not B	not B	not B								not B
Log Kow input		8.79	9.09	8.65								
Log BCF	C17Cl3											
B potential		2.65 not B	2.4 not B	1.74 not B	0.94 not B	0.92 not B	0.9 not B					not B
Log Kow input		8.51	8.63	8.77	8.65	8.65	8.94					
Log BCF	C17Cl4	3.04	1.12	1.23	1	1.03						
B potential		not B	not B	not B	not B	not B						not B
Log Kow input		8.01	8.25	8.16	8.14	8.14						
Log BCF	C17Cl5	3.21	3.1	2.94	1.08	2.33	1.86					
B potential		not B	not B	not B	not B	not B	not B					not B
Log Kow input		7.8	7.79	8.06	8.03	7.98	8.88					
Log BCF	C17Cl6	3.3	3.22	2.72	2.52	2.57	1.99					
B potential		B	not B	not B	not B	not B	not B					not B
Log Kow input		7.58	7.5	8.3	7.99	7.7	8.44					
BCF	C17Cl7	3.14	3.41	3.27	2.51	2.53	1.93	2.07	1.93	1.81		

	Congener group	Input structure										Overall conclusion
		1	2	3	4	5	6	7	8	9	10	
B potential		not B	B	not B	not B	not B	not B	not B	not B	not B		not B
Log Kow input		7.59	7.33	7.52	7.76	7.77	8.67	7.64	7.58	7.88		
Log BCF	C17Cl8	3.09	3.16	3.07	2.64	2.4	1.99					
B potential		not B	not B	not B	not B	not B	not B					not B
Log Kow input		7.58	7.73	7.71	7.53	7.79	7.73					
Log BCF	C17Cl9	3.14	3.23	3.1	2.4	2.34	2.29	1.77				
B potential		not B	not B	not B	not B	not B	not B	not B				not B
Log Kow input		7.56	7.6	7.66	7.76	7.9	8.02	7.8				
Log BCF	C17Cl10	2.94	3.02	2.49	2.43	2.32	1.73	1.81				
B potential		not B	not B	not B	not B	not B	not B	not B				not B
Log Kow input		7.76	7.87	7.93	7.78	8.13	8.01	7.97				
Log BCF	C17Cl11	2.94	2.35	2.35	2.19	1.75	1.74	1.64				
B potential		not B	not B	not B	not B	not B	not B	not B				not B
Log Kow input		8.14	7.88	7.94	8.08	8.01	8	8.1				
Log BCF	C17Cl12	2.79	2.74	2.66	2.07	2.09	1.53					
B potential		not B	not B	not B	not B	not B	not B					not B
Log Kow input		8.14	8.22	8.52	8.17	8.36	8.29					
Log BCF	C17Cl13	1.94	1.95	1.8	1.42	1.47						
B potential		not B	not B	not B	not B	not B						not B
Log Kow input		8.6	8.5	8.62	8.45	8.47						
Log BCF	C17Cl14	1.79	1.26	1.19	1.24							
B potential		not B	not B	not B	not B							not B
Log Kow input		8.86	8.71	8.81	8.93							
Log BCF	C17Cl15	1.14	1.18	1.1								
B potential		not B	not B	not B								not B
Log Kow input		9.07	9.07	9.17								
Log BCF	C17Cl16	1.08	1.11	1.03								
B potential		not B	not B	not B								not B
Log Kow input		9.41	9.41	9.52								

	Congener group	Input structure										Overall conclusion
		1	2	3	4	5	6	7	8	9	10	
Log BCF	C17Cl17	1										
B potential		not B										not B
Log Kow input		9.8										

Annex V – Growth correction of the BCF for a C_{15}, 51% Cl wt. substance

The background to the corrections made in this Annex is discussed in detail in EA (2011). The study performed by AstraZeneca (Thompson *et al.*, 2000) was originally summarised in EC (2005). The relevant kinetic parameters are summarised in Table 62.

Table 62: 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 7 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).

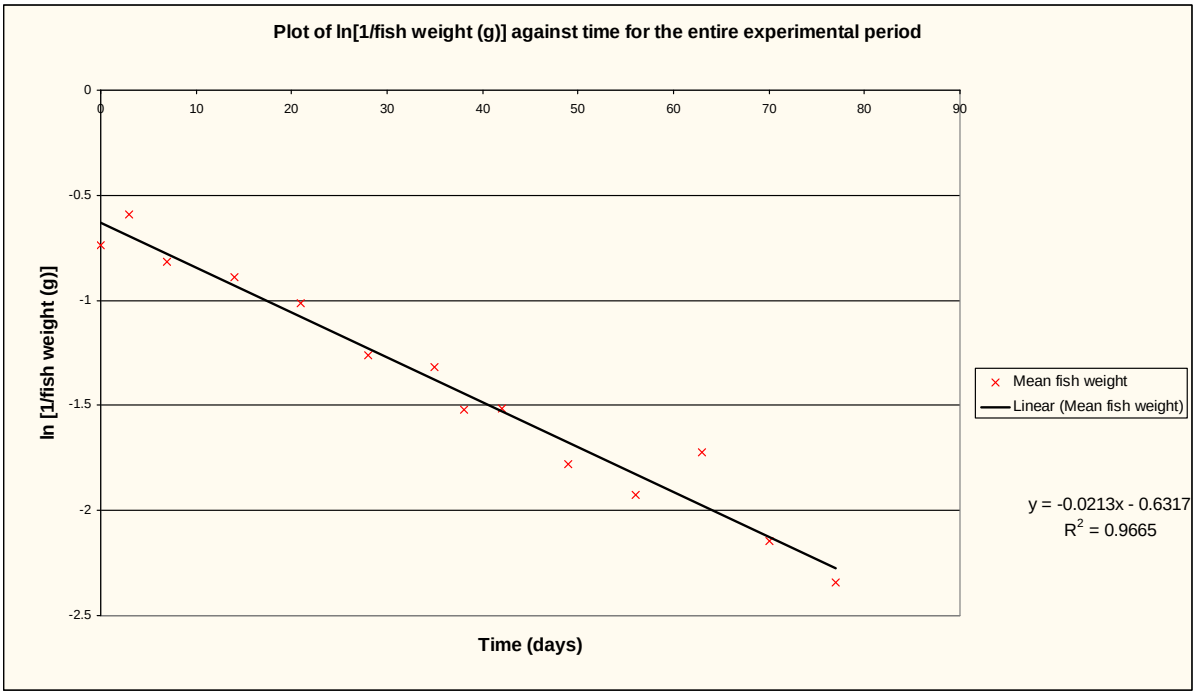


Figure 7: Determination of growth rate constant over the uptake and depuration phase

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 R^2 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 62.

Table 63: 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 Thompson *et al.*, (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 Thompson *et al.* (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[26]. 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 constant on the predicted growth corrected BCF is shown in Table 62 – the estimated BCF is slightly lower.

[26] 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.

Annex VI – Consideration of bioavailability in laboratory bioconcentration tests

MCCP have a low water solubility and a high log Kow. 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 minimise 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 MCCP 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)

Kow = octanol/water partition coefficient

0.35 and 0.08 are proportionality constants relating Kow 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 Kow 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 Kow 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 MCCP, 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 Kow. 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. 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 there is a possibility that POC or TOC could influence the freely dissolved concentration MCCP, 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.

Annex VII – Outcome of the statistic of the linear model for the BCF data for C_{14} chlorinated n-alkane, 45 % Cl wt. (Unpublished, 2010h) with the statistical software R

```
Call:
lm(formula = Cfish ~ days, data = xltable)

Residuals:
    Min      1Q  Median      3Q     Max
-224.94  -96.36  -13.94  119.07  264.46

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 1419.626    217.807   6.518 2.86e-05 ***
days          24.547      7.499   3.273  0.00666 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 156.9 on 12 degrees of freedom
Multiple R-squared:  0.4717,   Adjusted R-squared:  0.4277
F-statistic: 10.71 on 1 and 12 DF,  p-value: 0.006664
```

Annex VIII – Calculations performed on the dietary BMF study (Unpublished, 2019e)

The BMF_{kgL} values for the different congeners of the MCCP test substance[27] (including total substance) used in the study (Unpublished, 2019e) have been calculated in accordance with the approach set out in OECD TG 305 based on the following parameters:

Mean lipid fraction in fish (L_{fish}) and in food (L_{food})

According to OECD TG 305, the mean lipid fraction (w/w) in the fish and in the food are derived for both treatment and control groups (for food and control group fish this is usually from data measured at exposure start and end; for treatment group fish this is usually from data measured at end of exposure only). In some studies, fish lipid content may increase markedly; in such cases it is more appropriate to use a mean test fish lipid concentration calculated from the measured values at the end of exposure and end of depuration.

As the concentration in fish increased during the study, the mean test fish lipid concentration was calculated from the measured values at the end of exposure and end of depuration. In the study, the mean lipid fraction in fish was 5.793%.

For food group fish, the mean lipid fraction in the food was derived from data measured at exposure start and end. In the study, the mean lipid fraction in food was 16.35%.

Mean measured concentration of the test substance in the food or C_{food}

According to OECD TG 305, the mean measured concentration of the test substance in the food (C_{food}) is a measured variable in the study. The C_{food} was calculated based on concentrations reported during the test (14 day uptake and 0 day depuration). The C_{food} values for the different congeners and total substance (C_{14} chlorinated n-alkane, 50% Cl wt.) are reported in Table 64.

Table 64: Mean measured concentration of the test substance in the food (C_{food}) in **(µg/g** ww of food) or (mg/kg ww of food)

	$C_{14}Cl_3$	$C_{14}Cl_4$	$C_{14}Cl_5$	$C_{14}Cl_6$	$C_{14}Cl_7$	$C_{14}Cl_8$	$C_{14}Cl_9$	$C_{14}Cl_{10}$	$C_{14}Cl_{11}$	$C_{14}Cl_{12}$	$C_{14}Cl_{13}$	$C_{14}Cl_{14}$	C_{14} chlorinated n-alkane, 50% Cl wt.
C_{food}	0.01	0.53	3.93	5.90	3.90	1.47	0.44	0.14	0.06	0.03	0.01	0.01	16.43

Growth rate constant (k_g) subtraction method for growth correction

In accordance with OECD TG 305, a linear least squares correlation was calculated for the ln(fish weight) vs. day for each group (test(s) and control groups, individual data, not daily mean values) for the whole study, uptake and depuration phases.

The variances in the slopes of the lines were calculated and used to evaluate the statistical significance (p = 0.05) of the difference in the slopes (growth rate constants) using the emtrends function from the emmeans package in the R software.

Pairwise comparisons of the slopes between the different groups were performed following the Tukey method, as follows:

```
contrast                              estimate      SE  df t.ratio p.value
Control - Treated_Depuration         -0.00107 0.00294 174 -0.365  0.9291
Control - Treated_Uptake              0.00583 0.01288 174  0.452  0.8935
Treated_Depuration - Treated_Uptake   0.00690 0.01297 174  0.532  0.8557
```

Based on the above results from the R software, it is concluded that there is no statistically

[27] A GLP-certified OECD TG 305 dietary study using a C_{14} chlorinated n-alkane, 50% Cl wt. was performed. It was a liquid identified as tetradecane chlorinated 50% and contained a total chlorine content of 50.07% (w/w) (average value; with 3 to 14 chlorine atoms per molecule (equivalent to 35.32–72.98% Cl wt.). It was prepared by chlorination of n-tetradecane 99% and contained no stabiliser.

significant difference in the fish weight data analysis between the test (uptake phase and depuration phase) and control data. All the data (test uptake phase, test depuration phase and control) were pooled and an overall fish growth rate constant for the study (k_g) calculated as the overall slope of the linear correlation.

The overall fish growth rate constant for the study (k_g) was calculated using a linear model in the R software:

```
Call:
lm(formula = LN_Fish_Weight ~ Days, data = slopesgrowthrate)

Residuals:
     Min       1Q   Median       3Q      Max
-0.86680 -0.28393  0.04299  0.25790  0.88141

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 0.846203   0.040583   20.85   <2e-16 ***
Days        0.018794   0.001441   13.04   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3622 on 178 degrees of freedom
Multiple R-squared:  0.4886,   Adjusted R-squared:  0.4857
F-statistic:   170 on 1 and 178 DF,  p-value: < 2.2e-16
```

The overall fish growth rate constant for the study (k_g) is 0.018794.

It is worth noting that the following fish samples were excluded from the calculation of the growth rate as MCCP congeners were not detected in these samples: L1-WF19, L1-WF23 and L1-WF35.

Determination of depuration (loss) rate constant k_2

The depuration (loss) rate constants k_2 were calculated for all MCCP constituents (including total substance) by performing a linear regression of ln(concentration) versus time. The slope of the regression line is an estimate of the depuration rate constant k_2.

Sample “L1-WF35” has been excluded from the calculation of the depuration rate, as suggested by the laboratory, as the combination of the low lipid content and the low wet weight is indicative of a problem with this sample.

For C_{14} chlorinated n-alkane, 50% Cl wt., data points at day 56 with a concentration < LOD have been replaced to “LOD/2” (at other time, data points at a concentration < LOD have been excluded).

For all MCCP congeners, data points at a concentration < LOD have been excluded in the calculation of the depuration rate.

Table 65: Depuration rate constant k_2 for MCCP congener groups (including total substance)

	$C_{14}Cl_3$	$C_{14}Cl_4$	$C_{14}Cl_5$	$C_{14}Cl_6$	$C_{14}Cl_7$	$C_{14}Cl_8$	$C_{14}Cl_9$	$C_{14}Cl_{10}$	$C_{14}Cl_{11}$	$C_{14}Cl_{12}$	$C_{14}Cl_{13}$	$C_{14}Cl_{14}$	C_{14} chlorinated n-alkane, 50% Cl wt.
Best fit model used for the calculation of k_2	-	-	Box-cox power transformation model (see outcome bcmfR R-package)	Logarithm transformation model (see outcome bcmfR R-package)	Untransformed model (see outcome bcmfR R-package)	Logarithm transformation model (see outcome bcmfR R-package)	Box-cox power transformation model (see outcome bcmfR R-package)	Logarithm transformation model (see outcome bcmfR R-package)	Logarithm transformation model (see outcome bcmfR R-package)	-	-	-	Untransformed model (see outcome bcmfR R-package)
Depuration rate constant (k_2) (day^{-1})	K_2 not derived as these congeners were not detected	K_2 not derived as only two data points available. However, a lack of depuration cannot be excluded	0.0021	0.02302	0.026786	0.01244	0.01044	0.00962	0.01163	K_2 not derived as only two data points available. However, a lack of depuration cannot be excluded	K_2 not derived as only data points for two days are available. However, a lack of depuration cannot be excluded	K_2 not derived as these congeners were only detected at depuration day 3	0.02741

For C_{14} Cl_3 congeners, as this group of congeners was not detected during the test it was not possible to derive any depuration rate constant (k_2). For C_{14} Cl_{14} congeners, as this group of congeners was only detected at depuration day 3 it was not possible to derive any depuration rate constant (k_2).

For $C_{14}Cl_4$ and $C_{14}Cl_{12}$, only two data points were available for the calculation of the depuration rate constant (k_2). As it was not possible to conclude based on two data points, it was not possible to derive a k_2 value for these congeners. It is worth noting that the concentration of these congeners was increasing between depuration day 1 and day 3 thus suggesting that no depuration was occurring in *Oncorhynchus mykiss*. While it is not possible to conclude based on two data points, a lack of depuration in *Oncorhynchus mykiss* for $C_{14}Cl_4$ and $C_{14}Cl_{12}$ cannot be excluded. The same reasoning applies to $C_{14}Cl_{13}$ as only data for two days are available. As for the two other congeners, as the concentration of this group of congeners was increasing between depuration day 1 and day 3 thus suggesting that no depuration was occurring *Oncorhynchus mykiss*. While it is not possible to conclude based on data for two days only, a lack of depuration in *Oncorhynchus mykiss* for $C_{14}Cl_{13}$ cannot be excluded.

For $C_{14}Cl_5$, only 7 days of depuration have been used for the calculation of the k_2 as data points at the end of the depuration phase were all below the LOD and the only measured data at 28 days was excluded from the calculation as it was referring to sample L1-WF35. For $C_{14}Cl_5$, the depuration rate constant (k_2) calculated (0.0106, based on a linear regression) was lower than the overall fish growth rate constant for the study (k_g) (0.018794). That is why, for this group of congeners and in accordance with OECD TG 305, the mass approach was used in order to derive directly a mass based depuration rate corrected for growth (k_{2g}) (see further details in the following section 'The mass based depuration rate corrected for growth (k_{2g})'.

The “mass approach” was also applied to $C_{14}Cl_7$ (k_2 = 0.0174, based on a linear regression), $C_{14}Cl_8$ (k_2= 0.0124, based on a linear regression), $C_{14}Cl_9$ (k_2 = 0.0105, based on a linear regression), $C_{14}Cl_{10}$ (k_2 = 0.0096, based on a linear regression) and $C_{14}Cl_{11}$ (k_2 = 0.0116) as their k_2 values were lower than the overall fish growth rate constant for the study (k_g) (0.018794; see further details in the following section ‘The mass based depuration rate corrected for growth (k_{2g}))’.

The “mass approach” was not applied to $C_{14}Cl_6$ group of congeners as its k_2 value (0.02302) was higher than the overall fish growth rate constant for the study (k_g =0.018794). As a consequence, for $C_{14}Cl_6$ the depuration rate corrected for growth (or K_{2g}) was directly calculated using the “growth rate constant subtraction method for growth correction” as described in the OECD TG 305

The mass based depuration rate corrected for growth (k_{2g})

In Annex 5 of OECD TG 305 (section 7), it is reported that the ‘method for correcting growth dilution is subject to a lack of precision or sometimes does not work (for example for very slowly depurating substances tested in fast growing fish the derived depuration rate constant corrected for growth dilution, k_{2g}, may be very small and so the error in the two rate constants used to derive it become critical, and in some cases k_g estimates may be larger than k_2). In such cases an alternative approach (i.e. mass approach), which also works when first order growth kinetics have not been obeyed, can be used which avoids the need for the correction’.

The depuration rate growth corrected was calculated for $C_{14}Cl_5$ and C_{14} $Cl_{7\text{-}11}$ using the mass approach (as recommended in OECD TG 305). In accordance with OECD TG 305, ‘the depuration phase tissue concentrations (mass of test chemical/unit mass of fish) have been converted into mass of test chemical/fish: match concentrations and individual fish weights in tabular form (e.g.using a computer spreadsheet) and multiply each concentration by the total fish weight for that measurement to give a set of mass test chemical/fish for all depuration phase samples’. The k_{2g} for $C_{14}Cl_5$ and C_{14} $Cl_{7\text{-}11}$ was determined by using a linear regression.

Table 66: Depuration rate corrected for growth (K_{2g}) using the mass approach for $C_{14}Cl_5$ and $C_{14}Cl_7$ -Cl_{11}

	C_{14} Cl_5	C_{14} Cl_7	C_{14} Cl_8	C_{14} Cl_9	C_{14} Cl_{10}	C_{14} Cl_{11}
Depuration rate corrected for growth (k_{2g}) (day^{-1})	−0.0422 (no depuration; using a linear regression) According to best fit model: 0.0021 (Box-cox power transformation model and less conservative scenario with k_g=0 and k_2=k_{2g}, see outcome bcmfR R-package)	-0.0046 (no depuration; using a linear regression) According to best fit model: 0.00799 (Untransformed model, see outcome bcmfR R-package) or 0.026786 (untransformed model and less conservative scenario with k_g=0 and k_2=k_{2g}, see outcome	-0.0096 (no depuration; using a linear regression) According to best fit model: 0.01244 (Logarithm transformation model and less conservative scenario with k_g=0 and k_2=k_{2g}, see outcome bcmfR R-package)	-0.0111 (no depuration; using a linear regression) According to best fit model: 0.01044 (Box-cox power transformation model and less conservative scenario with k_g=0 and k_2=k_{2g}, see outcome bcmfR R-package)	-0.0116 (no depuration; using a linear regression) According to best fit model: 0.00962 (Logarithm transformation model and less conservative scenario with k_g=0 and k_2=k_{2g}, see outcome bcmfR R-package)	-0.0111 (no depuration; using a linear regression) According to best fit model: 0.01163 (Logarithm transformation model and less conservative scenario with k_g=0 and k_2=k_{2g}, see outcome bcmfR R-package)

		bcmfR R-package)				

Even by applying the mass approach, all K_{2g} values derived for $C_{14}Cl_5$ and C_{14} $Cl_{7\text{-}11}$ (using linear regressions) were all negative thus indicating a lack of depuration in *Oncorhynchus mykiss.*

Derivation of k_2, k_{2g} and BMF_{kgL} using the bcmfR R-package

The biomagnification factors (kinetic, growth corrected and lipid normalised) or BMF_{kgL} for MCCP congeners (including total substance) were calculated using the bcmfR R-package.
All the models run with the bcmfR R-package (Untransformed, Box-cox power and logarithm models, see below) are described in the Guidance document on Aspects of OECD TG 305 on Fish Bioaccumulation (OECD, 2017).

Table 67: Summary Table of the k_2, k_{2g} and BMF_{kgL} estimated with the best fit models for individual MCCP congeners and total substance using the bcmfR R-package

	C_{14} Cl_5	C_{14} Cl_6	C_{14} Cl_7	C_{14} Cl_8	C_{14} Cl_9	C_{14} Cl_{10}	C_{14} Cl_{11}	C_{14} chlorinated n-alkane, 50% Cl wt.
Best fit model	Box-Cox power transformation model	Logarithm transformation model	Untransformed model	Logarithm transformation model	Box-Cox power transformation model	Logarithm transformation model	Logarithm transformation model	Untransformed model
k_2 (day^{-1})	0.0021 Not statistically different from zero (Student t-test)	0.02302	0.026786	0.01244	0.01044	0.00962	0.01163	0.02741
k_{2g} (day^{-1})	0.0021 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.00422	0.00799 Or 0.026786 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.01244 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.01044 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.00962 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.01163 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.00861
BMF_{KgL}	0.6673 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.47292	0.42977 Or 0.12823 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.31626 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.47684 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.54647 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.33104 (less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	0.33303

It is worth noting, that BMF value could not be derived for $C_{14}Cl_3$, $C_{14}Cl_4$, $C_{14}Cl_{12}$, $C_{14}Cl_{13}$ and $C_{14}Cl_{14}$ as these congeners either were not detected and/or not enough frequently detected during the depuration phase.

For $C_{14}Cl_5$ and $C_{14}Cl_{7\text{-}11}$ as the growth rate constant (k_g) was higher than the depuration rate constant (k_2), the corresponding depuration rate growth corrected constant (k_{2g}) was negative thus the BMF derived from this negative k_{2g} was also negative. As the mass approach did not work in our case, the bcmfR R-package was re-run for $C_{14}Cl_5$ and $C_{14}Cl_{7\text{-}11}$ without correcting the depuration rate (k_2) for growth (k_g) and thus assuming that $k_2=k_{2g}$. This scenario ($k_g=0$ and $k_2=k_{2g}$) overestimates the depuration rate and the estimated BMF value will be underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then the group of congeners can be concluded as B and/or vB.

For $C_{14}Cl_6$, the BMF was directly derived using the bcmfR R-package following the "normal" approach (cf. the "growth rate constant subtraction method for growth correction" as described in the OECD TG 305) as the growth rate constant (k_g) was lower than the depuration rate constant (k_2).

All the results for the different group of congeners of MCCP and C_{14} chlorinated n-alkane, 50% Cl wt. using the bcmfR R-package are reported below:

Total substance (or C_{14} chlorinated n-alkane, 50 % Cl wt.):

Input data for C_{14} chlorinated n-alkane, 50% Cl wt.:

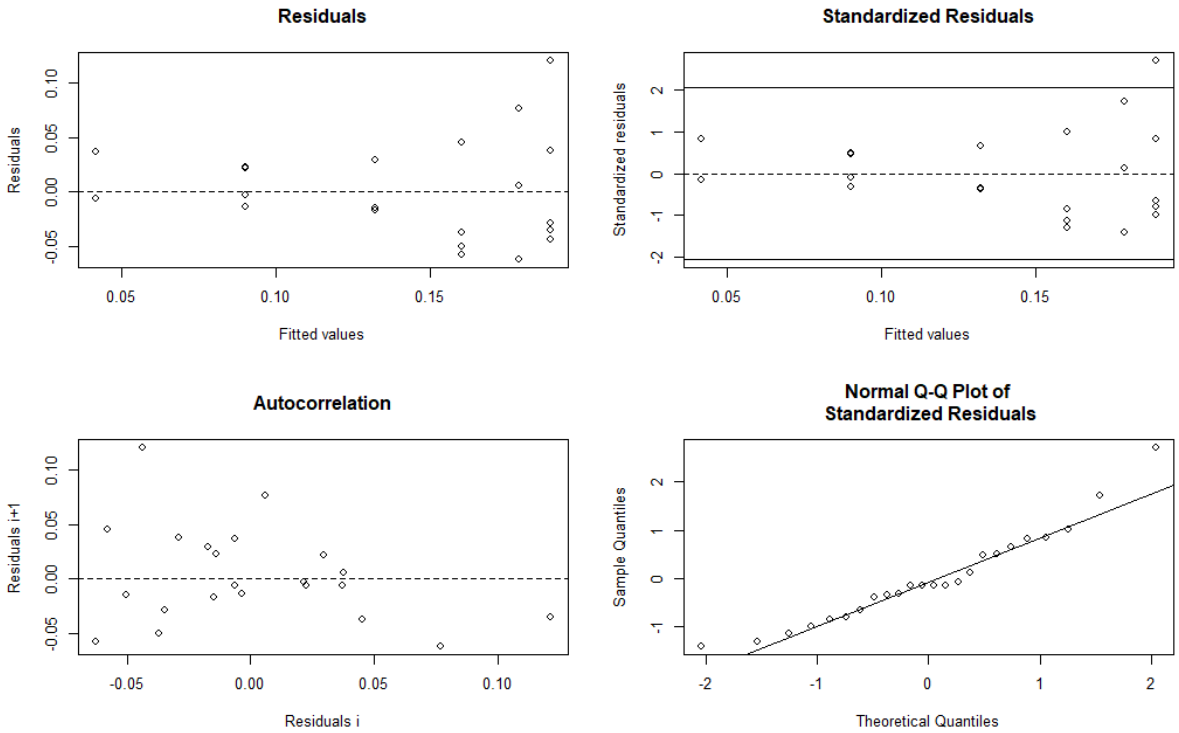
```
TEST.Dietary.Design:
              value              unit
cfood     16.430000        mgX/kgFood
ingestion  0.015000 kgFood/kgFish/day
tfeed     14.000000               day
lipidfood 16.350000           percent
lipidfish  5.793000           percent
tdepur     0.000000               day
tend      56.000000               day
kgrowth    0.018794             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1     0.1451
2          1     0.3101
3          1     0.1540
4          1     0.1599
5          1     0.2267
6          3     0.1849
7          3     0.2559
8          3     0.1164
9          7     0.1026
10         7     0.2055
11         7     0.1232
12         7     0.1101
13        14     0.1175
14        14     0.1153
15        14     0.1619
16        28     0.1115
17        28     0.0868
18        28     0.0764
19        28     0.1126
20        56     0.0355
21        56     0.0355
22        56     0.0355
23        56     0.0790
24        56     0.0355
```

UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()

Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.194174   0.015430  12.584 1.59e-11 ***
fitk2  0.027408   0.006551   4.184 0.000385 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.04437 on 22 degrees of freedom
```

```
Number of iterations to convergence: 3
Achieved convergence tolerance: 3.665e-06
```

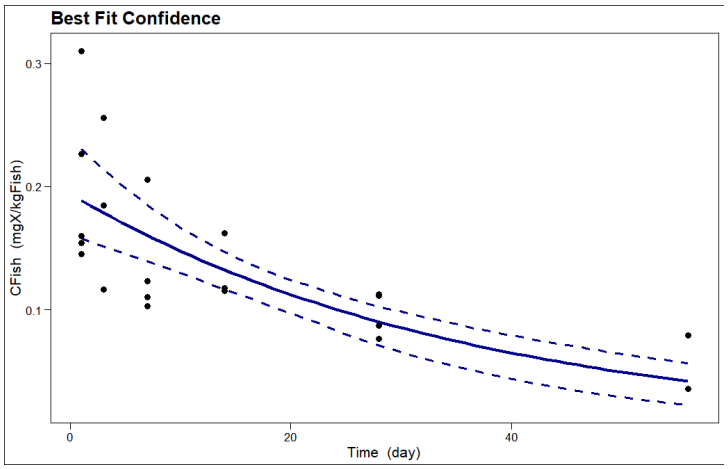
A k_2 value of 0.027408 is predicted with the untransformed model for C_{14} chlorinated n-alkane, 50% Cl wt.. This k_2 value is significantly different from zero (p=0.000385).




```
> ModelDiagnostics_Dietary()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.93934, p-value = 0.1577


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.33496, p-value = 0.7377
alternative hypothesis: two.sided
```

The run test indicates a *p-value* of 0.7377, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.1577) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```



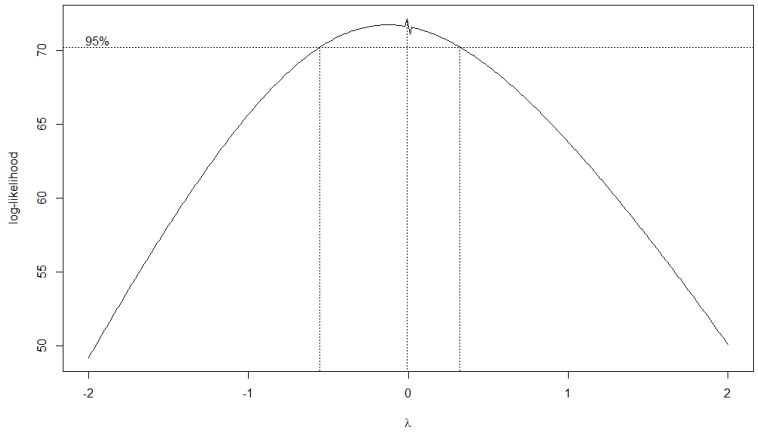

```
> SummTable_Dietary()
           Estimate Std.Error      2.5%     97.5%              unit
C0d         0.19417   0.01543   0.16393   0.22442        mgX/kgFish
k2          0.02741   0.00655   0.01457   0.04025             1/day
k2g         0.00861   0.00655  -0.00423   0.02145             1/day
kf          0.00102   0.00011    0.0008   0.00124 kgFood/kgFish/day
alpha       0.06776   0.00746   0.05314   0.08239                 -
BMFK        0.03709   0.00605   0.02522   0.04895     kgFood/kgFish
BMFKg       0.118     0.07959  -0.03799   0.27399     kgFood/kgFish
tHalfg     80.449    61.181   -39.465   200.36                day
BMFKgLipid  0.33303   0.22462  -0.10722   0.77329     kgFood/kgFish
```

A BMF_{KgL} of 0.33303 (95% Confidence interval: -0.10722–0.77329) is estimated with the untransformed model for C_{14} chlorinated n-alkane, 50% Cl wt.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
        fit     conflo     confup
-0.0100000 -0.5529664  0.3240101
```

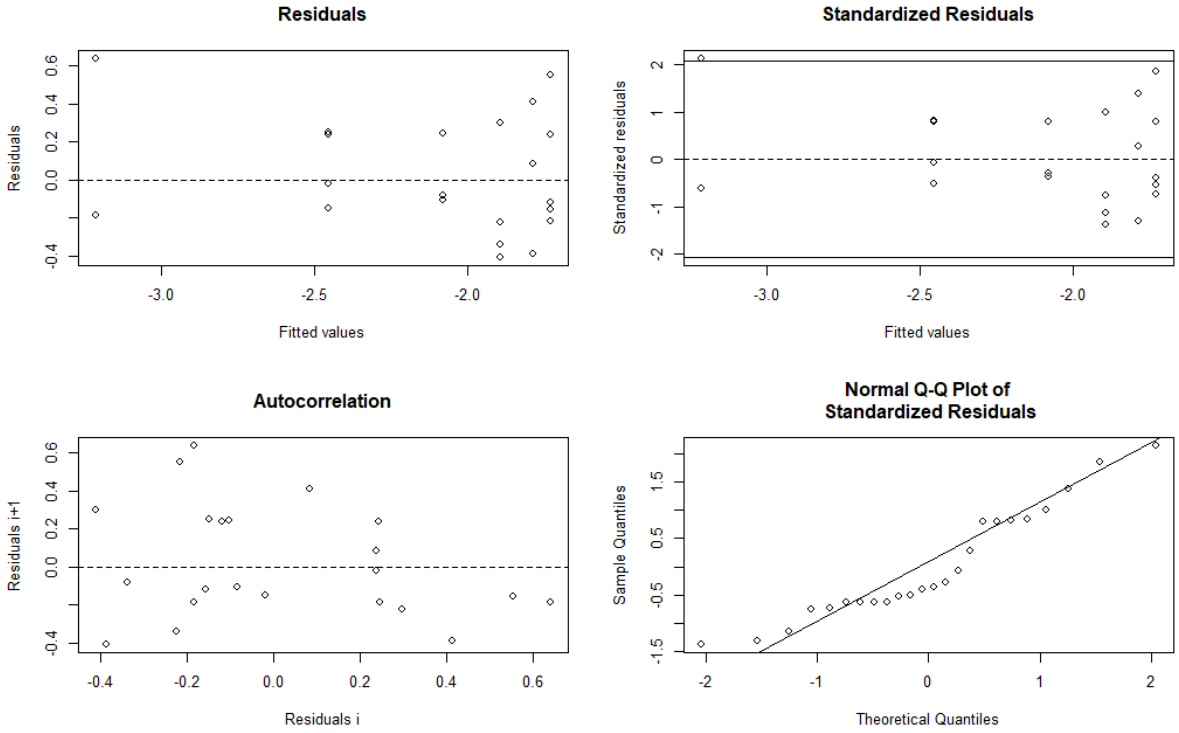
The estimated optimal λ value is -0.01 and its confidence interval is -0.553 up to 0.324. The most likely value (-0.01) is near the log transformation (0).




```
> FitModel_Dietary_BoxCox()

Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.184378   0.015302  12.049 3.68e-11 ***
fitk2  0.026236   0.002879   9.112 6.37e-09 ***
```

```
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2986 on 22 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 4.12e-07
```

A k_2 value of 0.026236 is predicted with the Box-Cox power transformation model for C_{14} chlorinated n-alkane, 50% Cl wt. This k_2 value is significantly different from zero ($p=6.37\times10^{-9}$).

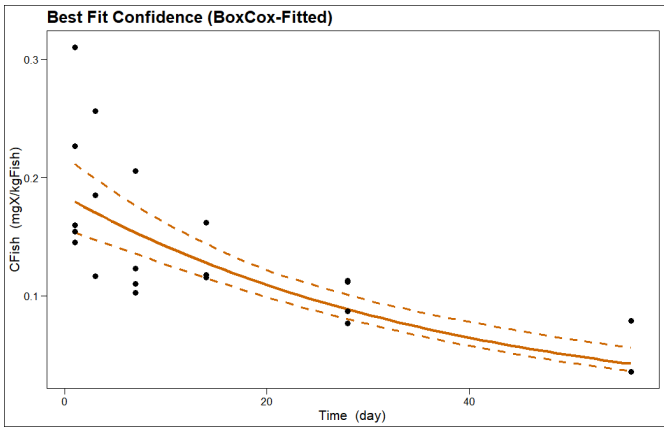


The Q-Q plot for the Box-Cox power transformation model is less attractive than for the untransformed model. No trend over time is indicated by the autocorrelation plot.

```
> ModelDiagnostics_Dietary_BoxCox()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.91755, p-value = 0.05158


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.33496, p-value = 0.7377
alternative hypothesis: two.sided
```

The run test indicates a *p-value* of 0.7377, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is slighty above 5%. The hypothesis that the error distribution is normal is not rejected. However, the Shapiro-wilk *p-value* with this model is less than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```



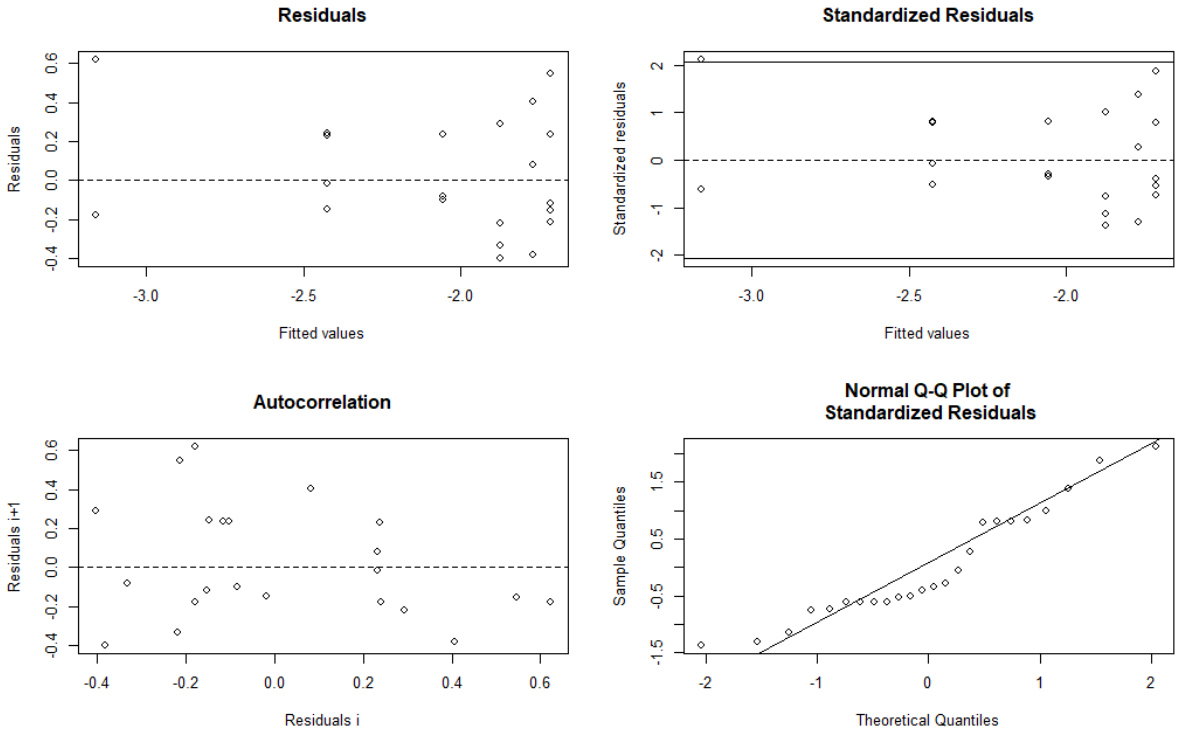

```
> SummTable_Dietary_BoxCox()
           Estimate Std.Error      2.5%     97.5%              unit
C0d         0.18438   0.0153   0.15439    0.21437        mgX/kgFish
k2          0.02624   0.00288  0.020593   0.03188             1/day
k2g         0.00744   0.00288  0.001799   0.01309             1/day
kf          0.00096   0.00009  0.000775   0.00114 kgFood/kgFish/day
alpha       0.06385   0.0062   0.051698   0.07601                 -
BMFK        0.03651   0.00249  0.031628   0.04138     kgFood/kgFish
BMFKg       0.12869   0.04065  0.049019   0.20836     kgFood/kgFish
tHalfg     93.114    36.023   22.51     163.72               day
BMFKgLipid  0.36321   0.11473  0.13835    0.58808     kgFood/kgFish
```

A BMF_{KgL} of 0.36321 (95% Confidence interval: 0.13835—0.58808) is estimated with the Box-Cox power transformation model for C_{14} chlorinated n-alkane, 50% Cl wt.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()

Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.184435   0.015271  12.077 3.51e-11 ***
fitk2  0.026232   0.002895   9.061 7.03e-09 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2923 on 22 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 4.352e-08
```

A k_2 value of 0.026232 is predicted with the logarithm transformation model. This k_2 value is significantly different from zero ($p = 7.03 \times 10^{-9}$).

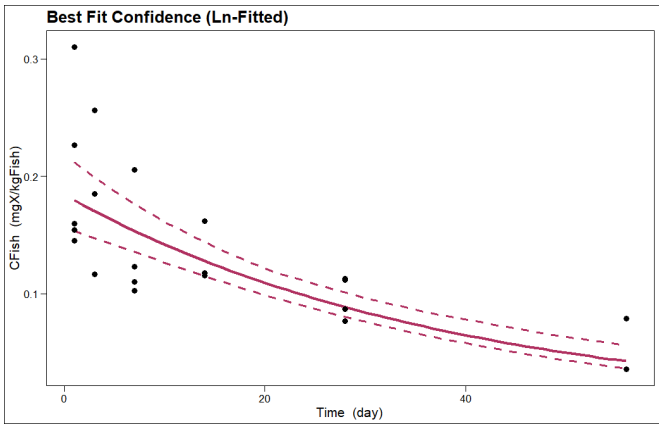


The Q-Q plot for the logarithm transformation model is less attractive than for the untransformed model. No trend over time is indicated by the autocorrelation plot.

```
> ModelDiagnostics_Dietary_Ln()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.91724, p-value = 0.05078


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.33496, p-value = 0.7377
alternative hypothesis: two.sided
```

The run test indicates a *p-value* of 0.7377, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is slighty above 5%. The hypothesis that the error distribution is normal is not rejected. However, the Shapiro-wilk *p-value* with this model is less than in the untransformed model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
            Estimate Std.Error      2.5%     97.5%              unit
C0d          0.18443   0.01527  0.1545     0.21437         mgX/kgFish
k2           0.02623   0.00289  0.020558   0.03191              1/day
k2g          0.00744   0.00289  0.001764   0.01311              1/day
kf           0.00096   0.00009  0.000776   0.00114 kgFood/kgFish/day
alpha        0.06387   0.00619  0.051731   0.07601                  -
BMFK         0.03652   0.00251  0.03161    0.04143      kgFood/kgFish
BMFKg        0.1288    0.04101  0.048421   0.20918      kgFood/kgFish
tHalfg      93.167    36.261   22.096    164.24                 day
BMFKgLipid   0.36352   0.11574  0.13666    0.59038      kgFood/kgFish
```

A BMF_{KgL} of 0.36352 (95% Confidence interval: 0.13666–0.59038) is estimated with the logarithm transformation model for C_{14} chlorinated n-alkane, 50% Cl wt.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for C_{14} chlorinated n-alkane, 50% Cl wt., an untransformed model is the best fit model to the data.

$C_{14}Cl_5$ group of congeners:

Input data for $C_{14}Cl_5$ group of congeners:

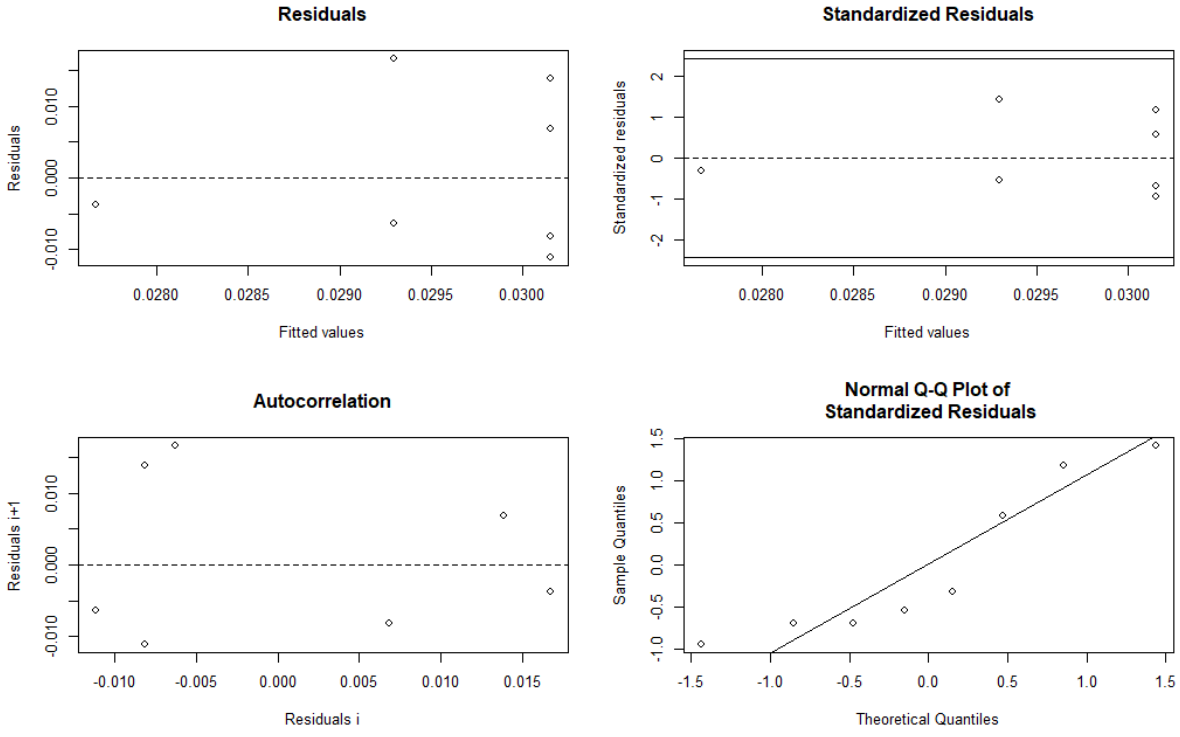
```
TEST.Dietary.Design:
              value              unit
cfood      3.930000        mgX/kgFood
ingestion  0.015000 kgFood/kgFish/day
tfeed     14.000000               day
lipidfood 16.350000           percent
lipidfish  5.793000           percent
tdepur     0.000000               day
tend      56.000000               day
kgrowth    0.018794             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
  time.data cfish.data
1         1      0.022
2         1      0.044
3         1      0.037
4         1      0.022
5         1      0.019
6         3      0.023
7         3      0.046
8         7      0.024
```

UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()

Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.030582   0.006467   4.729  0.00323 **
fitk2  0.014286   0.073910   0.193  0.85311
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.01175 on 6 degrees of freedom

Number of iterations to convergence: 4
Achieved convergence tolerance: 3.069e-06
```

A k_2 value of 0.014286 is predicted with the untransformation model for $C_{14}Cl_5$. The probability that the k_2 is not significantly different from zero is 0.85311 therefore it cannot be ruled out that $C_{14}Cl_5$ group of congeners is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification.

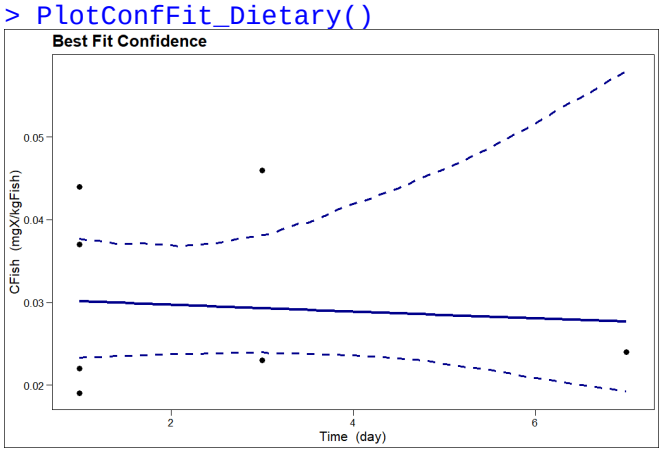
```
> ModelDiagnostics_Dietary()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.85355, p-value = 0.1035


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.20597, p-value = 0.8368
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates a *p-value* of 0.8368, confirming the interpretation of independent errors

in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is 0.1035 so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```




```
> SummTable_Dietary()
```

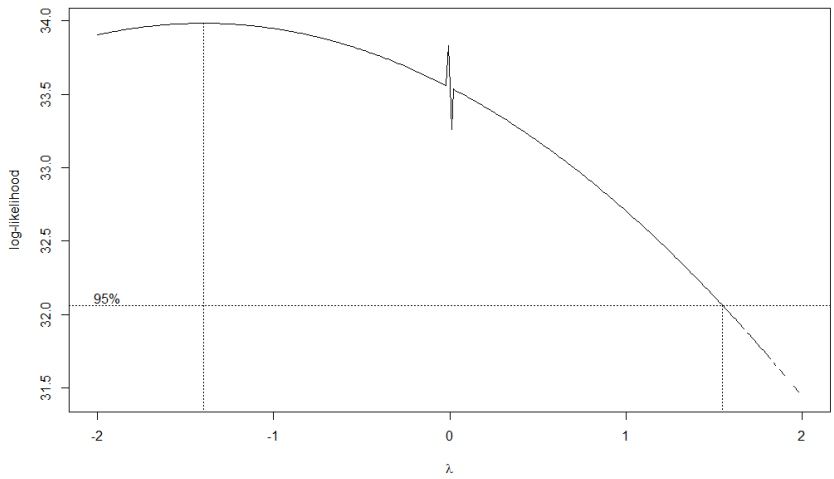
	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.03058	0.0065	0.018	0.043	mgX/kgFish
k2	0.01429	0.0739	-0.131	0.159	1/day
k2g	-0.00451	0.0739	-0.149	0.14	1/day
kf	0.00061	0.0004	0	0.001	kgFood/kgFish/day
alpha	0.04088	0.0275	-0.013	0.095	-
BMFK	0.04293	0.1939	-0.337	0.423	kgFood/kgFish
BMFKg	-0.13602	2.3195	-4.682	4.41	kgFood/kgFish
tHalfg	-153.71	2519.8	-5092.6	4785.2	day
BMFKgLipid	-0.38391	6.5466	-13.215	12.447	kgFood/kgFish

A depuration rate (k_2) of 0.01429 is predicted with the untransformation model for $C_{14}Cl_5$. The probability that the k_2 is not significantly different from zero is 0.85311 therefore it cannot be ruled out that $C_{14}Cl_5$ group of congeners is not depurated from rainbow trout thus it cannot be ruled that it has a high potential of biomagnification. This is confirmed by the negative depuration rate growth corrected (k_{2g}) of -0.00451 (suggesting no depuration) and the BMF_{KgL} of -0.38391 (95% Confidence interval: -13.215–12.447) derived by the untransformed model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
       fit    conflo    confup
-1.400000        NA  1.547243
```

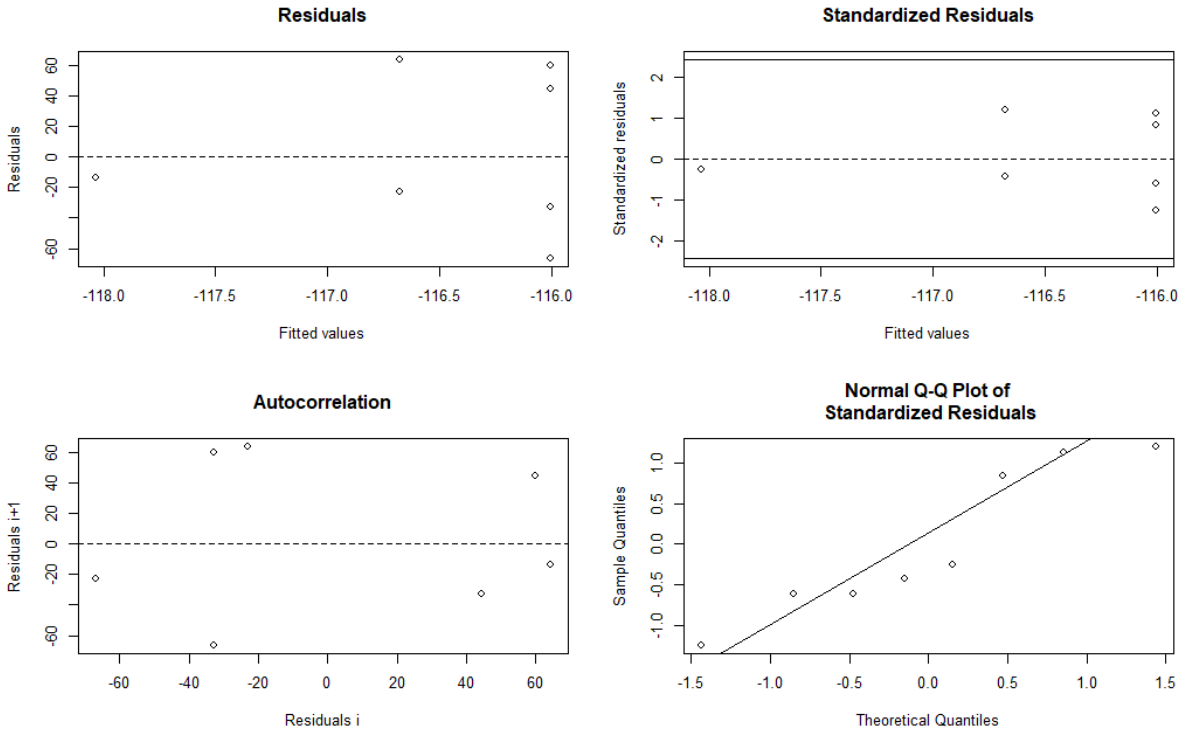
The estimated optimal λ value is -1.4 and its confidence interval is up to 1.547. The most likely value (-1.4) is near the reciprocal transformation (-1).



```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.026302   0.004570   5.755   0.0012 **
fitk2  0.002051   0.057365   0.036   0.9726
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 53.27 on 6 degrees of freedom

Number of iterations to convergence: 3
Achieved convergence tolerance: 6.181e-06
```

A k_2 value of 0.002051 is predicted with the Box-Cox power transformation model for $C_{14}Cl_5$. The probability that the k_2 is not significantly different from zero is 0.9726 therefore it cannot be ruled out that $C_{14}Cl_5$ group of congeners is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification.

```
> ModelDiagnostics_Dietary_BoxCox()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.88349, p-value = 0.2033


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.20597, p-value = 0.8368
alternative hypothesis: two.sided
```

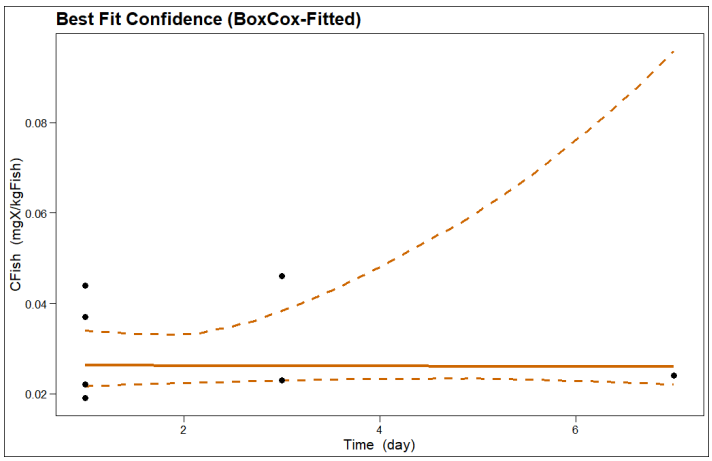


No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.8368, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2033), the

hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.0263	0.00457	0.0173	0.03526	mgX/kgFish
k2	0.00205	0.05736	-0.1104	0.11449	1/day
k2g	-0.01674	0.05736	-0.1292	0.09569	1/day
kf	0.00048	0.00026	0	0.001	kgFood/kgFish/day
alpha	0.03233	0.01753	-0.002	0.06669	-
BMFK	0.23644	6.4879	-12.48	12.953	kgFood/kgFish
BMFKg	-0.02896	0.11463	-0.2536	0.19572	kgFood/kgFish
tHalfg	-41.39	141.81	-319.34	236.56	day
BMFKgLipid	-0.08175	0.32354	-0.7159	0.55239	kgFood/kgFish

A depuration rate (k_2) of 0.002051 is predicted with the Box-Cox power transformation model for $C_{14}Cl_5$ group of congeners. The probability that the k_2 is not significantly different from zero is 0.9726 therefore it cannot be ruled out that C_{14} Cl_5 is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification. This is confirmed by the negative depuration rate growth corrected (k_{2g}) of -0.01674 (suggesting no depuration) and the BMF_{KgL} of -0.08175 (95% Confidence interval: -0.7159—0.55239) derived by the Box-Cox power transformation model.

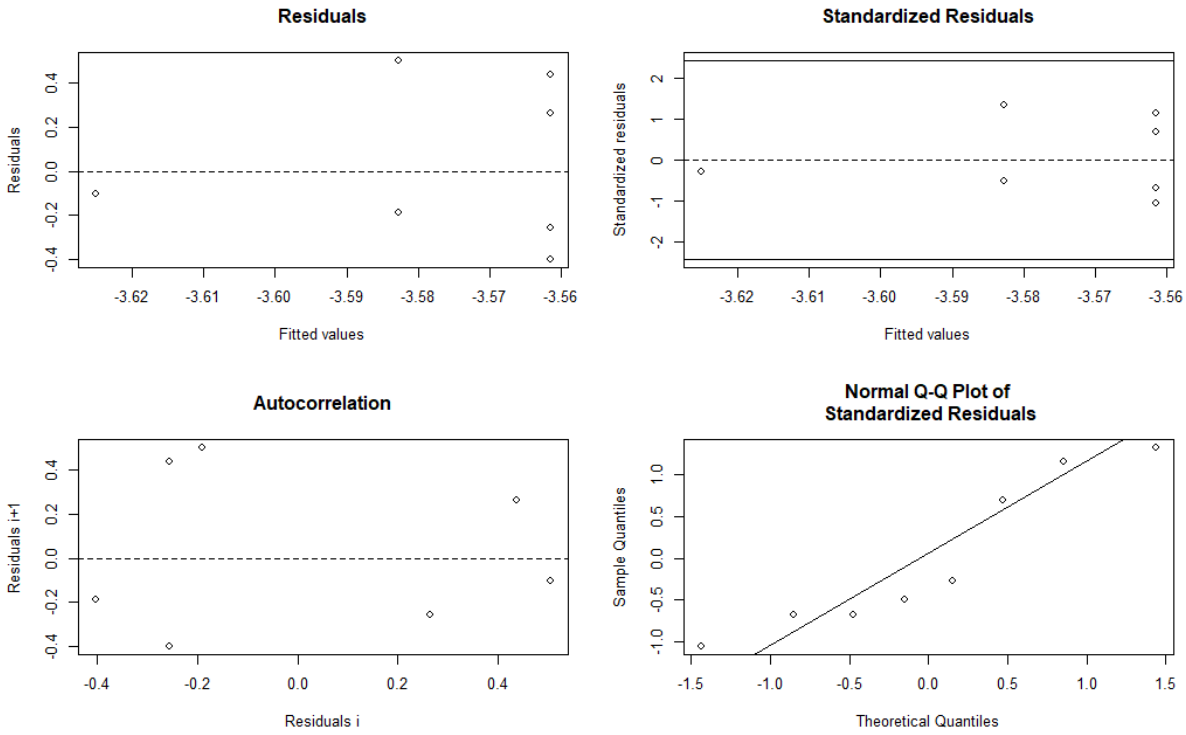
LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.028697   0.005787   4.959  0.00256 **
fitk2  0.010577   0.067221   0.157  0.88013
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3773 on 6 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 1.059e-07
```

A k_2 value of 0.010577 is predicted with the logarithm transformation model for $C_{14}Cl_5$. The probability that the k_2 is not significantly different from zero is 0.88013 therefore it cannot be ruled out that $C_{14}Cl_5$ group of congeners is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification.

```
> ModelDiagnostics_Dietary_Ln()
```

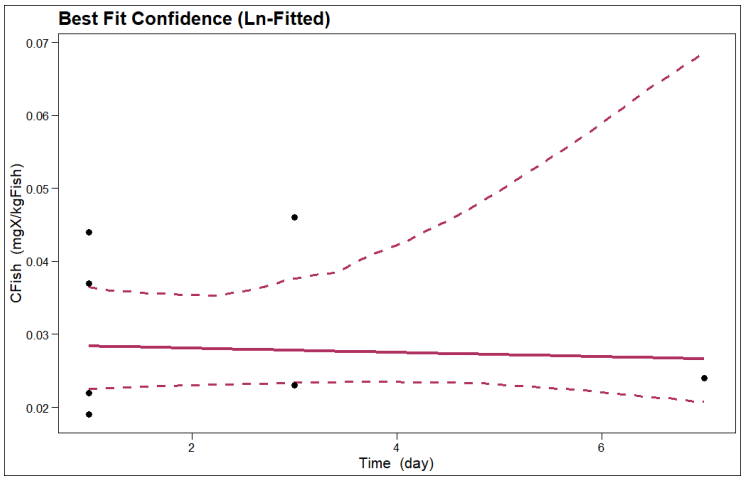
```
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.8718, p-value = 0.157


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.20597, p-value = 0.8368
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.8368, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.157), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is lower than in the Box-Cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
           Estimate Std.Error       2.5%     97.5%              unit
C0d          0.0287    0.0058     0.0174      0.04          mgX/kgFish
k2          0.01058    0.0672    -0.1212    0.1423               1/day
k2g        -0.00822    0.0672      -0.14    0.1235               1/day
kf          0.00056    0.0004    -0.0001    0.0012 kgFood/kgFish/day
alpha       0.03741    0.0234    -0.0084    0.0832                   -
BMFK        0.05305    0.3049    -0.5445    0.6506     kgFood/kgFish
BMFKg      -0.06829    0.6004    -1.2451    1.1085     kgFood/kgFish
tHalfg      -84.339    689.98   -1436.7      1268                 day
BMFKgLipid  -0.19274    1.6946    -3.5142    3.1287     kgFood/kgFish
```

A depuration rate (k_2) of 0.010577 is predicted with the logarithm transformation model for C_{14} Cl_5 congener. The probability that the k_2 is not significantly different from zero is 0.88013 therefore it cannot be ruled out that C_{14} Cl_5 is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification. This is confirmed by the negative depuration rate growth corrected (k_{2g}) of -0.00822 (suggesting no depuration) and the BMF_{KgL} of -0.19274 (95% Confidence interval: -3.5142–3.1287) derived by the Box-Cox power transformation model.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for C_{14} Cl_5 congener, the Box-Cox power transformation model is the best fit model to the data.

$C_{14}Cl_5$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

For C_{14} Cl_5 as the growth rate constant (k_g) was higher than the depuration rate constant (k_2), the corresponding depuration rate growth corrected constant (k_{2g}) was negative thus the BMF derived from this negative k_{2g} was also negative. As the mass approach did not work in our case, the bcmfR R-package was re-run for $C_{14}Cl_5$ without correcting the depuration rate (k_2) for growth (k_g) and thus assuming that $k_2=k_{2g}$. This scenario ($k_g=0$ and $k_2=k_{2g}$) overestimates the depuration rate and the estimated BMF value will be underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB.

Input data for C_{14} Cl_5 congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

```
TEST.Dietary.Design:
           value              unit
cfood      3.930        mgX/kgFood
ingestion  0.015 kgFood/kgFish/day
tfeed     14.000               day
lipidfood 16.350           percent
lipidfish  5.793           percent
tdepur     0.000               day
tend      56.000               day
kgrowth    0.000             1/day
```

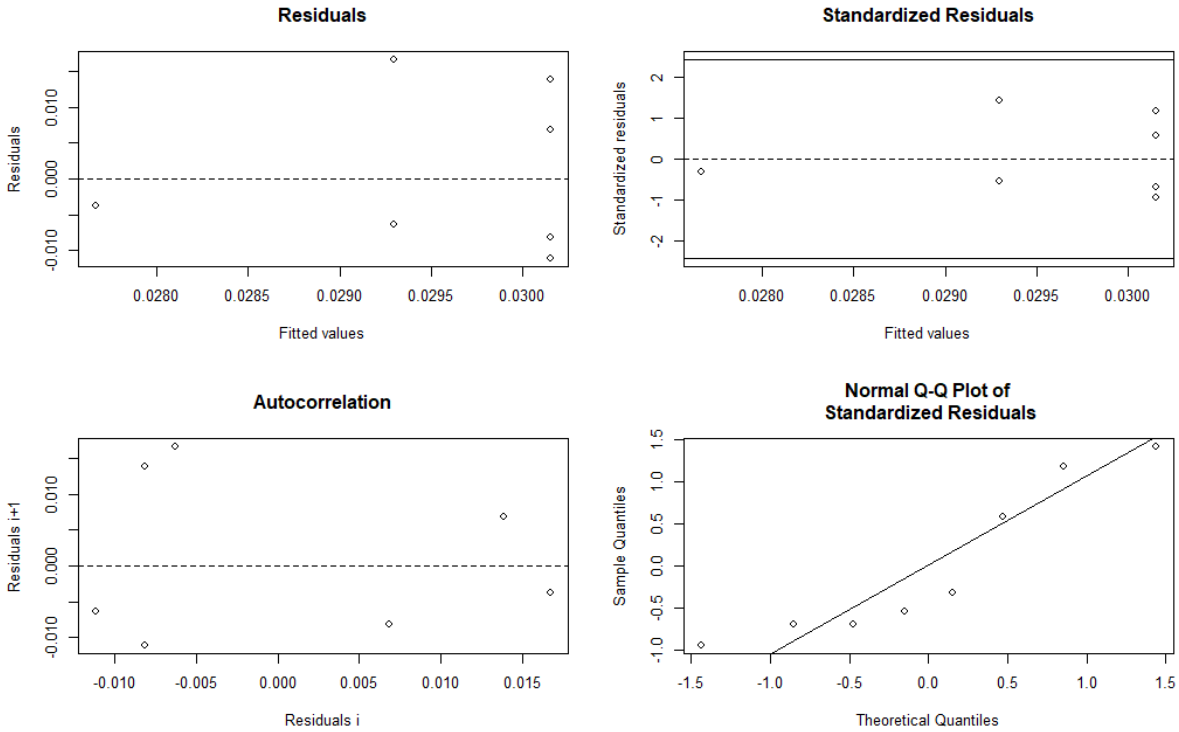
```
TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
  time.data cfish.data
1         1      0.022
2         1      0.044
3         1      0.037
4         1      0.022
5         1      0.019
6         3      0.023
7         3      0.046
8         7      0.024
```

UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()
Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.030582   0.006467   4.729  0.00323 **
fitk2  0.014286   0.073910   0.193  0.85311
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.01175 on 6 degrees of freedom

Number of iterations to convergence: 4
Achieved convergence tolerance: 3.069e-06
```

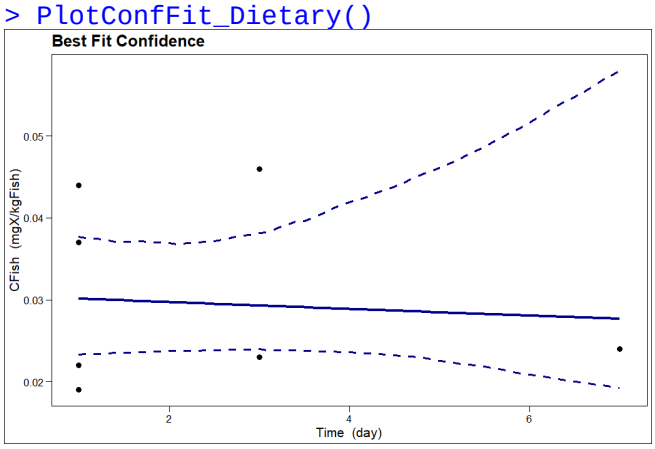
A k_2 value of 0.014286 is predicted with the untransformation model for $C_{14}Cl_5$. The probability that the k_2 is not significantly different from zero is 0.85311 therefore it cannot be ruled out that $C_{14}Cl_5$ group of congeners is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification.

```
> ModelDiagnostics_Dietary()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.85355, p-value = 0.1035


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.20597, p-value = 0.8368
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates a *p-value* of 0.8368, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is 0.1035 so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```



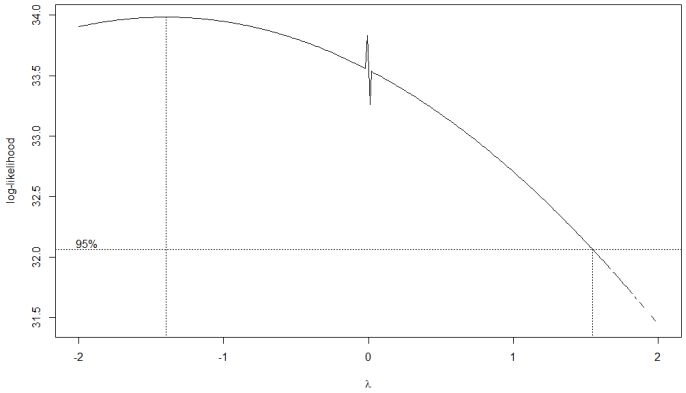

```
> SummTable_Dietary()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.03058	0.00647	0.0179	0.0433	mgX/kgFish
k2	0.01429	0.07391	-0.1306	0.1591	1/day
k2g	0.01429	0.07391	-0.1306	0.1591	1/day
kf	0.00061	0.00041	-0.0002	0.0014	kgFood/kgFish/day
alpha	0.04088	0.02752	-0.0131	0.0948	-
BMFK	0.04293	0.19393	-0.3372	0.423	kgFood/kgFish
BMFKg	0.04293	0.19393	-0.3372	0.423	kgFood/kgFish
tHalfg	48.511	250.98	-443.42	540.44	day
BMFKgLipid	0.12116	0.54734	-0.9516	1.194	kgFood/kgFish

A depuration rate (k_2) of 0.01429 (equal to the depuration rate growth corrected (k_{2g})) is predicted with the untransformation model for $C_{14}Cl_5$. The probability that the k_2 is not significantly different from zero is 0.85311, therefore it cannot be ruled out that $C_{14}Cl_5$ group of congeners is not depurated from rainbow trout thus it cannot be ruled that it has a high potential of biomagnification. A BMF_{KgL} of 0.12116 (95% Confidence interval: -0.9516—1.194) is derived by the untransformed model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
   fit    conflo    confup
-1.400000        NA  1.547243
```

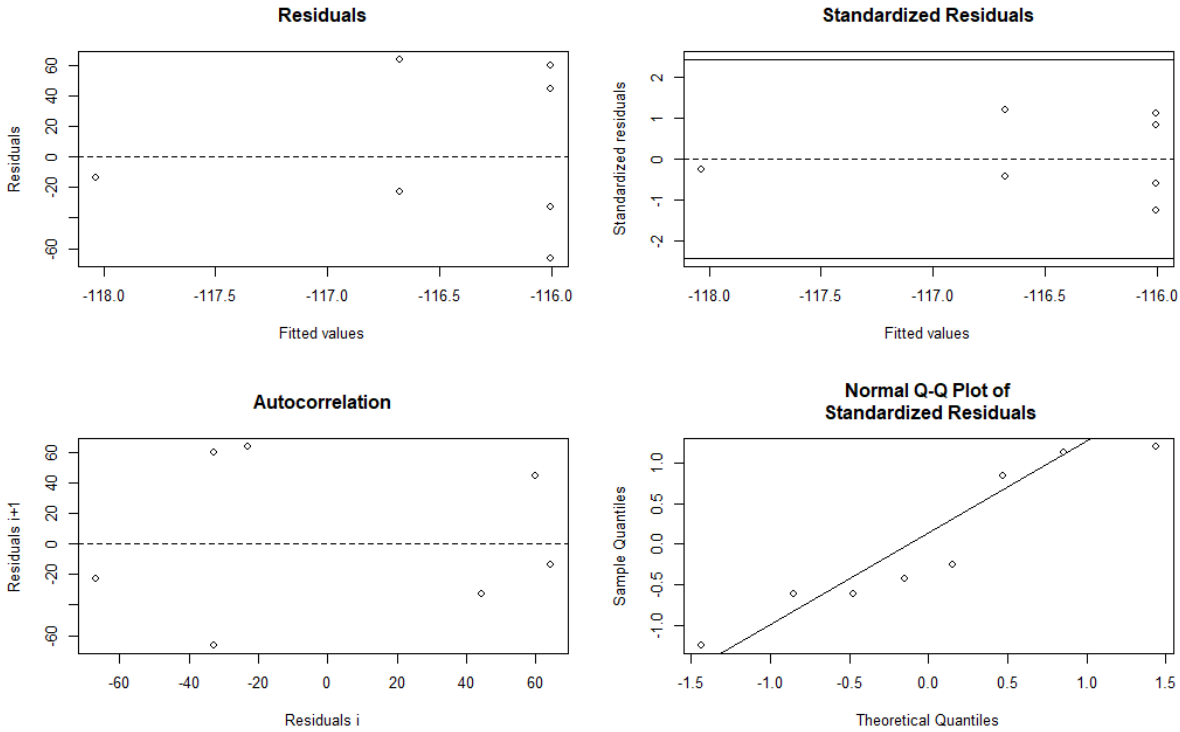


The estimated optimal λ value is -1.4 and its confidence interval is up to 1.547. The most likely value (-1.4) is near the reciprocal transformation (-1).

```
> FitModel_Dietary_BoxCox()


Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.026302   0.004570   5.755   0.0012 **
fitk2  0.002051   0.057365   0.036   0.9726
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 53.27 on 6 degrees of freedom

Number of iterations to convergence: 3
Achieved convergence tolerance: 6.181e-06
```

A k_2 value of 0.002051 is predicted with the Box-Cox power transformation model for $C_{14}Cl_5$. The probability that the k_2 is not significantly different from zero is 0.9726, therefore it cannot be ruled out that $C_{14}Cl_5$ group of congeners is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification.

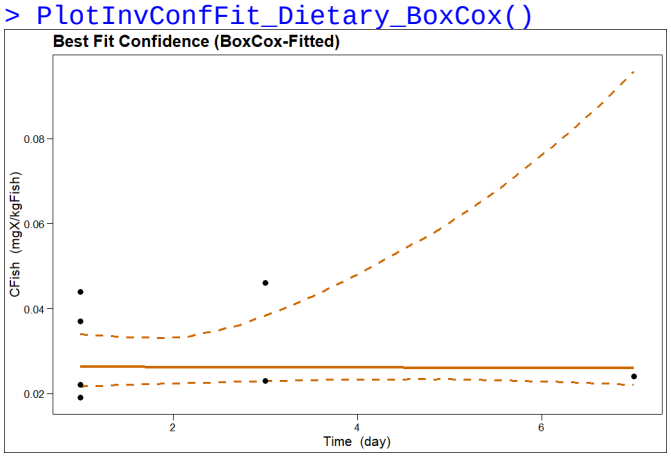
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.88349, p-value = 0.2033


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.20597, p-value = 0.8368
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.8368, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2033), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.0263	0.005	0.017	0.035	mgX/kgFish
k2	0.0021	0.057	-0.11	0.114	1/day
k2g	0.0021	0.057	-0.11	0.114	1/day
kf	0.0005	0	0	0.001	kgFood/kgFish/day
alpha	0.0323	0.018	-0.002	0.067	-
BMFK	0.2364	6.488	-12.48	12.953	kgFood/kgFish
BMFKg	0.2364	6.488	-12.48	12.953	kgFood/kgFish
tHalfg	337.89	9450.6	-18185	18861	day
BMFKgLipid	0.6673	18.311	-35.223	36.557	kgFood/kgFish

A depuration rate (k_2) of 0.002051 (equal to the depuration rate growth corrected (k_{2g})) is predicted with the Box-Cox power transformation model for $C_{14}Cl_5$ group of congeners. The probability that the k_2 is not significantly different from zero is 0.9726, therefore it cannot be

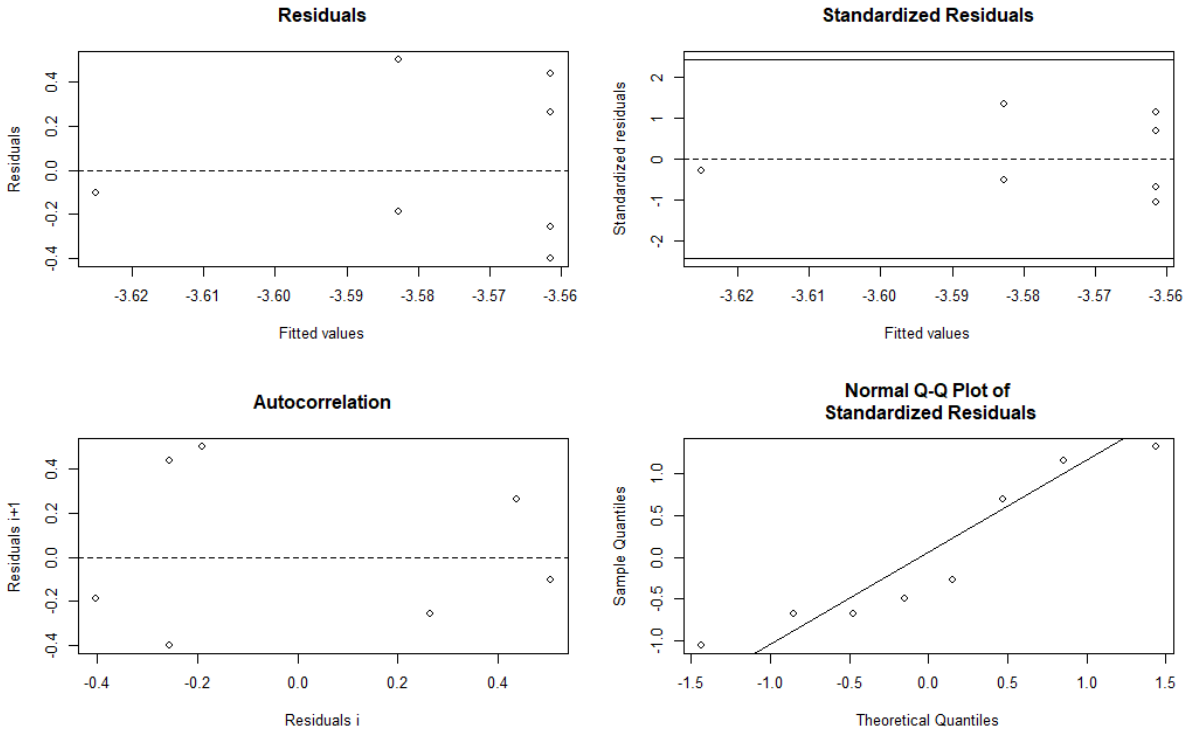
ruled out that C_{14} Cl_5 is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification. A BMF_{KgL} of 0.6673 (95% Confidence interval: -35.223—36.557) is derived by the Box-Cox power transformation model.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.028697   0.005787   4.959  0.00256 **
fitk2  0.010577   0.067221   0.157  0.88013
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3773 on 6 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 1.059e-07
```

A k_2 value of 0.010577 is predicted with the logarithm transformation model for $C_{14}Cl_5$. The probability that the k_2 is not significantly different from zero is 0.88013 therefore it cannot be ruled out that $C_{14}Cl_5$ group of congeners is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification.

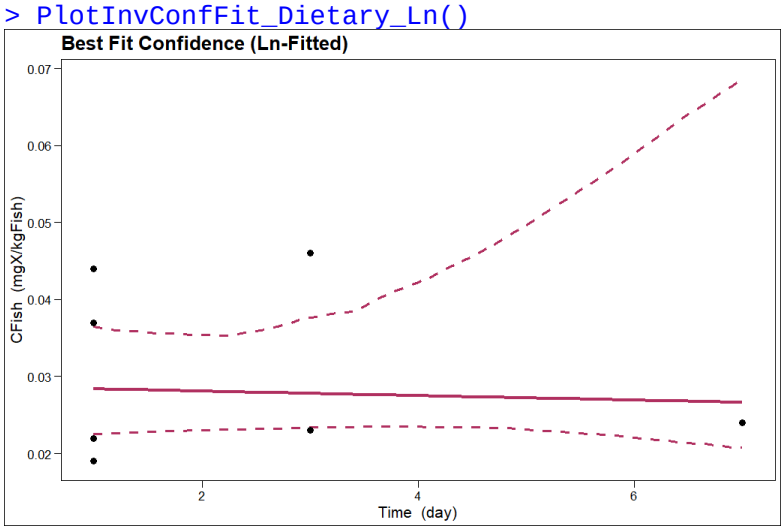
```
> ModelDiagnostics_Dietary_Ln()

-----
        Shapiro-Wilk normality test

data:  stdres
W = 0.8718, p-value = 0.157


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.20597, p-value = 0.8368
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.8368, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.157), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is lower than in the Box-Cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.0287	0.0058	0.0174	0.04	mgX/kgFish
k2	0.01058	0.0672	-0.1212	0.1423	1/day
k2g	0.01058	0.0672	-0.1212	0.1423	1/day
kf	0.00056	0.0004	-0.0001	0.0012	kgFood/kgFish/day
alpha	0.03741	0.0234	-0.0084	0.0832	-
BMFK	0.05305	0.3049	-0.5445	0.6506	kgFood/kgFish
BMFKg	0.05305	0.3049	-0.5445	0.6506	kgFood/kgFish
tHalfg	65.518	416.39	-750.6	881.64	day
BMFKgLipid	0.14973	0.8604	-1.5367	1.8362	kgFood/kgFish

A depuration rate (k_2) of 0.010577 (equal to the depuration rate growth corrected (k_{2g})) is predicted with the logarithm transformation model for C_{14} Cl_5 congener. The probability that the k_2 is not significantly different from zero is 0.88013, therefore it cannot be ruled out that C_{14} Cl_5 is not depurated from rainbow trout thus it cannot be ruled out that it has a high potential of biomagnification. A BMF_{KgL} of 0.14973 (95% Confidence interval: -1.5367—1.8362) derived by the Box-Cox power transformation model.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for C_{14} Cl_5 congener, the Box-Cox power transformation model is the best fit model to the data.

$C_{14}Cl_6$ group of congeners:

Input data for $C_{14}Cl_6$ group of congeners:

```
TEST.Dietary.Design:
               value              unit
cfood       5.900000         mgX/kgFood
ingestion   0.015000 kgFood/kgFish/day
tfeed      14.000000               day
lipidfood  16.350000           percent
lipidfish   5.793000           percent
tdepur      0.000000               day
tend       56.000000               day
kgrowth     0.018794             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1      0.042
2          1      0.096
3          1      0.031
4          1      0.045
5          1      0.063
6          3      0.054
7          3      0.080
8          3      0.033
9          7      0.028
10         7      0.059
11         7      0.032
12         7      0.032
13        14      0.032
14        14      0.030
15        14      0.045
16        28      0.029
17        28      0.028
```

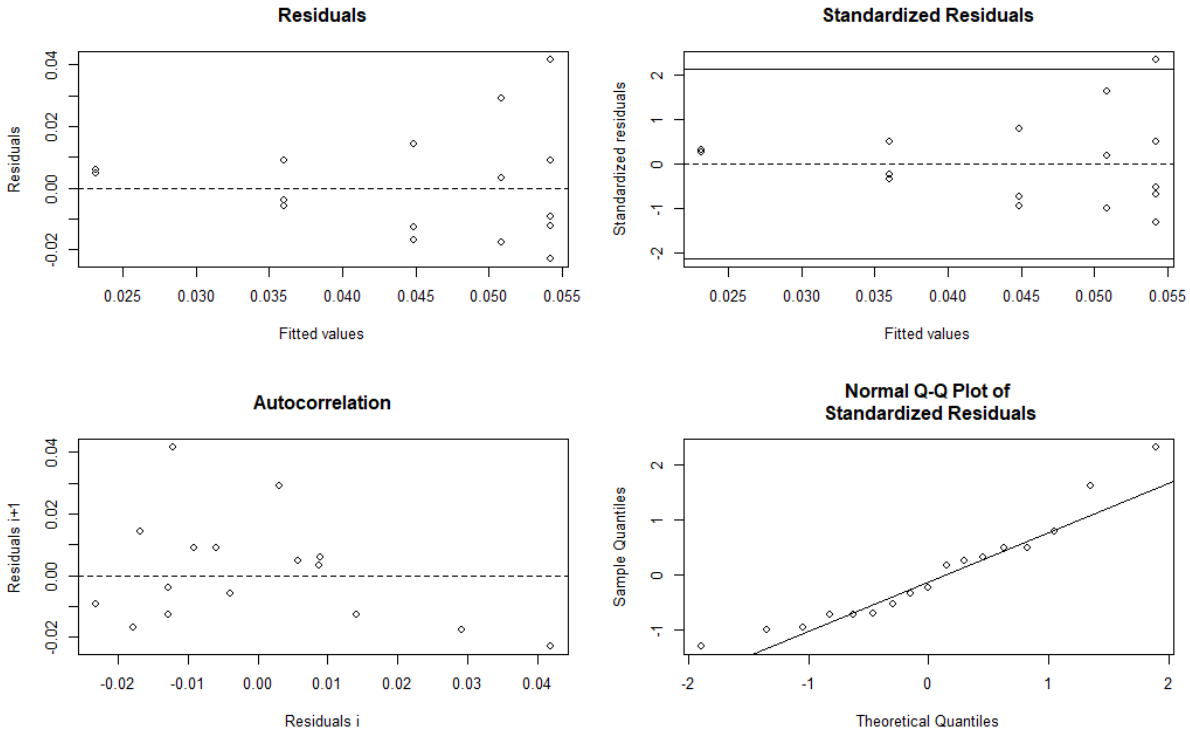
UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()

Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.055900   0.007038   7.942 9.41e-07 ***
fitk2  0.031434   0.016422   1.914   0.0749 .
---
```

```
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.01785 on 15 degrees of freedom

Number of iterations to convergence: 5
Achieved convergence tolerance: 1.638e-06
```

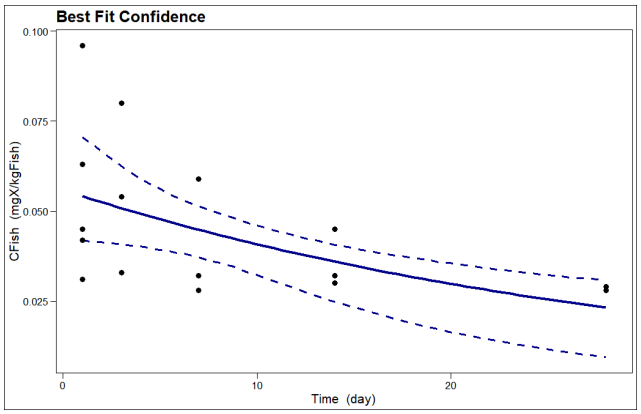
A k_2 value of 0.031434 is predicted with the untransformation model for $C_{14}Cl_6$ group of congeners. The probability that the k_2 is not significantly different from zero is 0.0749, therefore it cannot be ruled out that $C_{14}Cl_6$ group of congeners is not depurated from rainbow trout thus it cannot be ruled that it has a high potential of biomagnification.

```
> ModelDiagnostics_Dietary()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.92642, p-value = 0.1896


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.73946, p-value = 0.4596
alternative hypothesis: two.sided
```



The run test indicates a *p-value* of 0.4596, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.1896) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```

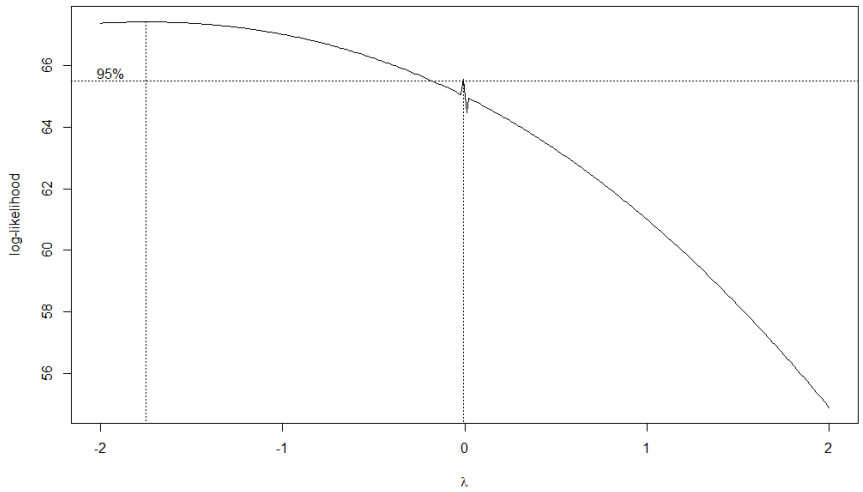



```
> SummTable_Dietary()
            Estimate Std.Error      2.5%     97.5%              unit
C0d           0.0559   0.00704   0.04211    0.0697         mgX/kgFish
k2            0.03143  0.01642  -0.00075    0.06362             1/day
k2g           0.01264  0.01642  -0.01955    0.04483             1/day
kf            0.00084  0.00018   0.00049    0.00118 kgFood/kgFish/day
alpha         0.05577  0.01181   0.03262    0.07892                 -
BMFK          0.02661  0.00922   0.00855    0.04467     kgFood/kgFish
BMFKg         0.06618  0.07372  -0.0783     0.21066     kgFood/kgFish
tHalfg       54.824   71.227   -84.781    194.43                 day
BMFKgLipid    0.18679  0.20805  -0.22099    0.59457     kgFood/kgFish
```

A BMF_{KgL} of 0.18679 (95% Confidence interval: -0.22099–0.59457) is estimated with the untransformed model for $C_{14}Cl_6$ group of congeners.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
         fit      conflo      confup
-1.75000000          NA -0.00906443
```



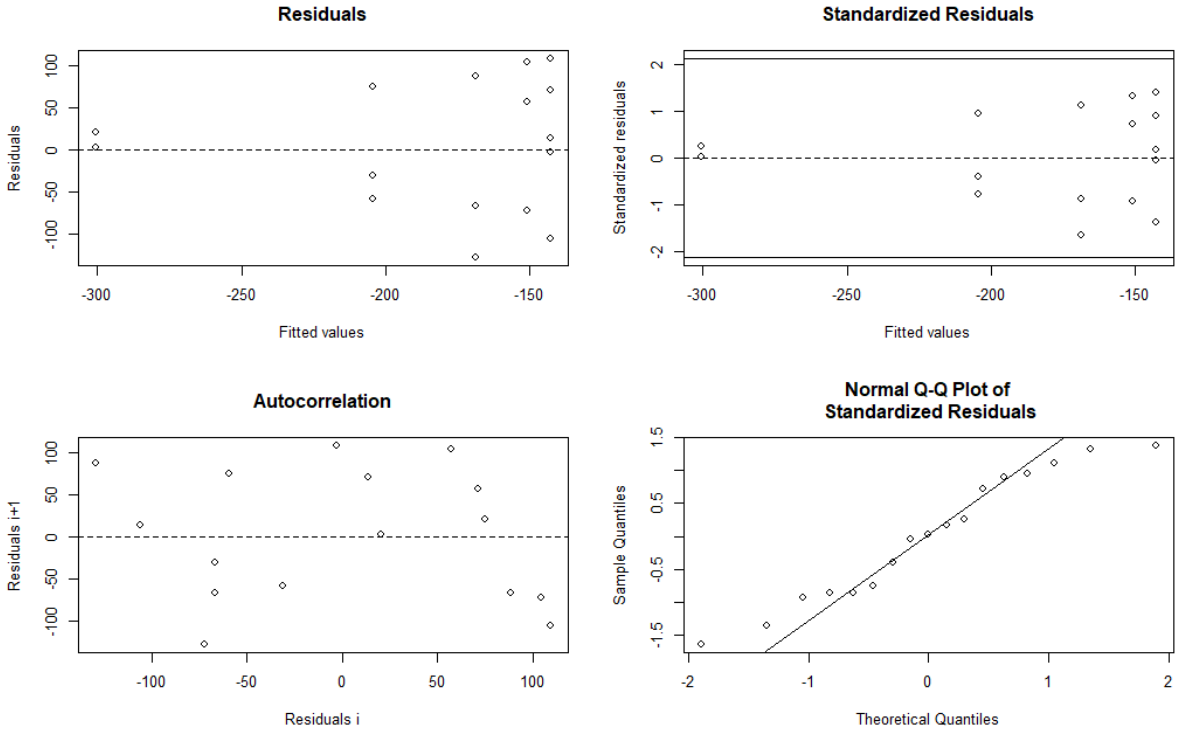
The estimated optimal λ value is -1.75 and its confidence interval is up to -0.009.

```
> FitModel_Dietary_BoxCox()

Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.043207   0.004037  10.703 2.03e-08 ***
fitk2  0.015689   0.005470   2.868   0.0117 *
---
```

```
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 78.14 on 15 degrees of freedom

Number of iterations to convergence: 4
Achieved convergence tolerance: 1.668e-06
```

A k_2 value of 0.015689 is predicted with the Box-Cox power transformation model for $C_{14}Cl_6$ group of congeners. This k_2 value is significantly different from zero (p=0.0117).

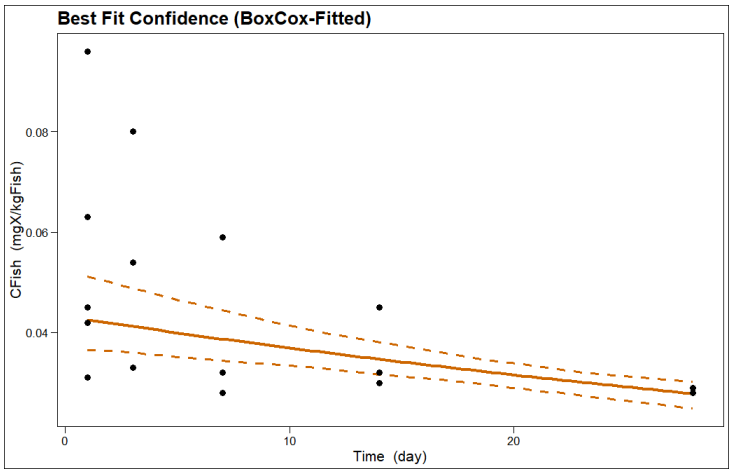
```
> ModelDiagnostics_Dietary_BoxCox()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.94522, p-value = 0.3854


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.73946, p-value = 0.4596
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p*-value of 0.4596, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is above 5% (0.3854). The hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
              Estimate Std.Error      2.5%    97.5%              unit
C0d             0.04321    0.004    0.0353   0.0511        mgX/kgFish
k2              0.01569   0.0055     0.005   0.0264             1/day
k2g            -0.00311   0.0055   -0.0138   0.0076             1/day
kf              0.00058   0.0001    0.0004   0.0007 kgFood/kgFish/day
alpha           0.03884   0.0048    0.0294   0.0483                 -
BMFK            0.03714   0.0091    0.0193    0.055      kgFood/kgFish
BMFKg          -0.18764   0.3514   -0.8764   0.5011      kgFood/kgFish
tHalfg      -223.18     393.17   -993.79   547.43                day
BMFKgLipid     -0.52958   0.9918   -2.4734   1.4143      kgFood/kgFish
```

A BMF_{KgL} of -0.52958 (95% Confidence interval: -2.4734—1.4143) is estimated with the Box-Cox power transformation model for $C_{14}Cl_6$ group of congeners.

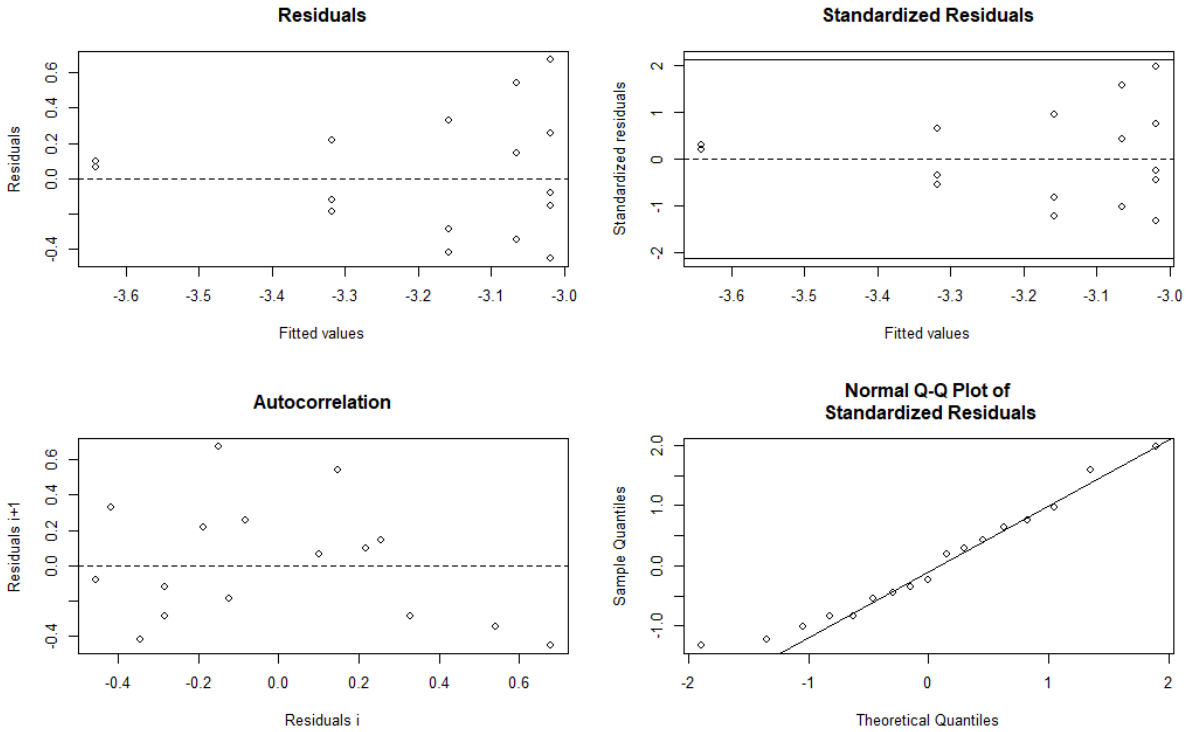
LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()

Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.049957   0.005753   8.684 3.09e-07 ***
fitk2  0.023016   0.009724   2.367   0.0318 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3412 on 15 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 8.035e-08
```

A k_2 value of 0.023016 is predicted with the logarithm transformation model. This k_2 value is significantly different from zero (p=0.0318).

```
> ModelDiagnostics_Dietary_Ln()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.95575, p-value = 0.5536


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.73946, p-value = 0.4596
```

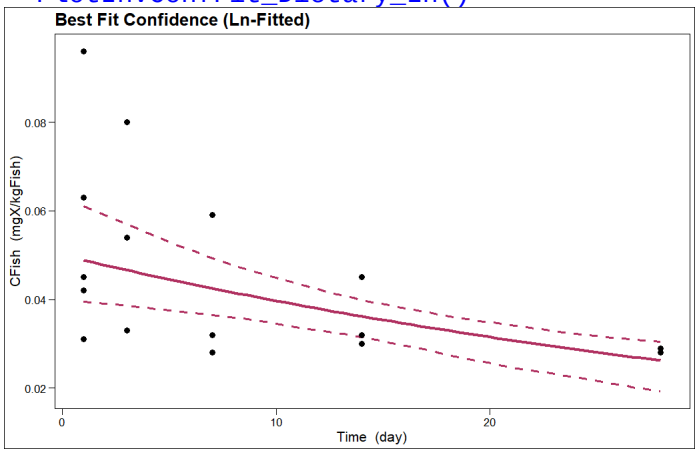
```
alternative hypothesis: two.sided
```



The Q-Q plot for the logarithm transformation model is more attractive than for the untransformed model and the Box-Cox power transformation model. No trend over time is indicated by the autocorrelation plot.

The run test indicates *p-value* of 0.4596, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.5536). The hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model and than in the Box-Cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.04996	0.0058	0.0387	0.0612	mgX/kgFish
k2	0.02302	0.0097	0.004	0.0421	1/day
k2g	0.00422	0.0097	-0.0148	0.0233	1/day
kf	0.00071	0.0001	0.0005	0.0009	kgFood/kgFish/day
alpha	0.04717	0.0079	0.0318	0.0626	-
BMFK	0.03074	0.0089	0.0133	0.0482	kgFood/kgFish
BMFKg	0.16756	0.362	-0.5419	0.877	kgFood/kgFish
tHalfg	164.13	378	-576.75	905.02	day
BMFKgLipid	0.47292	1.0216	-1.5294	2.4752	kgFood/kgFish

A depuration rate growth corrected (k_{2g}) of 0.00422 and a BMF_{KgL} of 0.47292 (95% Confidence interval: -1.5294–2.4752) are estimated with the logarithm transformation model for $C_{14}Cl_6$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_6$, the logarithm transformed model is the best fit model to the data.

$C_{14}Cl_7$ group of congeners:

Input data for $C_{14}Cl_7$ group of congeners:

```
TEST.Dietary.Design:
              value              unit
cfood      3.900000        mgX/kgFood
ingestion  0.015000 kgFood/kgFish/day
tfeed     14.000000               day
lipidfood 16.350000           percent
lipidfish  5.793000           percent
tdepur     0.000000               day
tend      56.000000               day
kgrowth    0.018794             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1      0.041
2          1      0.094
3          1      0.050
4          1      0.048
5          1      0.076
6          3      0.019
7          3      0.058
8          3      0.069
9          3      0.037
10         7      0.032
11         7      0.066
12         7      0.039
13         7      0.034
14        14      0.037
15        14      0.018
16        14      0.022
17        14      0.036
18        14      0.051
19        28      0.036
20        28      0.028
21        28      0.022
22        28      0.036
23        56      0.022
```

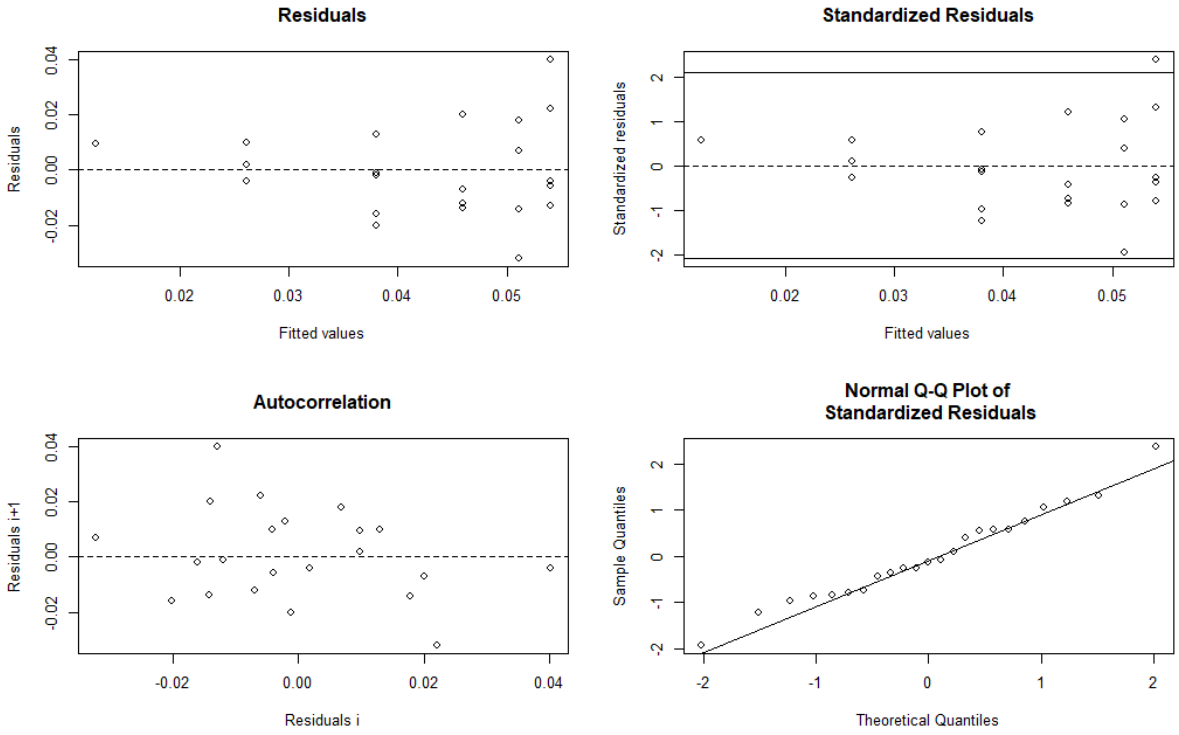
UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()

Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.055408   0.005846   9.477 4.92e-09 ***
fitk2  0.026786   0.010304   2.600   0.0167 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.01667 on 21 degrees of freedom
```

```
Number of iterations to convergence: 6
Achieved convergence tolerance: 7.211e-06
```

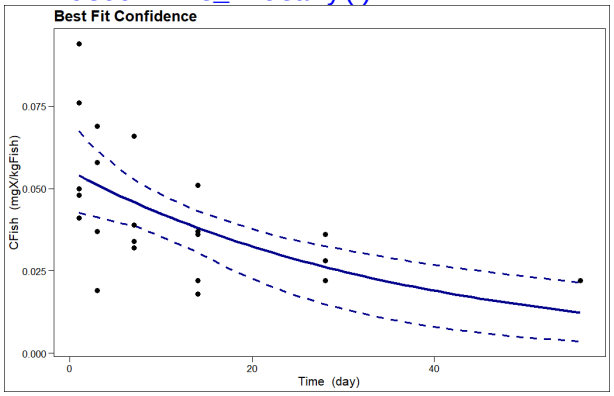
A k_2 value of 0.026786 is predicted with the untransformation model for C_{14} Cl_7 congener. This k_2 value is significantly different from zero (p=0.0167).

```
> ModelDiagnostics_Dietary()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.98011, p-value = 0.9081


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.13227, p-value = 0.8948
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates *p-value* of 0.8948, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.9081) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```

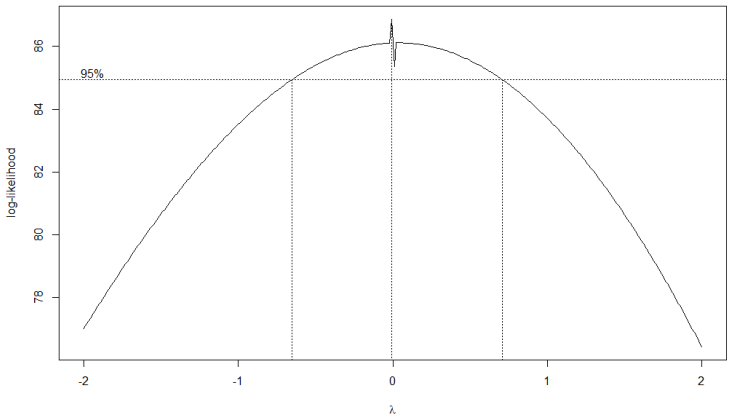


```
> SummTable_Dietary()
           Estimate Std.Error       2.5%     97.5%              unit
C0d         0.05541   0.00585    0.04395   0.06687        mgX/kgFish
k2          0.02679    0.0103    0.00659   0.04698             1/day
k2g         0.00799    0.0103     -0.0122   0.02819             1/day
kf          0.00122   0.00019    0.00084   0.00159 kgFood/kgFish/day
alpha       0.08113   0.01284    0.05597   0.10629                 -
BMFK        0.04543   0.01184    0.02223   0.06864     kgFood/kgFish
BMFKg       0.15227   0.17595   -0.19258   0.49713     kgFood/kgFish
tHalfg     86.714   111.8     -132.42    305.84               day
BMFKgLipid  0.42977   0.49659   -0.54354   1.4031      kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of 0.00799 and a BMF_{KgL} of 0.42977 (95% Confidence interval: -0.54354—1.4031) are estimated for $C_{14}Cl_7$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()

      fit     conflo     confup
-0.0100000 -0.6523538  0.7077635
```



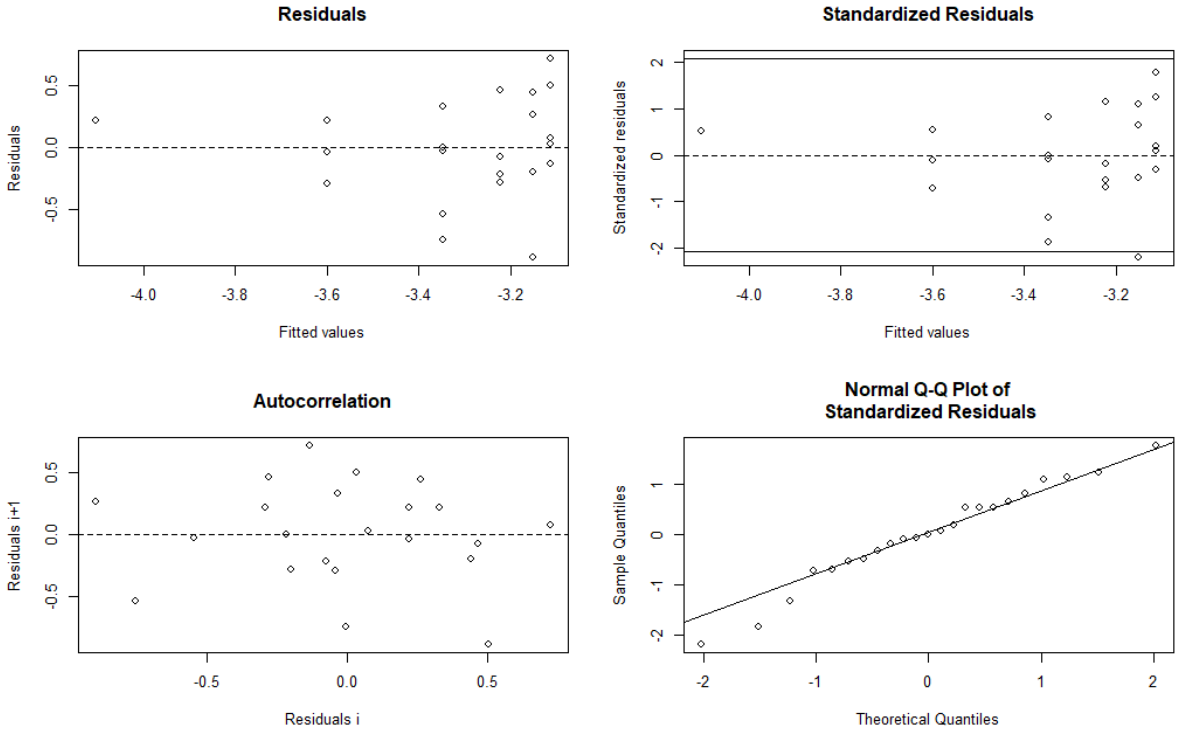
The estimated optimal λ value is -0.01 and its confidence interval is -0.6523 up to 0.7077. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.047407   0.005299   8.946 1.31e-08 ***
fitk2  0.017360   0.006168   2.814   0.0104 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.4049 on 21 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 5.101e-06
```

A k_2 value of 0.017360 is predicted with the Box-Cox power transformation model. This k_2 value is significantly different from zero (p=0.0104).

```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test
```

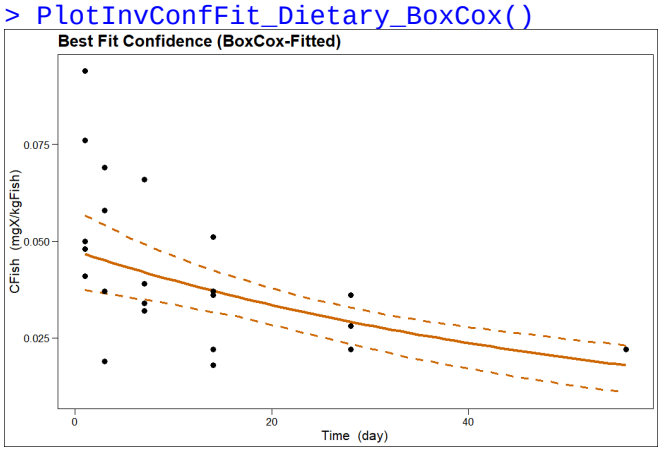
```
data:  stdres
W = 0.97361, p-value = 0.7745


------
        Runs Test

data:  as.factor(run)
Standard Normal = -1.0599, p-value = 0.2892
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.2892, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7745), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is lower than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
      Estimate Std.Error      2.5%    97.5%              unit
C0d     0.0474    0.0053     0.037    0.058         mgX/kgFish
k2      0.0174    0.0062     0.005    0.029              1/day
k2g    -0.0014    0.0062    -0.014    0.011              1/day
kf      0.001     0.0001     0.001    0.001 kgFood/kgFish/day
```

```
alpha         0.0652    0.0093     0.047    0.084                  -
BMFK          0.0563    0.0142     0.029    0.084     kgFood/kgFish
BMFKg        -0.6819    3.0132    -6.588    5.224     kgFood/kgFish
tHalfg     -483.15   2077.8    -4555.6   3589.3                day
BMFKgLipid   -1.9245    8.5043   -18.593   14.744     kgFood/kgFish
```

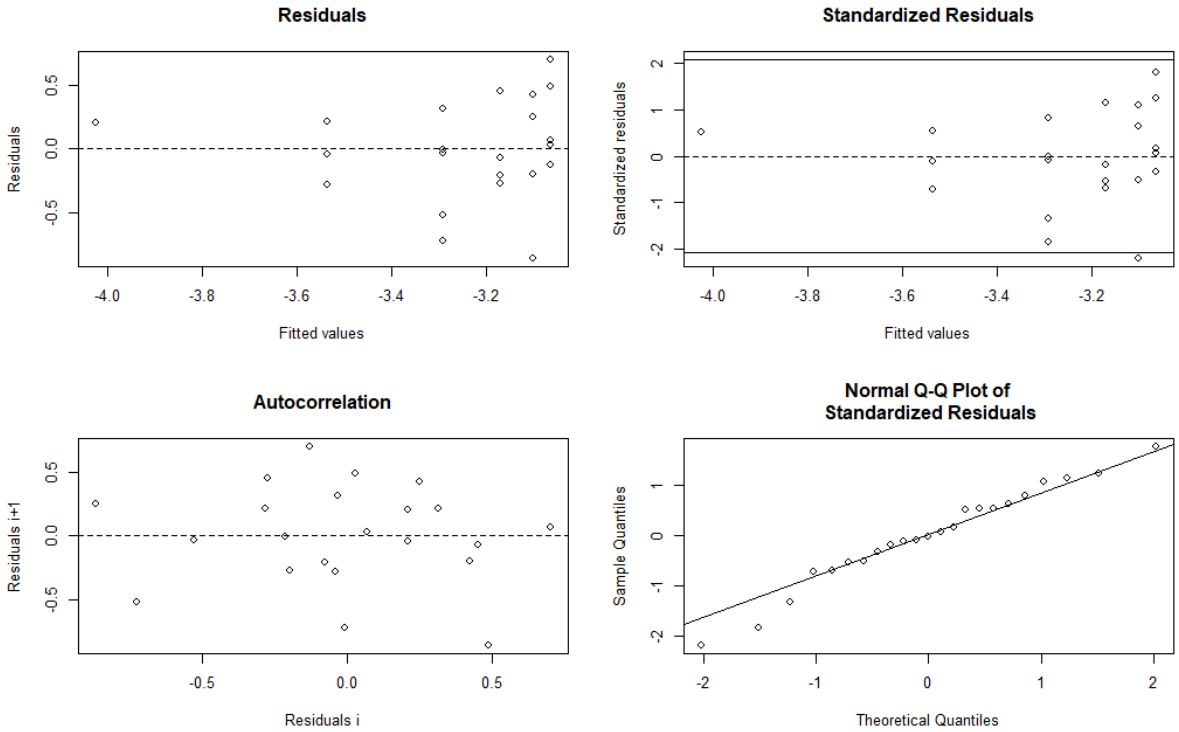
A depuration rate growth corrected (k_{2g}) of -0.0014 and a BMF_{KgL} of -1.9245 (95% Confidence interval: -18.593—14.744) are estimated with the Box-Cox power transformation model for $C_{14}Cl_7$ congener.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()

Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.047477   0.005304   8.951  1.3e-08 ***
fitk2  0.017423   0.006191   2.814   0.0104 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3919 on 21 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 7.541e-08
```

A k_2 value of 0.017423 is predicted with the logarithm transformation model for $C_{14}Cl_7$ group of congeners. This k_2 value is significantly different from zero ($p=0.0104$).

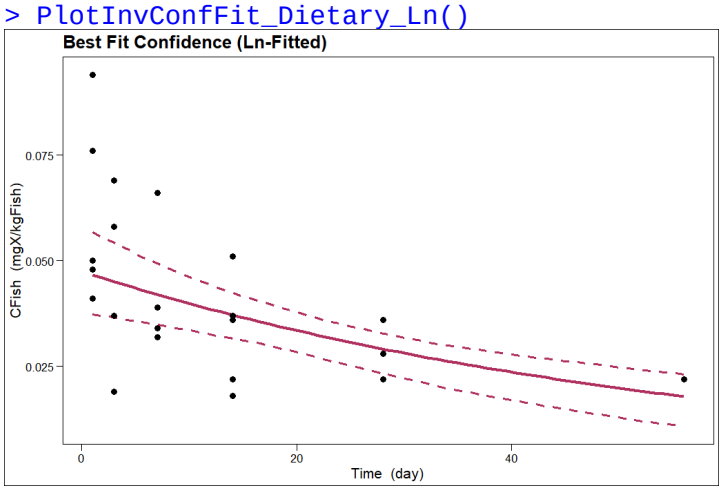
```
> ModelDiagnostics_Dietary_Ln()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.97409, p-value = 0.7856


------
        Runs Test

data:  as.factor(run)
Standard Normal = -1.0599, p-value = 0.2892
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.2892, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7856), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is lower than in the untransformed model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
   Estimate Std.Error      2.5%    97.5%              unit
C0d   0.0475    0.0053     0.037    0.058         mgX/kgFish
k2    0.0174    0.0062     0.005     0.03              1/day
k2g  -0.0014    0.0062    -0.014    0.011              1/day
kf    0.001     0.0001     0.001    0.001 kgFood/kgFish/day
alpha 0.0653    0.0094     0.047    0.084                  -
BMFK  0.0562    0.0141     0.029    0.084     kgFood/kgFish
BMFKg -0.7145   3.3105    -7.203    5.774     kgFood/kgFish
tHalfg -505.33  2281.4   -4976.8   3966.2               day
BMFKgLipid -2.0167 9.3435 -20.33   16.297     kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of -0.0014 and a BMF_{KgL} of -2.0167 (95% Confidence interval: -20.33–16.297) are estimated with the logarithm transformation model for $C_{14}Cl_7$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_7$ group of congeners, the untransformed model is the best fit model to the data.

$C_{14}Cl_7$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

For $C_{14}Cl_7$ as the growth rate constant (k_g) was higher than the depuration rate constant (k_2), the corresponding depuration rate growth corrected constant (k_{2g}) was negative when using the logarithm model and the Box-Cox power transformation models thus the BMF derived from this negative k_{2g} was also negative. However, the BMF derived using the untransformed model was positive. The untransformed model was considered to be the best fit model for $C_{14}Cl_7$ group of congeners. As the mass approach did not work in our case, and in order to confirm the outcome of the untransformed model, the bcmfR R-package was re-run for $C_{14}Cl_7$ without correcting the depuration rate (k_2) for growth (k_g) and thus assuming that $k_2=k_{2g}$. This scenario ($k_g=0$ and $k_2=k_{2g}$) overestimates the depuration rate and the estimated BMF value will be underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB.

Input data for $C_{14}Cl_7$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

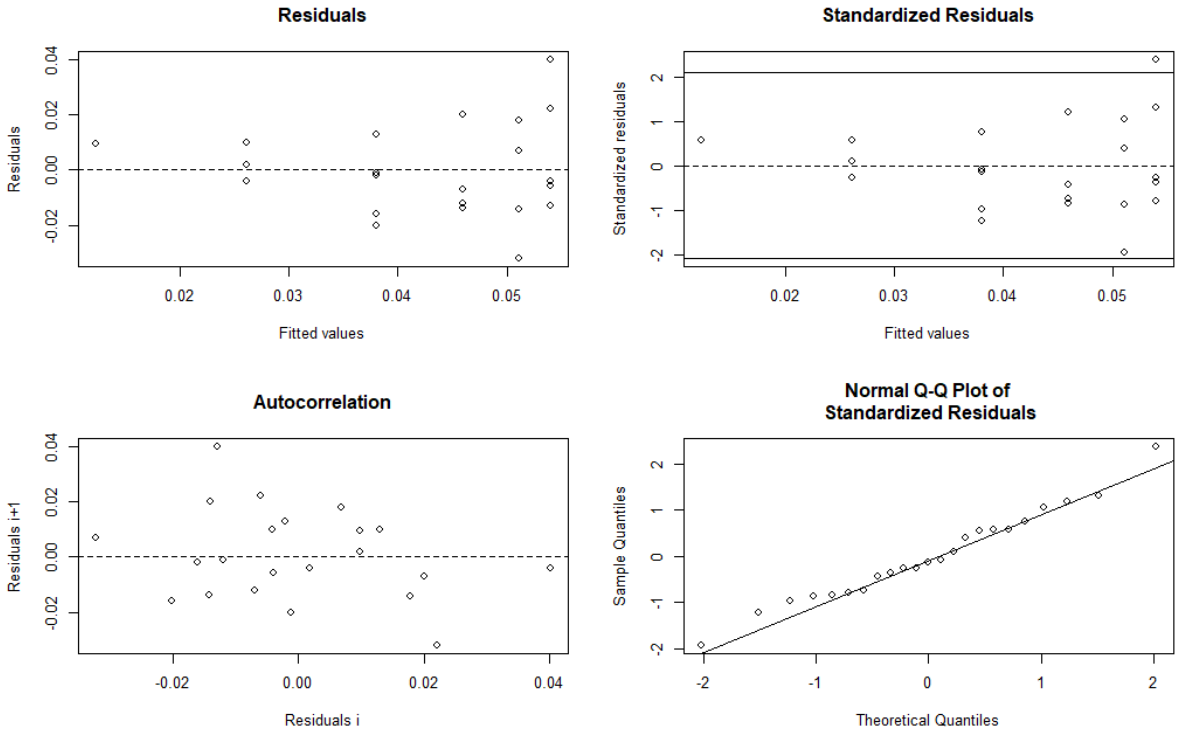
```
TEST.Dietary.Design:
            value              unit
cfood       3.900        mgX/kgFood
ingestion   0.015 kgFood/kgFish/day
tfeed      14.000               day
lipidfood  16.350           percent
lipidfish   5.793           percent
tdepur      0.000               day
tend       56.000               day
kgrowth     0.000             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1      0.041
2          1      0.094
3          1      0.050
4          1      0.048
5          1      0.076
6          3      0.019
7          3      0.058
8          3      0.069
9          3      0.037
10         7      0.032
11         7      0.066
12         7      0.039
13         7      0.034
14        14      0.037
15        14      0.018
16        14      0.022
17        14      0.036
18        14      0.051
19        28      0.036
20        28      0.028
21        28      0.022
22        28      0.036
23        56      0.022
```

UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()
Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.055408   0.005846   9.477 4.92e-09 ***
fitk2  0.026786   0.010304   2.600   0.0167 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.01667 on 21 degrees of freedom

Number of iterations to convergence: 6
Achieved convergence tolerance: 7.211e-06
```

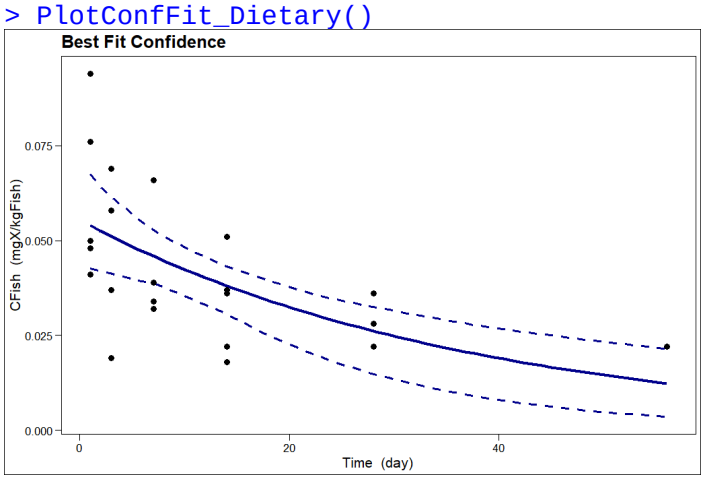
A k_2 value of 0.026786 is predicted with the untransformation model for $C_{14}Cl_7$ group of congeners. This k_2 value is significantly different from zero (p=0.0167).

```
> ModelDiagnostics_Dietary()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.98011, p-value = 0.9081


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.13227, p-value = 0.8948
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates *p-value* of 0.8948, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.9081) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```

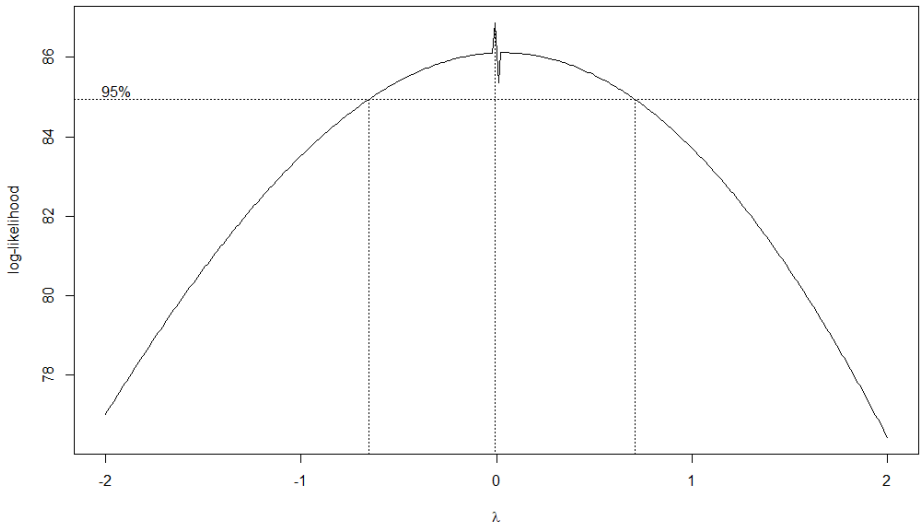



```
> SummTable_Dietary()
             Estimate Std.Error     2.5%    97.5%              unit
C0d          0.055408  0.005846 0.043949  0.06687        mgX/kgFish
k2           0.026786  0.010304 0.00659   0.04698             1/day
k2g          0.026786  0.010304 0.00659   0.04698             1/day
kf           0.001217  0.000193 0.00084   0.00159 kgFood/kgFish/day
alpha        0.081129  0.012837 0.055969  0.10629                 -
BMFK         0.045432  0.01184  0.022226  0.06864     kgFood/kgFish
BMFKg        0.045432  0.01184  0.022226  0.06864     kgFood/kgFish
tHalfg      25.872     9.9523   6.3654   45.378               day
BMFKgLipid   0.12823   0.033417 0.06273   0.19372     kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of 0.026786 (equal to k_2) and a BMF_{KgL} of 0.12823 (95% Confidence interval: 0.06273–0.19372) are estimated for $C_{14}Cl_7$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
fit      conflo     confup
-0.0100000 -0.6523538  0.7077635
```



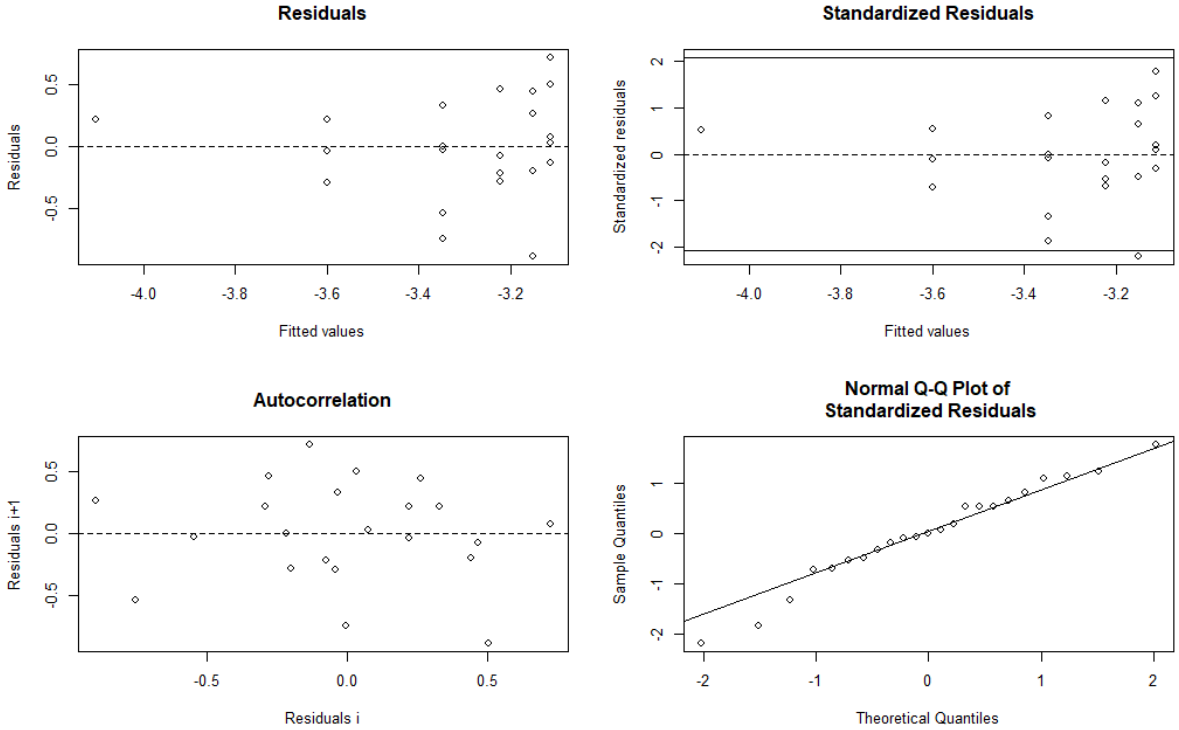
The estimated optimal λ value is -0.01 and its confidence interval is -0.652 up to 0.708. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)
```

```
Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.047407   0.005299   8.946 1.31e-08 ***
fitk2  0.017360   0.006168   2.814   0.0104 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.4049 on 21 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 5.101e-06
```

A k_2 value of 0.017360 is predicted with the Box-Cox power transformation model. This k_2 value is significantly different from zero (p=0.0104).

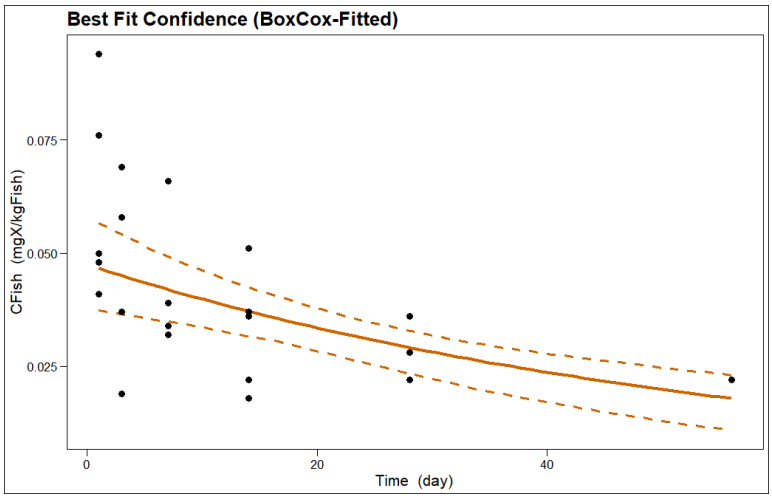
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.97361, p-value = 0.7745


------
        Runs Test

data:  as.factor(run)
Standard Normal = -1.0599, p-value = 0.2892
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.2892, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7745), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is lower than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
            Estimate Std.Error      2.5%    97.5%              unit
C0d          0.04741  0.005299  0.03702   0.05779        mgX/kgFish
k2           0.01736  0.006168  0.00527   0.02945             1/day
k2g          0.01736  0.006168  0.00527   0.02945             1/day
kf           0.00098   0.00014  0.000703  0.00125 kgFood/kgFish/day
alpha         0.0652  0.009343  0.04689   0.08351                 -
BMFK         0.05634  0.014157  0.028591  0.08409     kgFood/kgFish
BMFKg        0.05634  0.014157  0.028591  0.08409     kgFood/kgFish
tHalfg     39.92    14.185    12.118    67.722               day
BMFKgLipid   0.15901  0.039957  0.080696  0.23733     kgFood/kgFish
```

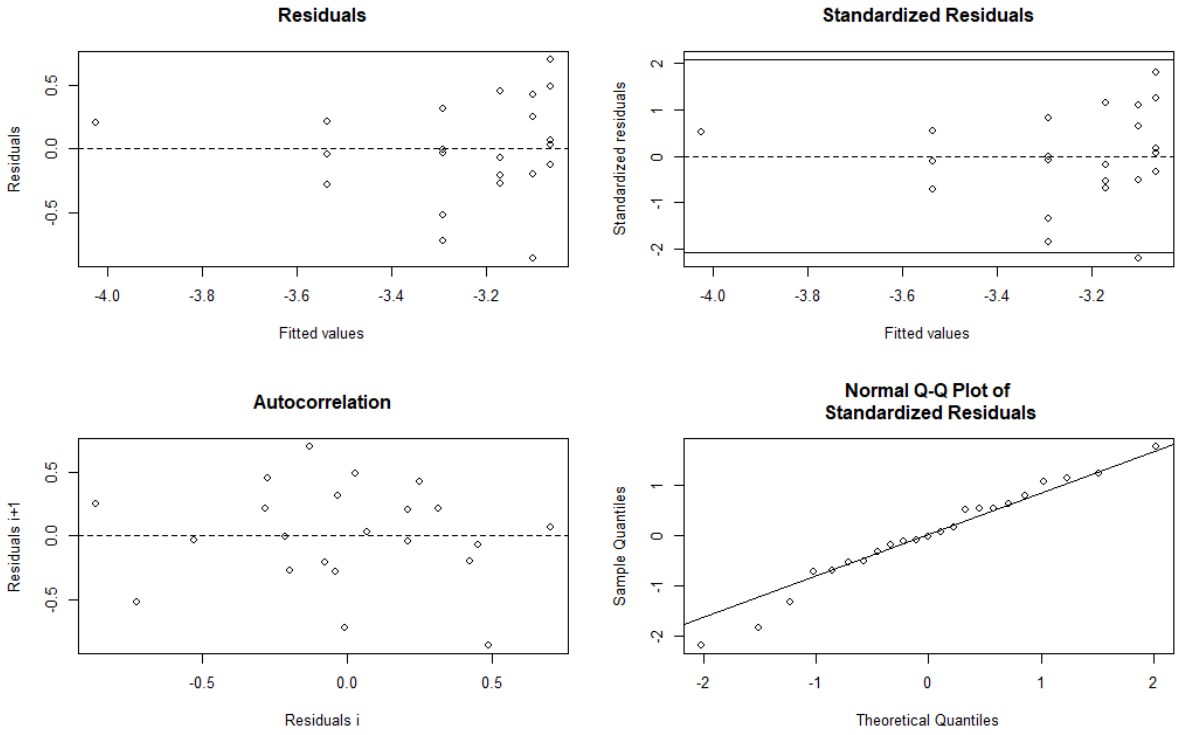
A depuration rate growth corrected (k_{2g}) of 0.01736 (equal to k_2) and a BMF_{KgL} of 0.15901 (95% Confidence interval: 0.080696–0.23733) are estimated with the Box-Cox power transformation model for $C_{14}Cl_7$ group of congeners.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.047477   0.005304   8.951  1.3e-08 ***
fitk2  0.017423   0.006191   2.814   0.0104 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3919 on 21 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 7.541e-08
```

A k_2 value of 0.017423 is predicted with the logarithm transformation model for $C_{14}Cl_7$ group of congeners. This k_2 value is significantly different from zero (p=0.0104).

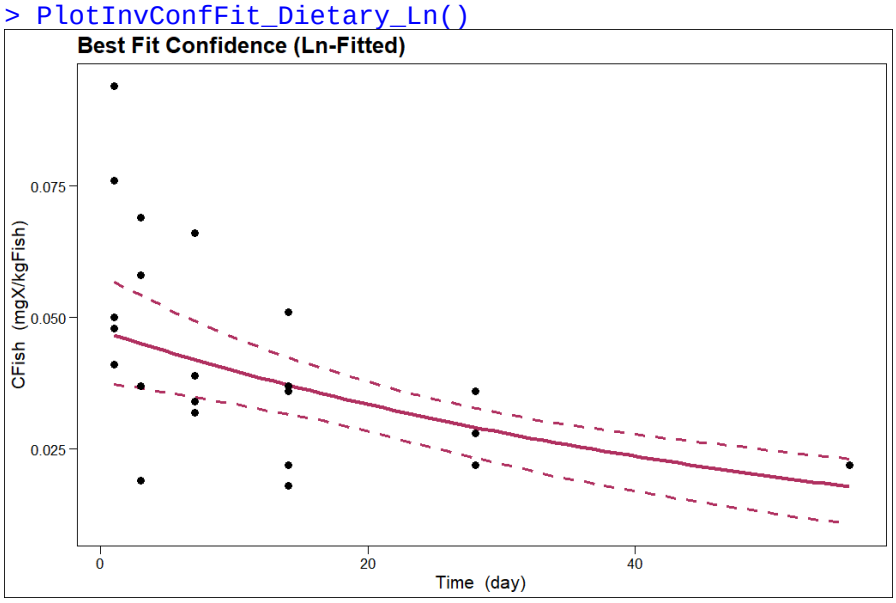
```
> ModelDiagnostics_Dietary_Ln()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.97409, p-value = 0.7856


------
        Runs Test

data:  as.factor(run)
Standard Normal = -1.0599, p-value = 0.2892
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.2892, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7856), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is lower than in the untransformed model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.04748	0.005304	0.037081	0.05787	mgX/kgFish
k2	0.01742	0.006191	0.005288	0.02956	1/day
k2g	0.01742	0.006191	0.005288	0.02956	1/day
kf	0.00098	0.00014	0.000705	0.00126	kgFood/kgFish/day
alpha	0.06533	0.009364	0.046974	0.08368	-
BMFK	0.05624	0.014132	0.028544	0.08394	kgFood/kgFish
BMFKg	0.05624	0.014132	0.028544	0.08394	kgFood/kgFish
tHalfg	39.776	14.135	12.071	67.48	day
BMFKgLipid	0.15874	0.039885	0.080563	0.23691	kgFood/kgFish

A depuration rate growth corrected (k_{2g}) of 0.01742 (equal to k_2) and a BMF_{KgL} of 0.15874 (95% Confidence interval: 0.080563–0.23691) are estimated with the logarithm transformation model for $C_{14}Cl_7$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_7$ group of congeners, the untransformed model is the best fit model to the data.

$C_{14}Cl_8$ group of congeners:

Input data for $C_{14}Cl_8$ group of congeners:

```
TEST.Dietary.Design:
              value              unit
cfood      1.470000        mgX/kgFood
ingestion  0.015000 kgFood/kgFish/day
tfeed     14.000000               day
lipidfood 16.350000           percent
lipidfish  5.793000           percent
tdepur     0.000000               day
tend      56.000000               day
kgrowth    0.018794             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1      0.023
2          1      0.048
3          1      0.024
4          1      0.027
5          1      0.044
6          3      0.012
7          3      0.032
8          3      0.035
9          3      0.021
10         7      0.019
11         7      0.037
12         7      0.024
13         7      0.019
14        14      0.022
15        14      0.012
16        14      0.015
17        14      0.022
18        14      0.030
19        28      0.022
20        28      0.017
21        28      0.013
22        28      0.024
23        56      0.016
```

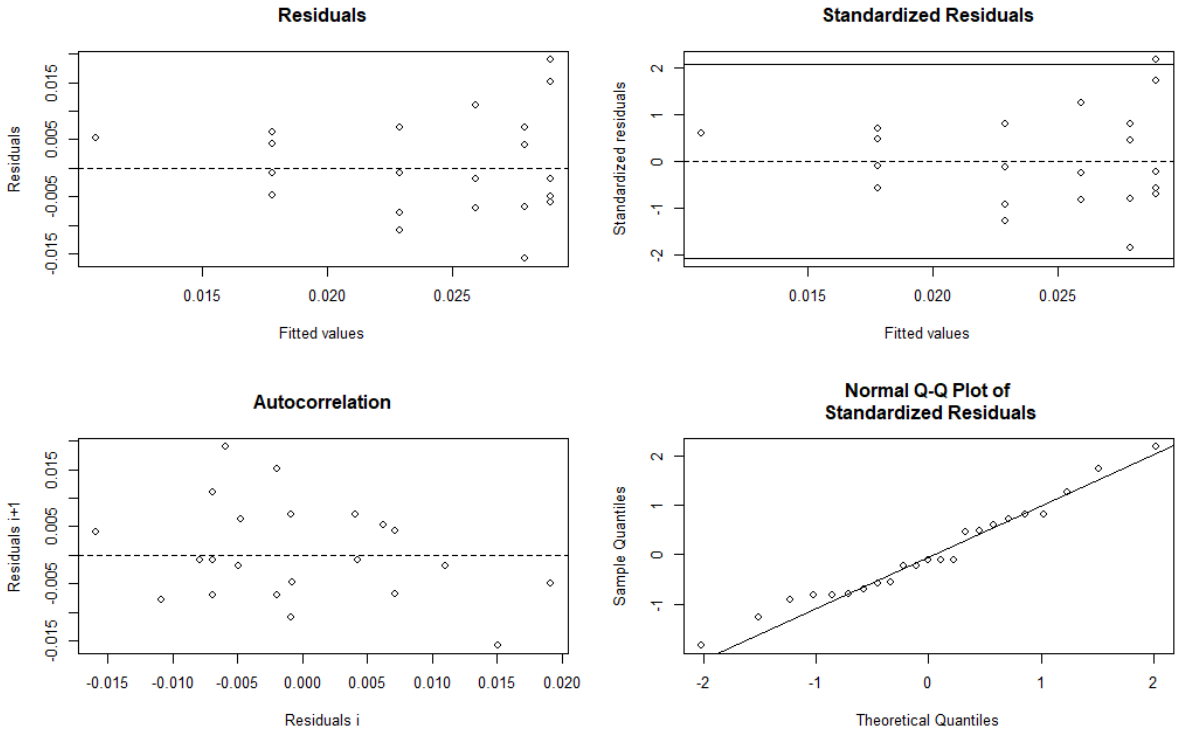
UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()
Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.029456   0.002872  10.255 1.24e-09 ***
fitk2  0.017999   0.008091   2.225   0.0372 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

```
Residual standard error: 0.008688 on 21 degrees of freedom

Number of iterations to convergence: 5
Achieved convergence tolerance: 9.485e-06
```

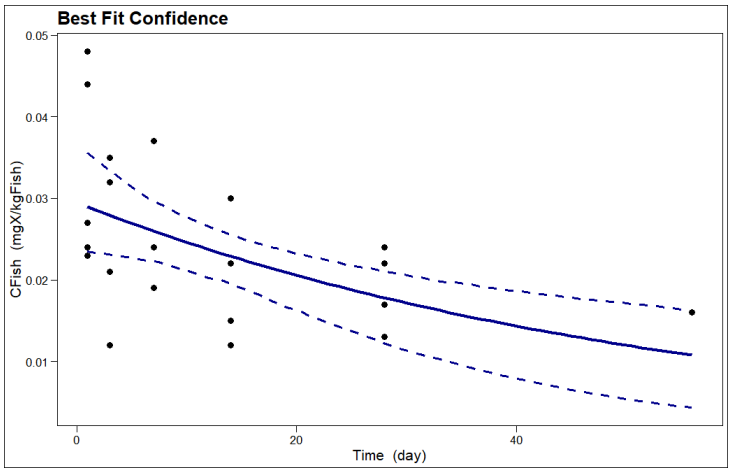
A k_2 value of 0.017999 is predicted with the untransformation model for $C_{14}Cl_8$ group of congeners. This k_2 value is significantly different from zero (p=0.0372).

```
> ModelDiagnostics_Dietary()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.97053, p-value = 0.7018


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.019525, p-value = 0.9844
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates *p-value* of 0.9844, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7018) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```

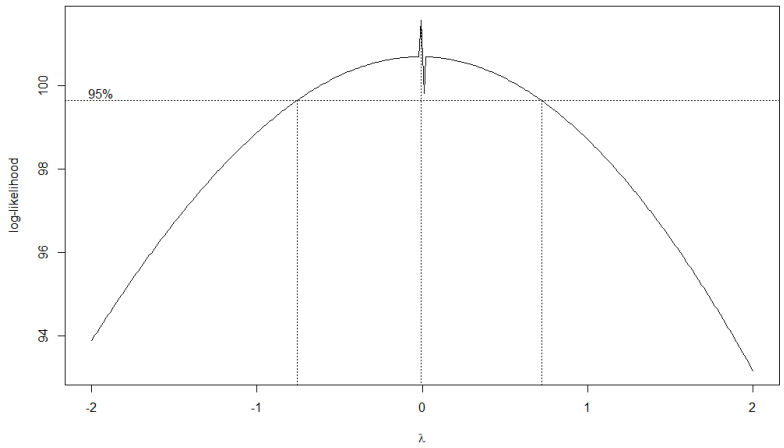



```
> SummTable_Dietary()

Estimate Std.Error       2.5%     97.5%              unit
C0d          0.0295     0.003     0.024     0.035        mgX/kgFish
k2           0.018      0.008     0.002     0.034             1/day
k2g         -0.0008     0.008    -0.017     0.015             1/day
kf           0.0016     0         0.001     0.002 kgFood/kgFish/day
alpha        0.1079     0.015     0.078     0.137                 -
BMFK         0.09       0.031     0.03      0.15      kgFood/kgFish
BMFKg       -2.0367    20.969   -43.136    39.063     kgFood/kgFish
tHalfg    -871.68    8871.1   -18259     16516                 day
BMFKgLipid  -5.7483    59.183   -121.75    110.25     kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of -0.0008 and a BMF_{KgL} of -5.7483 are estimated for $C_{14}Cl_8$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
fit      conflo     confup
-0.0100000 -0.7590848  0.7219265
```



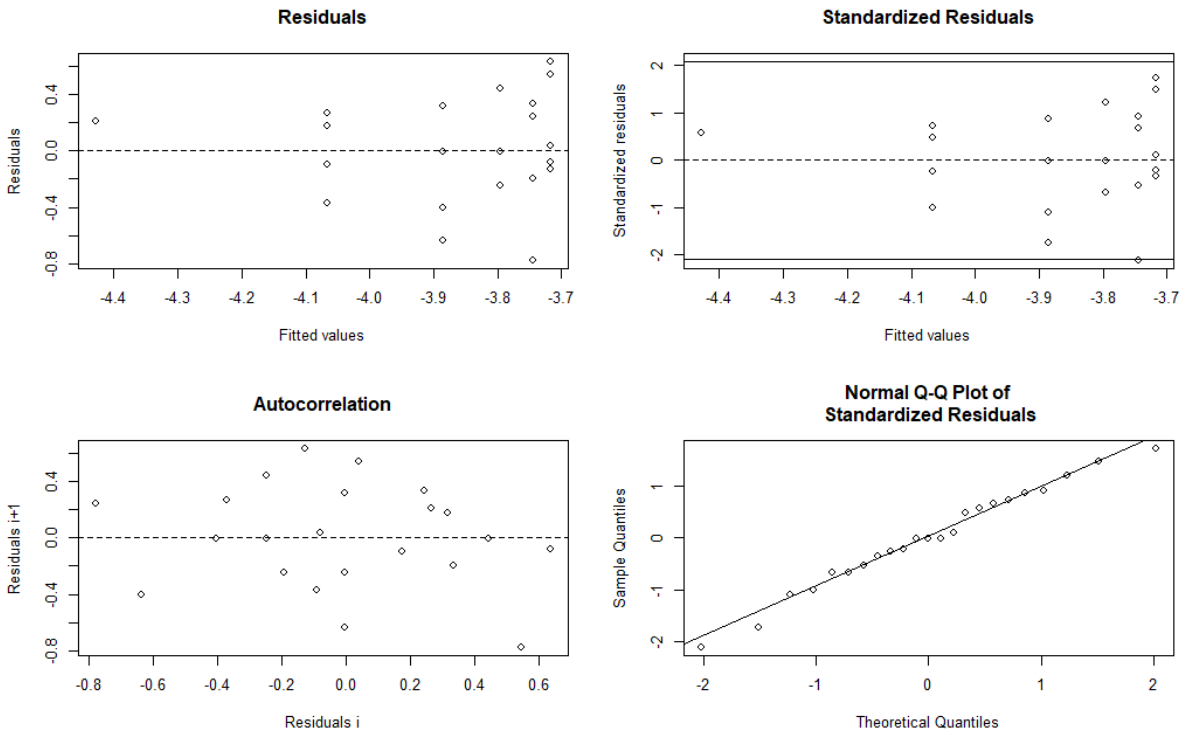
The estimated optimal λ value is -0.01 and its confidence interval is -0.7590848 up to 0.7219265. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.026307   0.002646   9.942 2.14e-09 ***
fitk2  0.012402   0.005557   2.232   0.0366 *
```

```
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3663 on 21 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 2.812e-06
```

A k_2 value of 0.012402 is predicted with the Box-Cox power transformation model for $C_{14}Cl_8$ group of congeners. This k_2 value is significantly different from zero (p=0.0366).

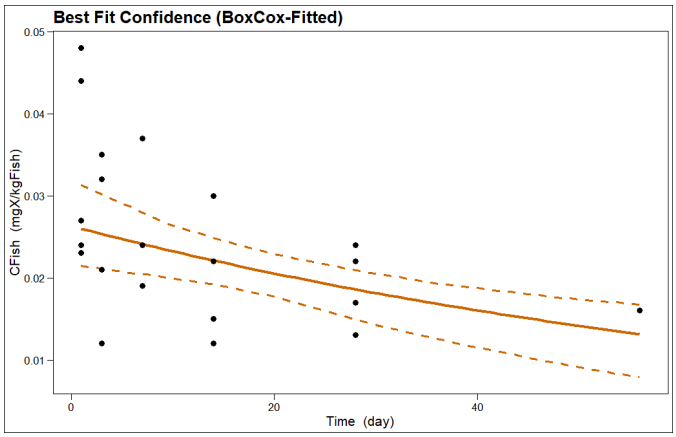
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.9836, p-value = 0.9574


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.13227, p-value = 0.8948
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot. The Q-Q plot for the Box-Cox power transformation model is more attractive than for the untransformed model.

The run test indicates a *p-value* of 0.8948, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.9574), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
             Estimate Std.Error       2.5%    97.5%              unit
C0d           0.02631   0.00265    0.02112  0.03149        mgX/kgFish
k2            0.0124    0.00556    0.00151  0.02329             1/day
k2g          -0.00639   0.00556   -0.01728  0.0045              1/day
kf            0.00139   0.00018    0.00104  0.00175 kgFood/kgFish/day
alpha         0.09283   0.01201    0.0693   0.11636                 -
BMFK          0.11227   0.03924    0.03537  0.18918     kgFood/kgFish
BMFKg        -0.21786   0.21319   -0.6357   0.19999     kgFood/kgFish
tHalfg     -108.42     94.264   -293.18    76.335               day
BMFKgLipid   -0.61487   0.60169   -1.7942   0.56445     kgFood/kgFish
```

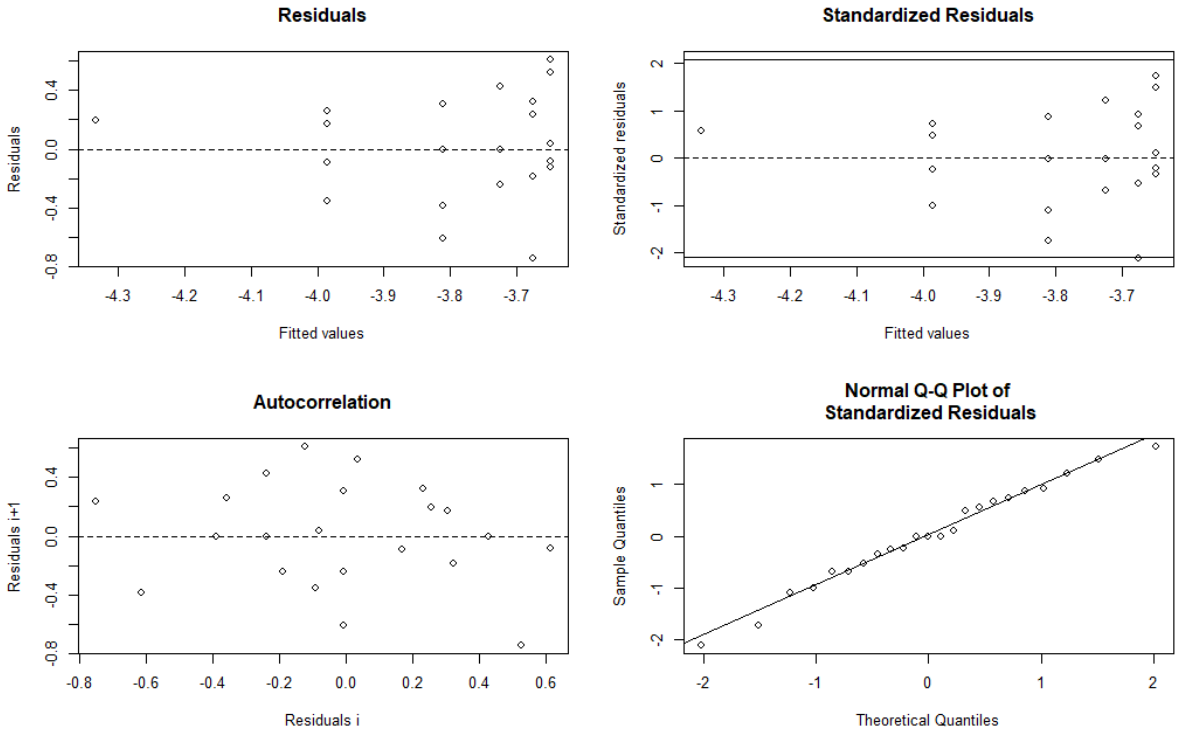
A depuration rate growth corrected (k_{2g}) of -0.00639 and a BMF_{KgL} of -0.61487 (95% Confidence interval: -1.7942—0.56445) are estimated with the Box-Cox power transformation model for $C_{14}Cl_8$ group of congeners.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()

Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.026335   0.002648   9.946 2.13e-09 ***
fitk2  0.012443   0.005572   2.233   0.0366 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3527 on 21 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 1.358e-07
```

A k_2 value of 0.012443 is predicted with the logarithm transformation model for $C_{14}Cl_8$ group of congeners. This k_2 value is significantly different from zero (p=0.0366).

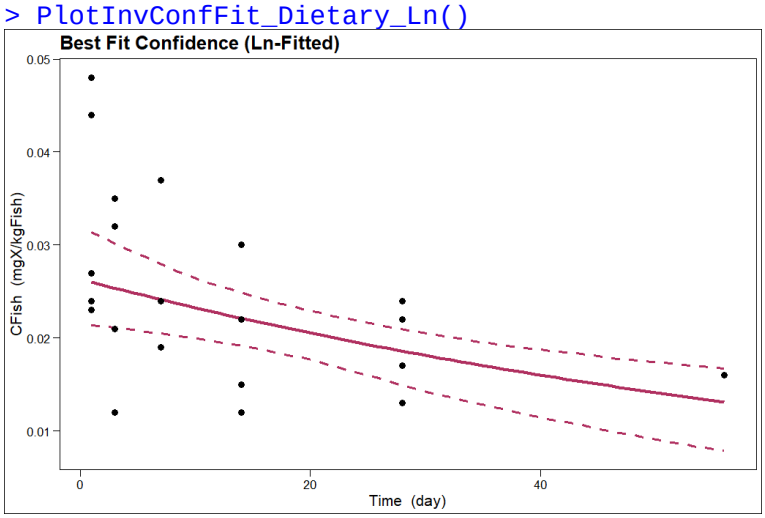
```
> ModelDiagnostics_Dietary_Ln()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.98389, p-value = 0.9606


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.13227, p-value = 0.8948
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.8948, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.9606), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model and than in the Box-cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
```

	Estimate	Std.Error	2.5%	97.5%		unit
C0d	0.02633	0.00265	0.02115	0.03152		mgX/kgFish
k2	0.01244	0.00557	0.00152	0.02336		1/day
k2g	-0.00635	0.00557	-0.01727	0.00457		1/day
kf	0.00139	0.00018	0.00104	0.00175		kgFood/kgFish/day
alpha	0.09296	0.01203	0.06938	0.11653		-
BMFK	0.11206	0.03913	0.03536	0.18875		kgFood/kgFish
BMFKg	-0.21955	0.21661	-0.64411	0.205		kgFood/kgFish
tHalfg	-109.12	95.743	-296.78	78.535		day
BMFKgLipid	-0.61966	0.61135	-1.8179	0.57858		kgFood/kgFish

A depuration rate growth corrected (k_{2g}) of -0.00635 and a BMF_{KgL} of -0.61966 (95% Confidence interval: -1.8179–0.57858) are estimated with the logarithm transformation model for C_{14} Cl_8 congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_8$ group of congeners, the logarithm transformed model is the best fit model to the data.

$C_{14}Cl_8$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

For $C_{14}Cl_8$ as the growth rate constant (k_g) was higher than the depuration rate constant (k_2), the corresponding depuration rate growth corrected constant (k_{2g}) was negative thus the BMF derived from this negative k_{2g} was also negative. As the mass approach did not work in our case, the bcmfR R-package was re-run for $C_{14}Cl_8$ without correcting the depuration rate (k_2) for growth (k_g) and thus assuming that $k_2=k_{2g}$. This scenario ($k_g=0$ and $k_2=k_{2g}$) overestimates the depuration rate and the estimated BMF value will be underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB.

Input data for $C_{14}Cl_8$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

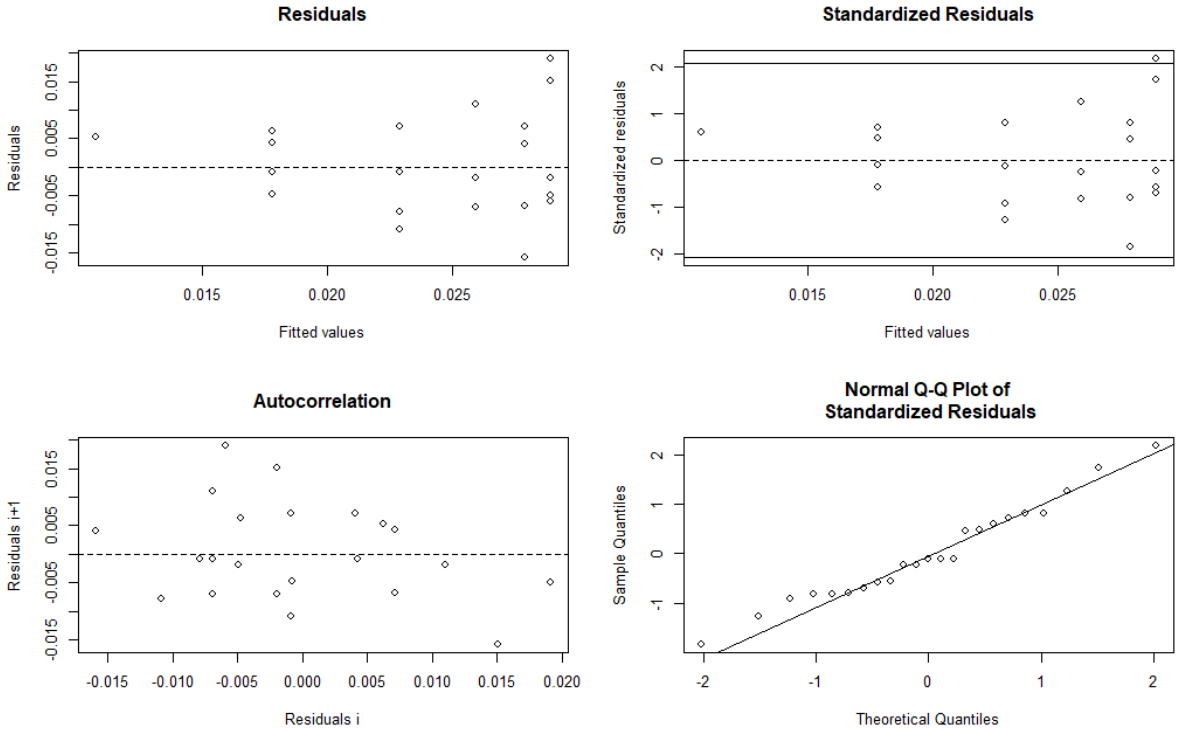
```
TEST.Dietary.Design:
           value              unit
cfood      1.470        mgX/kgFood
ingestion  0.015 kgFood/kgFish/day
tfeed     14.000               day
lipidfood 16.350           percent
lipidfish  5.793           percent
tdepur     0.000               day
tend      56.000               day
kgrowth    0.000             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1      0.023
2          1      0.048
3          1      0.024
4          1      0.027
5          1      0.044
6          3      0.012
7          3      0.032
8          3      0.035
9          3      0.021
10         7      0.019
11         7      0.037
12         7      0.024
13         7      0.019
14        14      0.022
15        14      0.012
16        14      0.015
17        14      0.022
18        14      0.030
19        28      0.022
20        28      0.017
21        28      0.013
22        28      0.024
23        56      0.016
```

UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()


Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.029456   0.002872  10.255 1.24e-09 ***
fitk2  0.017999   0.008091   2.225   0.0372 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.008688 on 21 degrees of freedom

Number of iterations to convergence: 5
Achieved convergence tolerance: 9.485e-06
```

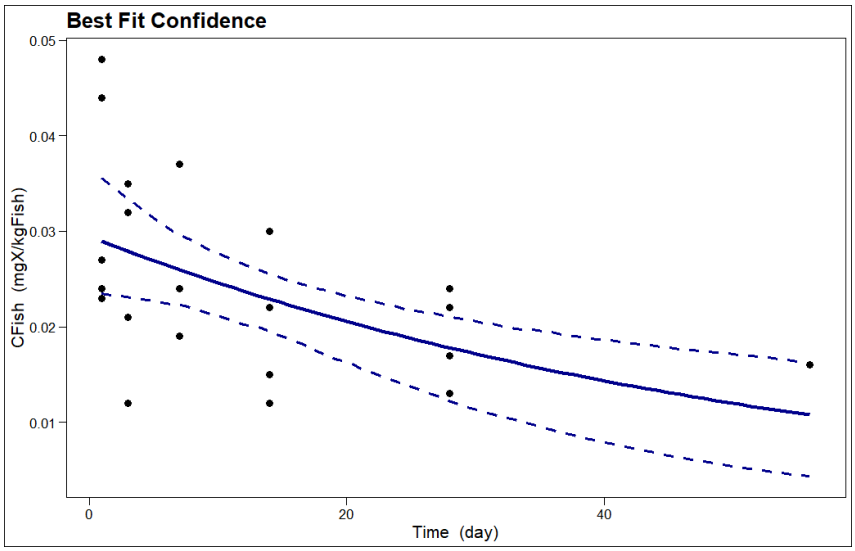
A k_2 value of 0.017999 is predicted with the untransformation model for $C_{14}Cl_8$ group of congeners. This k_2 value is significantly different from zero (p=0.0372).

```
> ModelDiagnostics_Dietary()
-----
        Shapiro-Wilk normality test

data:  stdres
W = 0.97053, p-value = 0.7018


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.019525, p-value = 0.9844
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates *p-value* of 0.9844, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7018) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```

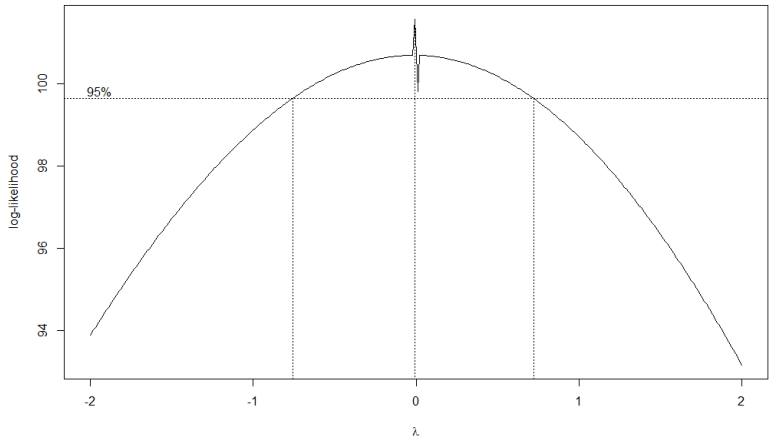



```
> SummTable_Dietary()
           Estimate Std.Error     2.5%    97.5%             unit
C0d         0.02946  0.002872 0.023826  0.03509        mgX/kgFish
k2          0.018    0.008091 0.002141  0.03386             1/day
k2g         0.018    0.008091 0.002141  0.03386             1/day
kf          0.00162  0.000226 0.001177  0.00206 kgFood/kgFish/day
alpha       0.10795  0.015042 0.078465  0.13743                 -
BMFK        0.08996  0.030509 0.030163  0.14976     kgFood/kgFish
BMFKg       0.08996  0.030509 0.030163  0.14976     kgFood/kgFish
tHalfg     38.502   17.308    4.5792   72.425               day
BMFKgLipid  0.2539   0.086107 0.085132  0.42267     kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of 0.018 (equal to k_2) and a BMF_{KgL} of 0.2539 are estimated for $C_{14}Cl_8$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
    fit     conflo     confup
-0.0100000 -0.7590848  0.7219265
```



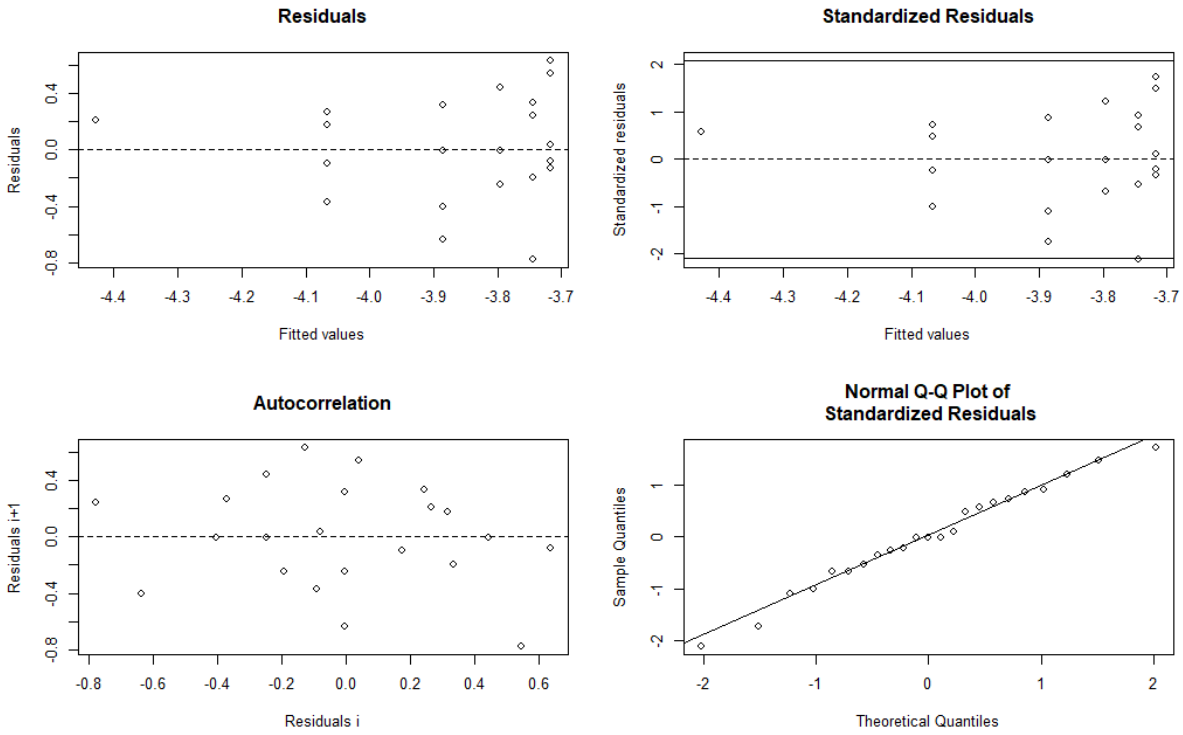
The estimated optimal λ value is -0.01 and its confidence interval is -0.759 up to 0.722. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
```

```
fitc0d 0.026307   0.002646   9.942 2.14e-09 ***
fitk2  0.012402   0.005557   2.232   0.0366 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3663 on 21 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 2.812e-06
```

A k_2 value of 0.012402 is predicted with the Box-Cox power transformation model for $C_{14}Cl_8$ group of congeners. This k_2 value is significantly different from zero (p=0.0366).

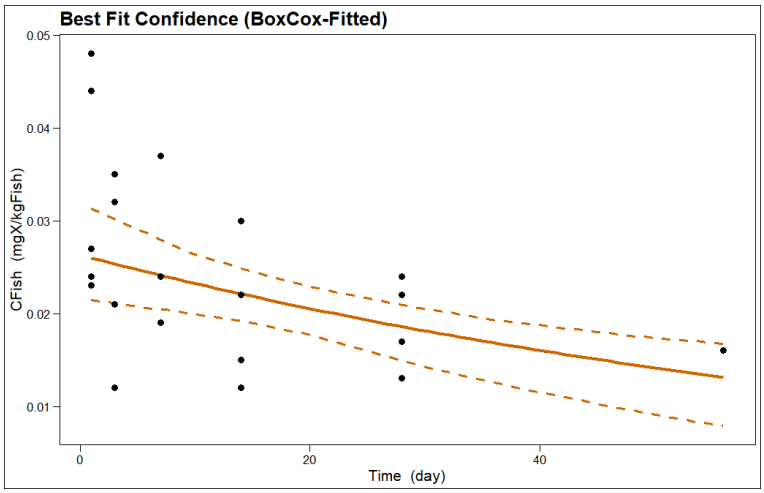
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.9836, p-value = 0.9574


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.13227, p-value = 0.8948
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot. The Q-Q plot for the Box-Cox power transformation model is more attractive than for the untransformed model.

The run test indicates a *p-value* of 0.8948, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.9574), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
            Estimate Std.Error     2.5%     97.5%              unit
C0d          0.02631  0.002646 0.021121   0.03149        mgX/kgFish
k2           0.0124   0.005557 0.001511   0.02329             1/day
k2g          0.0124   0.005557 0.001511   0.02329             1/day
kf           0.00139  0.00018  0.001039   0.00175 kgFood/kgFish/day
alpha        0.09283  0.012006 0.069298   0.11636                 -
BMFK         0.11227  0.039238 0.035366   0.18918     kgFood/kgFish
BMFKg        0.11227  0.039238 0.035366   0.18918     kgFood/kgFish
tHalfg      55.876   25.035    6.8068   104.95               day
BMFKgLipid   0.31688  0.11074  0.099816   0.53394     kgFood/kgFish
```

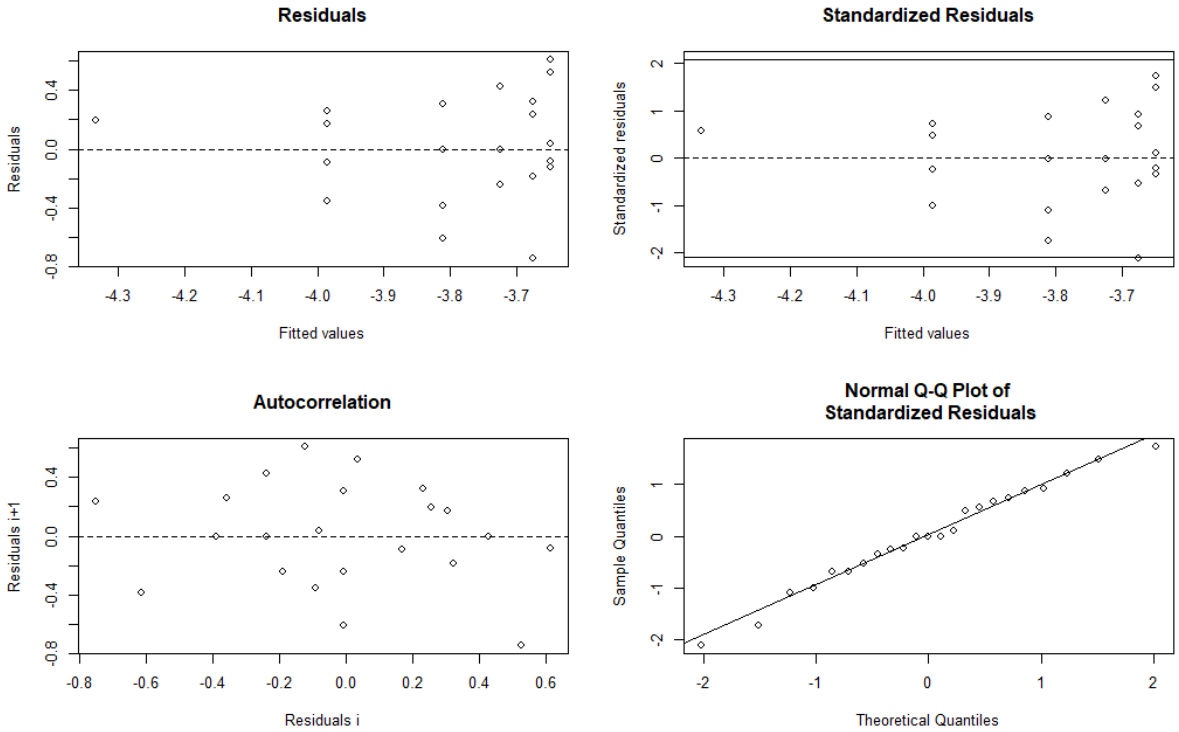
A depuration rate growth corrected (k_{2g}) of 0.0124 (equal to k_2) and a BMF_{KgL} of 0.31688 (95% Confidence interval: 0.099816—0.53394) are estimated with the Box-Cox power transformation model for $C_{14}Cl_8$ group of congeners.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
       Estimate Std. Error t value Pr(>|t|)
fitc0d 0.026335   0.002648   9.946 2.13e-09 ***
fitk2  0.012443   0.005572   2.233   0.0366 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3527 on 21 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 1.358e-07
```

A k_2 value of 0.012443 is predicted with the logarithm transformation model for $C_{14}Cl_8$ group of congeners. This k_2 value is significantly different from zero (p=0.0366).

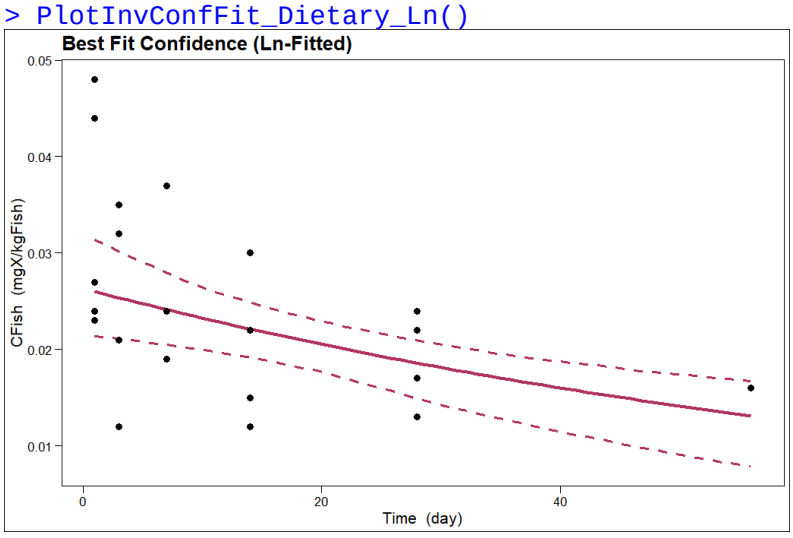
```
> ModelDiagnostics_Dietary_Ln()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.98389, p-value = 0.9606


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.13227, p-value = 0.8948
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.8948, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.9606), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model and than in the Box-cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.02633	0.002648	0.021145	0.03152	mgX/kgFish
k2	0.01244	0.005572	0.001522	0.02336	1/day
k2g	0.01244	0.005572	0.001522	0.02336	1/day
kf	0.00139	0.00018	0.001041	0.00175	kgFood/kgFish/day
alpha	0.09296	0.012026	0.069385	0.11653	-
BMFK	0.11206	0.03913	0.03536	0.18875	kgFood/kgFish
BMFKg	0.11206	0.03913	0.03536	0.18875	kgFood/kgFish
tHalfg	55.693	24.94	6.811	104.57	day
BMFKgLipid	0.31626	0.11044	0.099799	0.53273	kgFood/kgFish

A depuration rate growth corrected (k_{2g}) of 0.01244 (equal to k_2) and a BMF_{KgL} of 0.31626 (95% Confidence interval: 0.099799–0.53273) are estimated with the logarithm transformation model for $C_{14}Cl_8$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_8$ group of congeners, the logarithm transformed model is the best fit model to the data.

$C_{14}Cl_9$ group of congeners:

Input data for $C_{14}Cl_9$ group of congeners:

```
TEST.Dietary.Design:
              value              unit
cfood      0.440000        mgX/kgFood
ingestion  0.015000 kgFood/kgFish/day
tfeed     14.000000               day
lipidfood 16.350000           percent
lipidfish  5.793000           percent
tdepur     0.000000               day
tend      56.000000               day
kgrowth    0.018794             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1     0.0085
2          1     0.0162
3          1     0.0093
4          1     0.0102
5          1     0.0157
6          3     0.0111
7          3     0.0119
8          3     0.0075
9          7     0.0070
10         7     0.0132
11         7     0.0094
12         7     0.0068
13        14     0.0086
14        14     0.0053
15        14     0.0064
16        14     0.0087
17        14     0.0113
18        28     0.0086
19        28     0.0068
20        28     0.0052
21        28     0.0093
22        56     0.0071
```

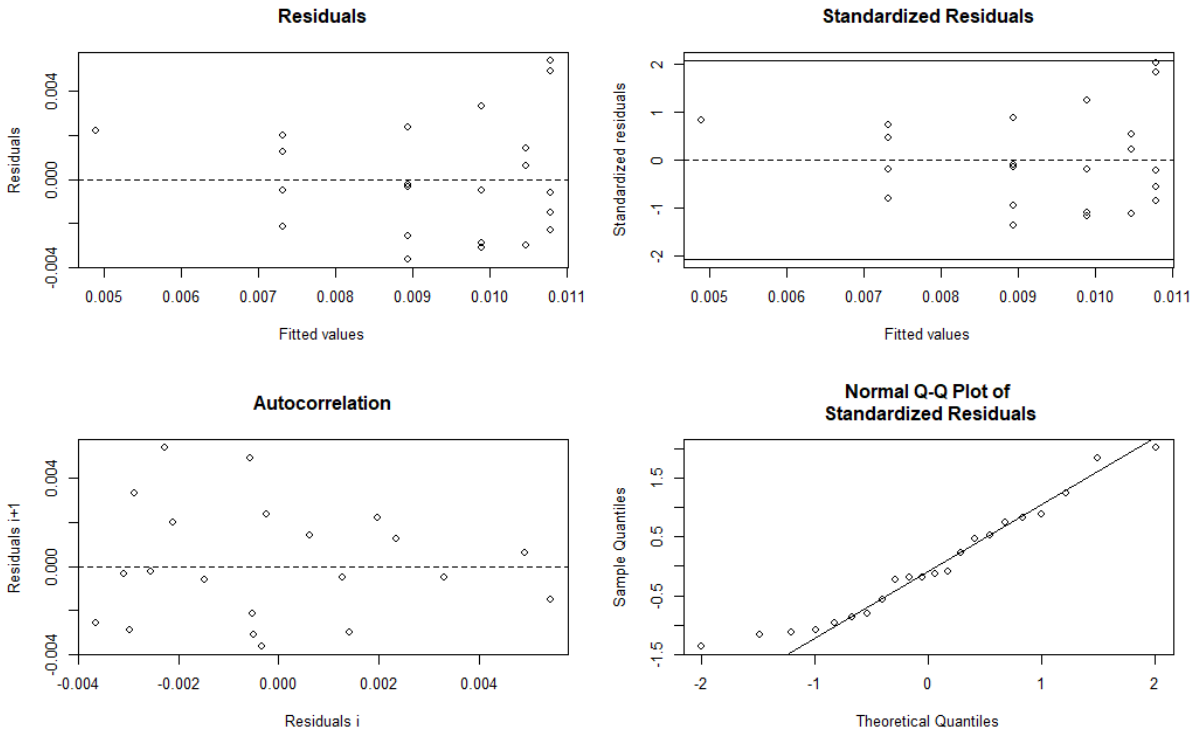
UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()
Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0109330  0.0008897  12.289 8.92e-11 ***
fitk2  0.0143495  0.0061084   2.349   0.0292 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.002668 on 20 degrees of freedom
```

```
Number of iterations to convergence: 5
Achieved convergence tolerance: 8.346e-06
```

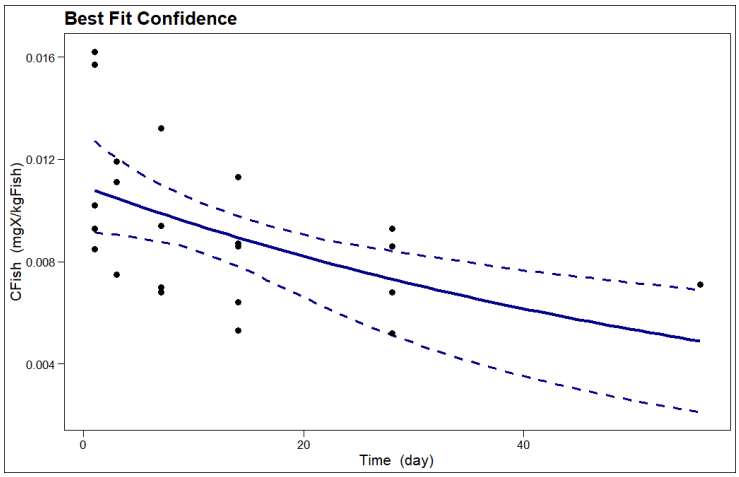
A k_2 value of 0.0143495 is predicted with the untransformation model for $C_{14}Cl_9$ group of congeners. This k_2 value is significantly different from zero (p=0.0292).

```
> ModelDiagnostics_Dietary()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.94677, p-value = 0.2722


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.74069, p-value = 0.4589
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates a *p-value* of 0.4589, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2722) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```




```
> SummTable_Dietary()
             Estimate Std.Error      2.5%     97.5%              unit
C0d           0.01093   0.00089    0.0092   0.01268        mgX/kgFish
k2            0.01435   0.00611    0.0024   0.02632             1/day
k2g          -0.00444   0.00611   -0.0164   0.00753             1/day
kf            0.00196   0.00022    0.0015   0.00239 kgFood/kgFish/day
alpha         0.13061   0.01479    0.1016   0.15959                 -
BMFK          0.13653   0.04581    0.0467   0.22632     kgFood/kgFish
BMFKg        -0.44079   0.64851   -1.7119   0.8303      kgFood/kgFish
tHalfg     -155.92    214.3     -575.94   264.1                 day
BMFKgLipid   -1.2441    1.8303    -4.8315   2.3434      kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of -0.00444 and a BMF_{KgL} of -1.2441 (95% Confidence interval: -4.8315—2.3434) are estimated for $C_{14}Cl_9$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
   fit      conflo     confup
-0.0100000 -1.0103384  0.7214893
```

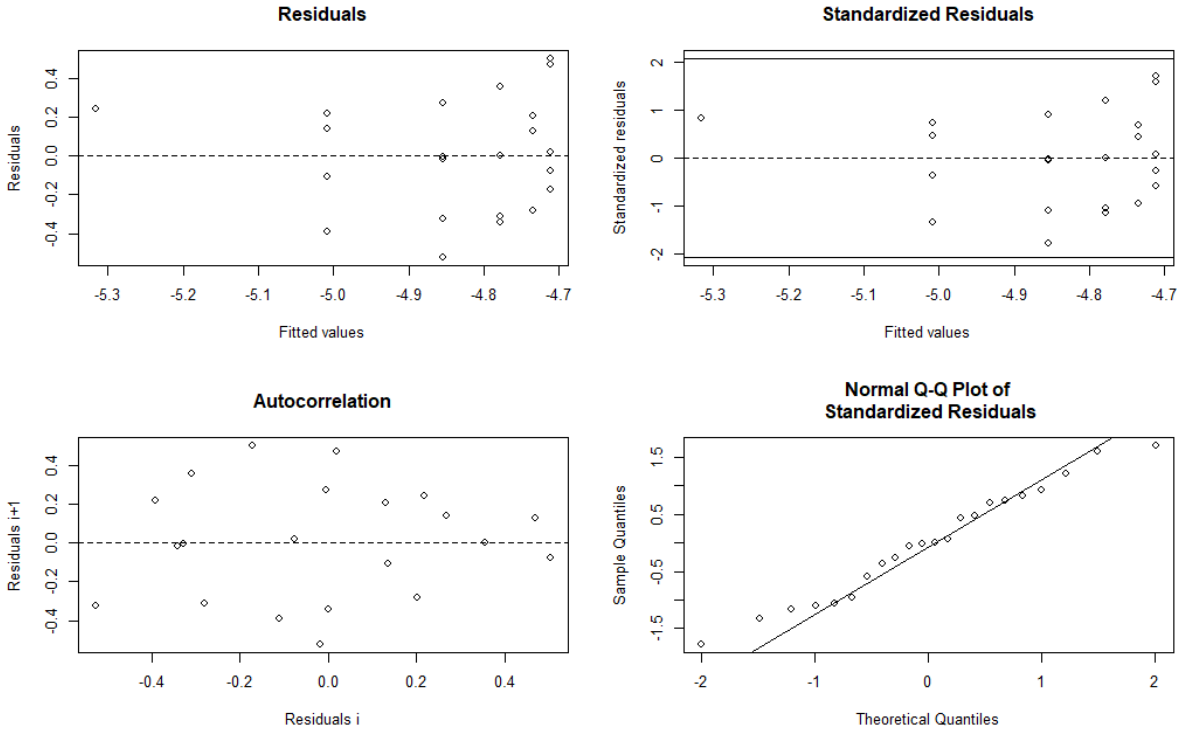
The estimated optimal λ value is -0.01 and its confidence interval is -1.0103384 up to 0.7214893. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0101115  0.0008365  12.089 1.19e-10 ***
```

```
fitk2   0.0104433   0.0044748    2.334    0.0302 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2942 on 20 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 3.522e-06
```

A k_2 value of 0.0104433 is predicted with the Box-Cox power transformation model for $C_{14}Cl_9$ group of congeners. This k_2 value is significantly different from zero (p=0.0302).

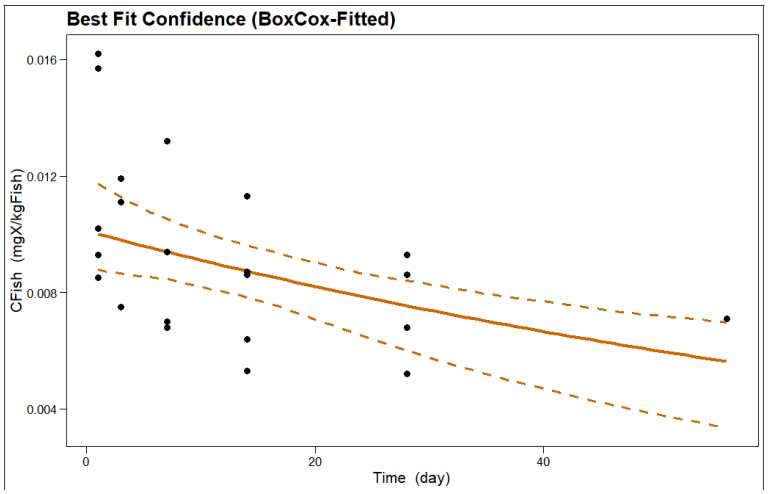
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.97319, p-value = 0.7836


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.87386, p-value = 0.3822
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.3822, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7836), the
hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
Estimate Std.Error       2.5%    97.5%               unit
C0d          0.01011   0.00084    0.00847 0.011751         mgX/kgFish
k2           0.01044   0.00447    0.00167 0.019214              1/day
k2g         -0.00835   0.00447   -0.01712 0.00042               1/day
kf           0.00176   0.00019    0.0014  0.002131 kgFood/kgFish/day
alpha        0.11763   0.01249    0.09315 0.1421                   -
BMFK         0.16895   0.05846    0.05437 0.28353       kgFood/kgFish
BMFKg       -0.21129   0.13235   -0.47069 0.048119      kgFood/kgFish
tHalfg     -82.987    44.469   -170.15    4.1723               day
BMFKgLipid  -0.59633   0.37354   -1.3285  0.13581       kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of -0.00835 and a BMF_{KgL} of -0.59633 (95% Confidence interval: -1.3285—0.13581) are estimated with the Box-Cox power transformation model for $C_{14}Cl_9$ group of congeners.

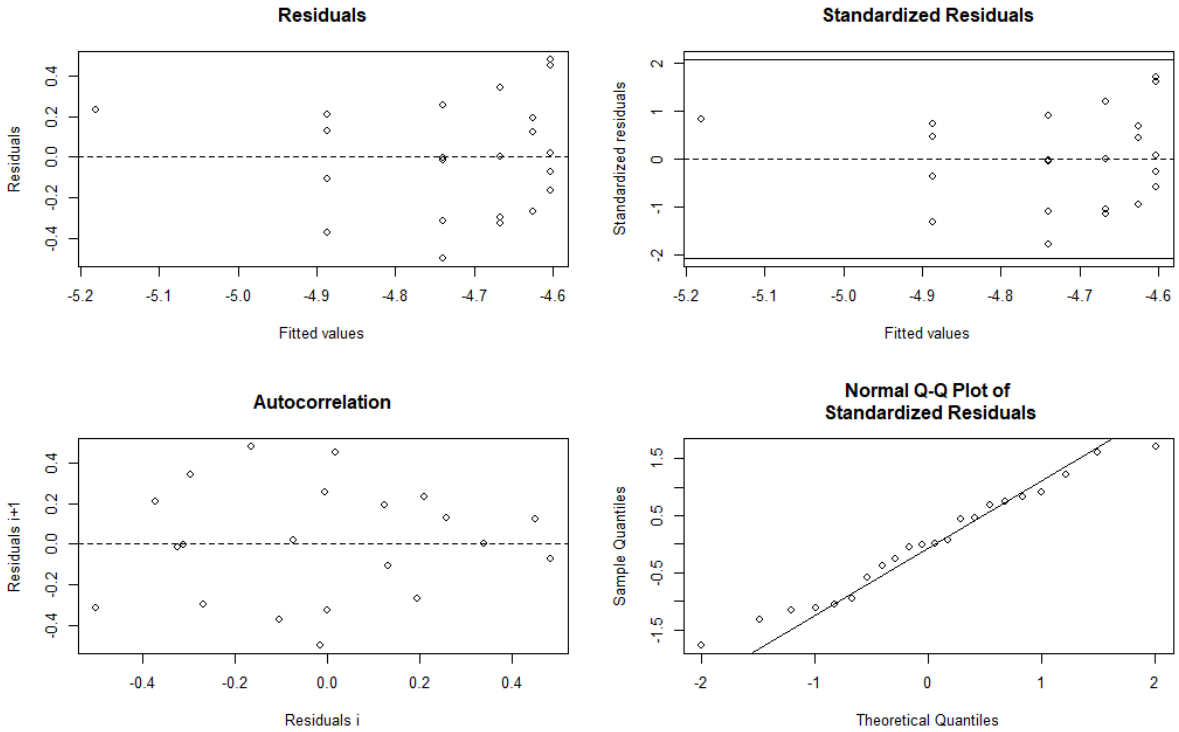
LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0101189  0.0008369  12.091 1.19e-10 ***
fitk2  0.0104727  0.0044855   2.335   0.0301 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2807 on 20 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 4.369e-07
```

A k_2 value of 0.0104727 is predicted with the logarithm transformation model for $C_{14}Cl_9$ group of congeners. This k_2 value is significantly different from zero (p=0.0301).

```
> ModelDiagnostics_Dietary_Ln()


------
        Shapiro-Wilk normality test

data:  stdres
W = 0.97305, p-value = 0.7805


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.84144, p-value = 0.4001
```

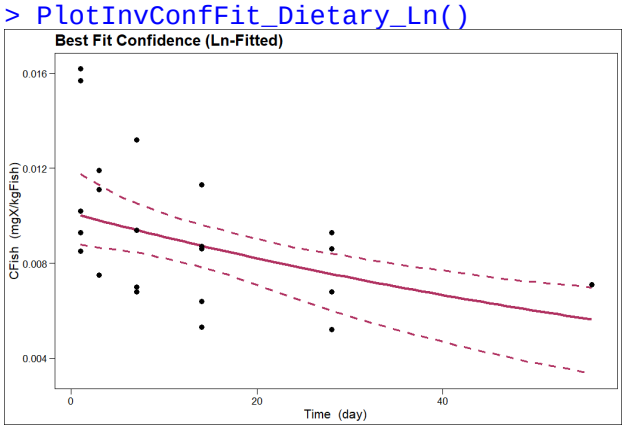
```
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.4001, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7805), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is slightly lower than in the Box-cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
            Estimate Std.Error       2.5%    97.5%             unit
C0d          0.01012   0.00084    0.00848 0.011759         mgX/kgFish
k2           0.01047   0.00449    0.00168 0.019264              1/day
k2g         -0.00832   0.00449   -0.01711 0.00047               1/day
kf           0.00177   0.00019     0.0014  0.002134 kgFood/kgFish/day
alpha        0.11774   0.0125      0.09323 0.14224                  -
BMFK         0.16863   0.05831     0.05434 0.28293       kgFood/kgFish
BMFKg       -0.21223   0.13362    -0.47414 0.04967       kgFood/kgFish
tHalfg     -83.281    44.892    -171.27    4.7068              day
BMFKgLipid  -0.599     0.37714    -1.3382  0.14019       kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of -0.00832 and a BMF_{KgL} of -0.599 (95% Confidence interval: -1.3382–0.14019) are estimated with the logarithm transformation model for $C_{14}Cl_9$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_9$ group of congeners, the Box-Cox power transformation model is the best fit model to the data.

$C_{14}Cl_9$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

Input data for $C_{14}Cl_9$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

```
TEST.Dietary.Design:
           value              unit
cfood      0.440        mgX/kgFood
ingestion  0.015 kgFood/kgFish/day
tfeed     14.000               day
lipidfood 16.350           percent
lipidfish  5.793           percent
tdepur     0.000               day
tend      56.000               day
kgrowth    0.000             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1     0.0085
2          1     0.0162
3          1     0.0093
4          1     0.0102
5          1     0.0157
6          3     0.0111
7          3     0.0119
8          3     0.0075
9          7     0.0070
10         7     0.0132
11         7     0.0094
12         7     0.0068
13        14     0.0086
14        14     0.0053
15        14     0.0064
16        14     0.0087
17        14     0.0113
18        28     0.0086
19        28     0.0068
20        28     0.0052
21        28     0.0093
22        56     0.0071
```

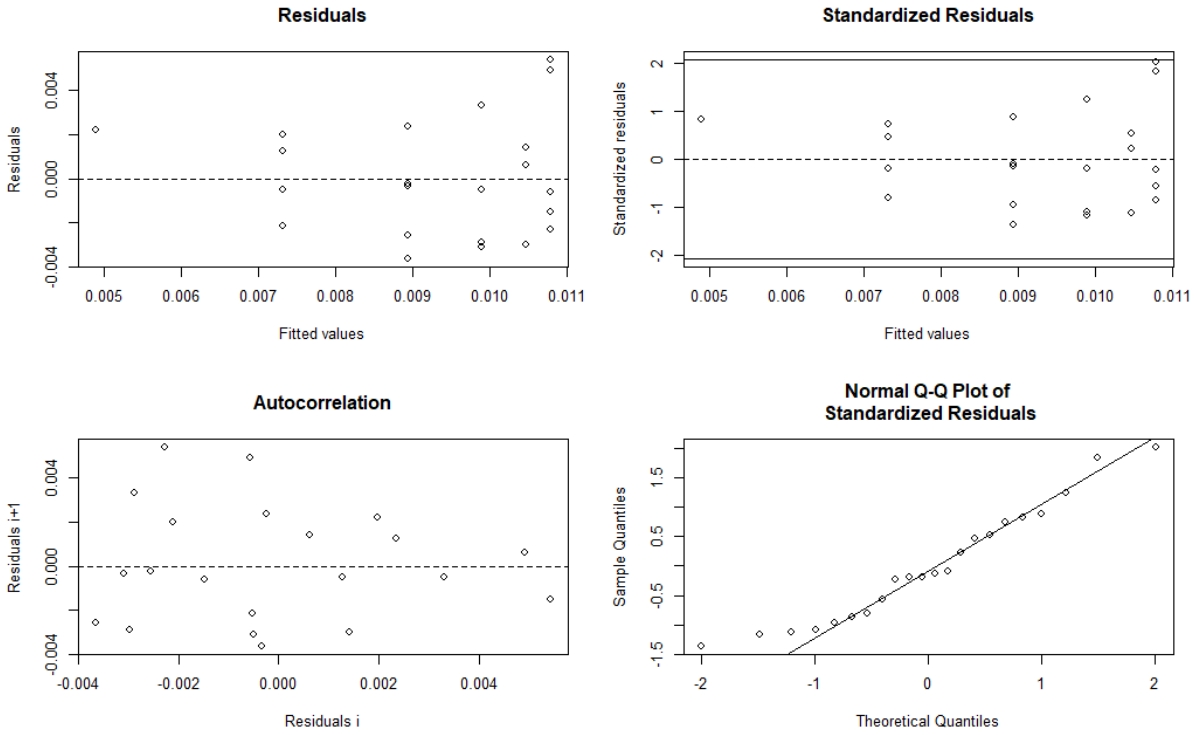
UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()
Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0109330  0.0008897  12.289 8.92e-11 ***
fitk2  0.0143495  0.0061084   2.349   0.0292 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.002668 on 20 degrees of freedom

Number of iterations to convergence: 5
Achieved convergence tolerance: 8.346e-06
```

A k_2 value of 0.0143495 is predicted with the untransformation model for $C_{14}Cl_9$ group of

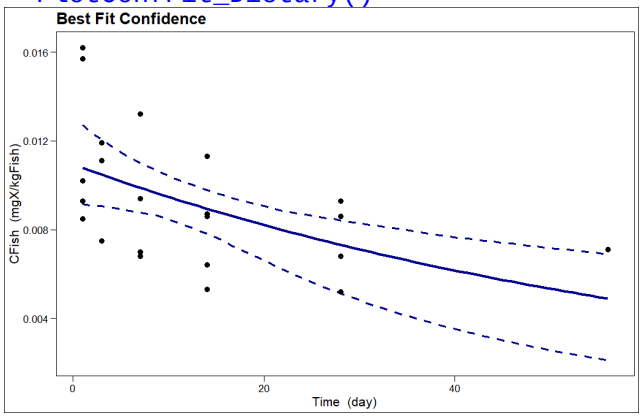
congeners. This k_2 value is significantly different from zero (p=0.0292).

```
> ModelDiagnostics_Dietary()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.94677, p-value = 0.2722


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.74069, p-value = 0.4589
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates a *p-value* of 0.4589, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2722) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```



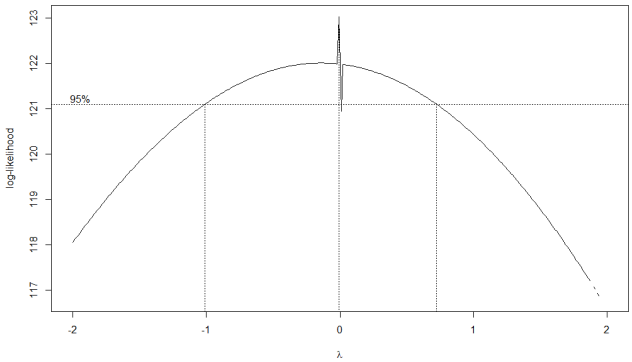

```
> SummTable_Dietary()
           Estimate Std.Error     2.5%    97.5%            unit
C0d         0.01093   0.00089  0.009189  0.01268       mgX/kgFish
```

```
k2           0.01435  0.006108 0.002377  0.02632            1/day
k2g          0.01435  0.006108 0.002377  0.02632            1/day
kf           0.00196  0.000222 0.001524  0.00239 kgFood/kgFish/day
alpha        0.13061  0.014787 0.10162   0.15959                -
BMFK         0.13653  0.045813 0.046733  0.22632     kgFood/kgFish
BMFKg        0.13653  0.045813 0.046733  0.22632     kgFood/kgFish
tHalfg      48.294   20.558    7.9999   88.589               day
BMFKgLipid   0.38533  0.1293   0.1319    0.63876     kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of 0.01435 (equal to k_2) and a BMF_{KgL} of 0.38533 (95% Confidence interval: 0.1319—0.63876) are estimated for $C_{14}Cl_9$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
       fit      conflo      confup
-0.0100000 -1.0103384  0.7214893
```



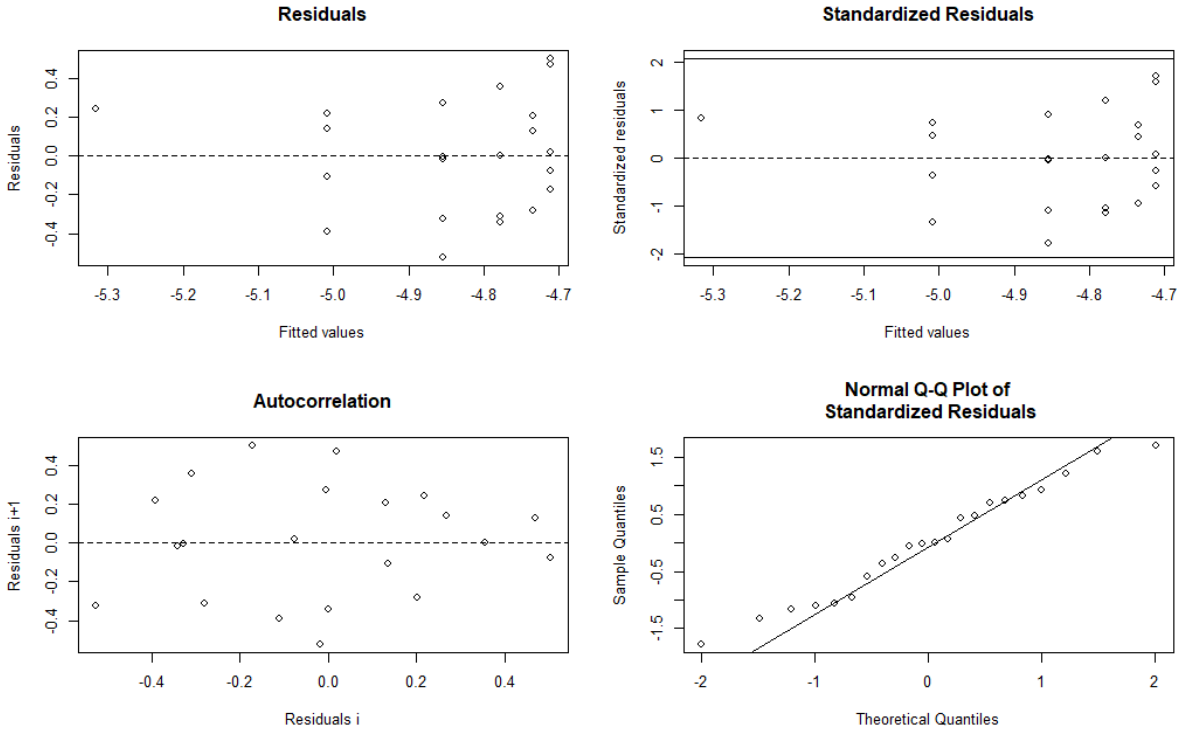
The estimated optimal λ value is -0.01 and its confidence interval is -1.0103 up to 0.7215. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()


Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0101115  0.0008365  12.089 1.19e-10 ***
fitk2  0.0104433  0.0044748   2.334   0.0302 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2942 on 20 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 3.522e-06
```

A k_2 value of 0.0104433 is predicted with the Box-Cox power transformation model for $C_{14}Cl_9$ group of congeners. This k_2 value is significantly different from zero (p=0.0302).

```
> ModelDiagnostics_Dietary_BoxCox()


------
        Shapiro-Wilk normality test

data:  stdres
W = 0.97319, p-value = 0.7836
```

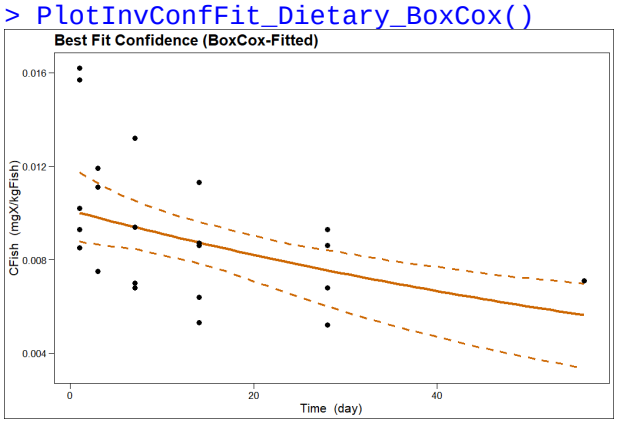
```
------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.87386, p-value = 0.3822
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.3822, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7836), the
hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
          Estimate Std.Error      2.5%     97.5%             unit
C0d        0.01011  0.000836  0.008472   0.01175        mgX/kgFish
k2         0.01044  0.004475  0.001673   0.01921             1/day
k2g        0.01044  0.004475  0.001673   0.01921             1/day
kf         0.00176  0.000187  0.001397   0.00213 kgFood/kgFish/day
alpha      0.11763  0.012486  0.093154   0.1421                  -
BMFK       0.16895   0.05846  0.054369   0.28353     kgFood/kgFish
BMFKg      0.16895   0.05846  0.054369   0.28353     kgFood/kgFish
tHalfg      66.359    28.434    10.628    122.09              day
BMFKgLipid 0.47684     0.165   0.15345   0.80024     kgFood/kgFish
```

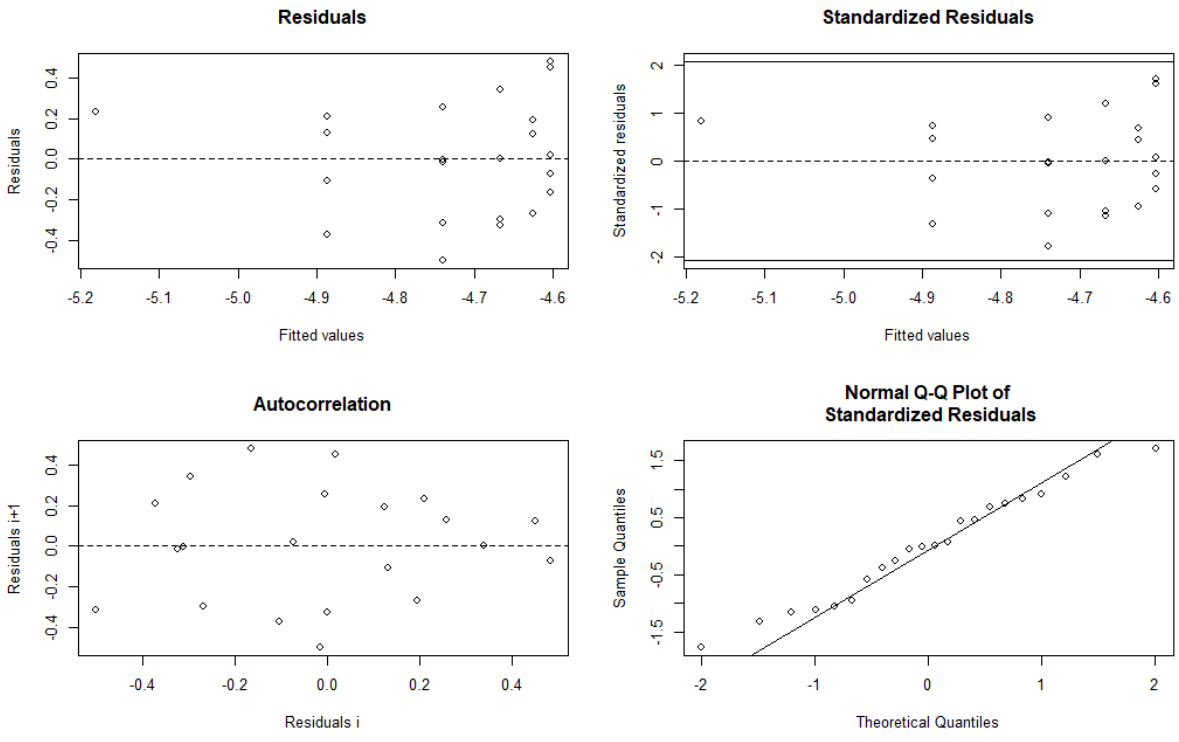
A depuration rate growth corrected (k_{2g}) of 0.01044 (equal to k_2) and a BMF_{KgL} of 0.47684 (95% Confidence interval: 0.15345–0.80024) are estimated with the Box-Cox power transformation model for $C_{14}Cl_9$ group of congeners.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0101189  0.0008369  12.091 1.19e-10 ***
fitk2  0.0104727  0.0044855   2.335   0.0301 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2807 on 20 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 4.369e-07
```

A k_2 value of 0.0104727 is predicted with the logarithm transformation model for $C_{14}Cl_9$ group of congeners. This k_2 value is significantly different from zero (p=0.0301).

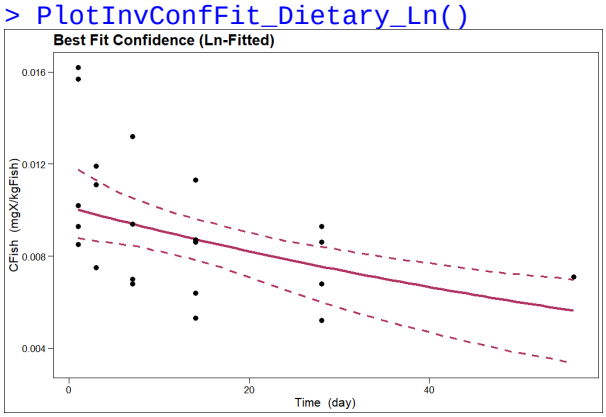
```
> ModelDiagnostics_Dietary_Ln()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.97305, p-value = 0.7805


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.84144, p-value = 0.4001
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.4001, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.7805), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is slightly lower than in the Box-cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
            Estimate Std.Error      2.5%     97.5%              unit
C0d          0.01012  0.000837  0.008479   0.01176        mgX/kgFish
k2           0.01047  0.004485  0.001681   0.01926             1/day
k2g          0.01047  0.004485  0.001681   0.01926             1/day
kf           0.00177  0.000188  0.001398   0.00213 kgFood/kgFish/day
alpha        0.11774  0.012502  0.093232   0.14224                 -
BMFK         0.16863  0.058313  0.054339   0.28293     kgFood/kgFish
BMFKg        0.16863  0.058313  0.054339   0.28293     kgFood/kgFish
tHalfg      66.172   28.341    10.623    121.72                day
BMFKgLipid   0.47595  0.16458   0.15336    0.79853     kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of 0.01047 (equal to k_2) and a BMF_{KgL} of 0.47595 (95% Confidence interval: 0.15336–0.79853) are estimated with the logarithm transformation model for $C_{14}Cl_9$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_9$ group of congeners, the Box-Cox power transformation model is the best fit model to the data.

$C_{14}Cl_{10}$ group of congeners:

Input data for $C_{14}Cl_{10}$ group of congeners:

```
TEST.Dietary.Design:
              value              unit
cfood      0.140000        mgX/kgFood
ingestion  0.015000 kgFood/kgFish/day
tfeed     14.000000               day
lipidfood 16.350000           percent
lipidfish  5.793000           percent
tdepur     0.000000               day
tend      56.000000               day
kgrowth    0.018794             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1     0.0030
2          1     0.0053
3          1     0.0033
```

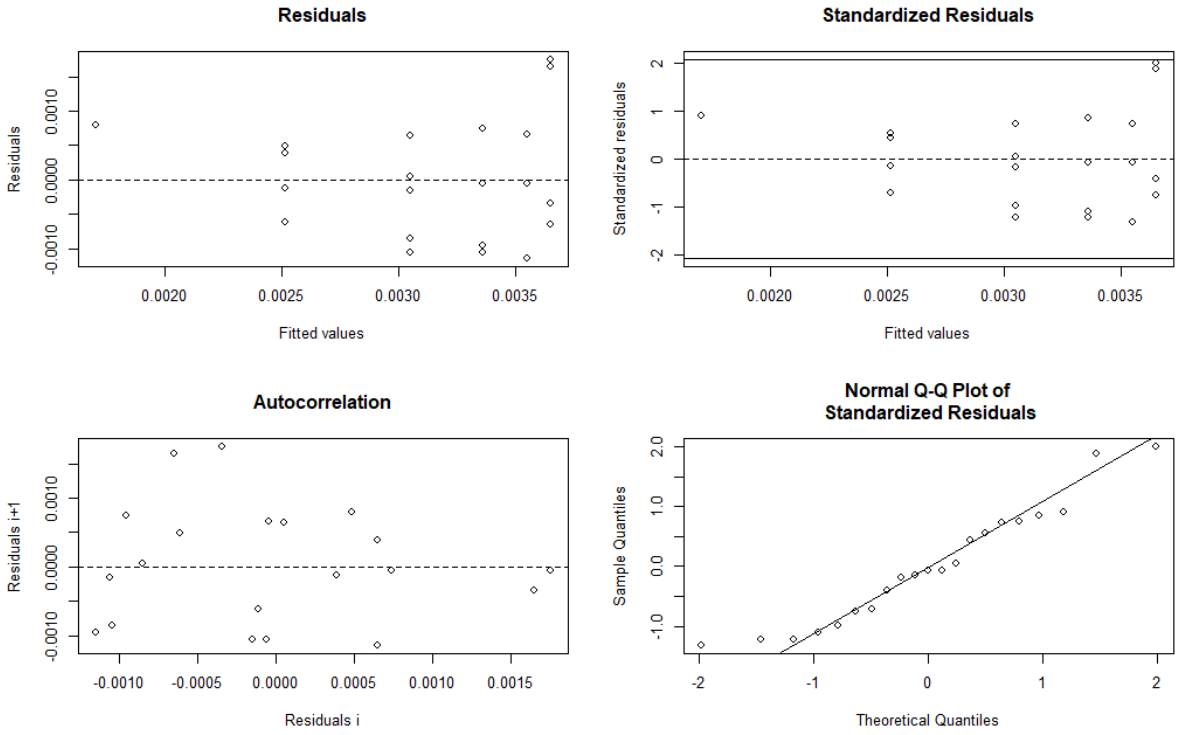
```
4          1     0.0054
5          3     0.0035
6          3     0.0042
7          3     0.0024
8          7     0.0024
9          7     0.0041
10         7     0.0033
11         7     0.0023
12        14     0.0029
13        14     0.0020
14        14     0.0022
15        14     0.0031
16        14     0.0037
17        28     0.0029
18        28     0.0024
19        28     0.0019
20        28     0.0030
21        56     0.0025
```

UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()
Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0036978  0.0003036  12.180 2.01e-10 ***
fitk2  0.0137770  0.0059081   2.332   0.0309 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.000869 on 19 degrees of freedom

Number of iterations to convergence: 6
Achieved convergence tolerance: 2.379e-06
```

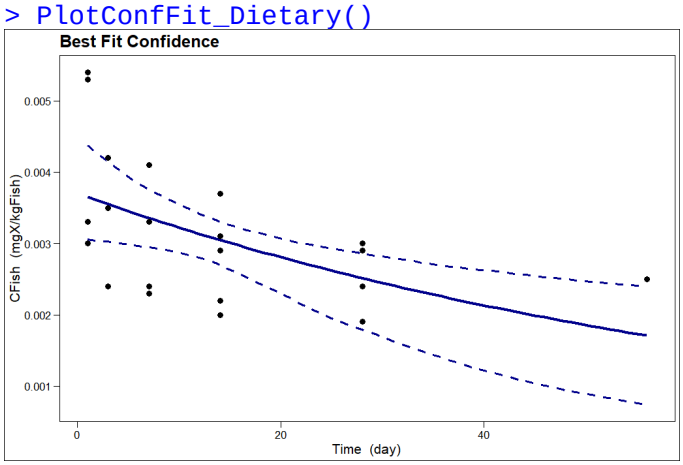
A k_2 value of 0.0137770 is predicted with the untransformation model for $C_{14}Cl_{10}$ group of congeners. This k_2 value is significantly different from zero (p=0.0309).

```
> ModelDiagnostics_Dietary()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.94216, p-value = 0.2403


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.32686, p-value = 0.7438
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates *p-value* of 0.7438, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2403) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```

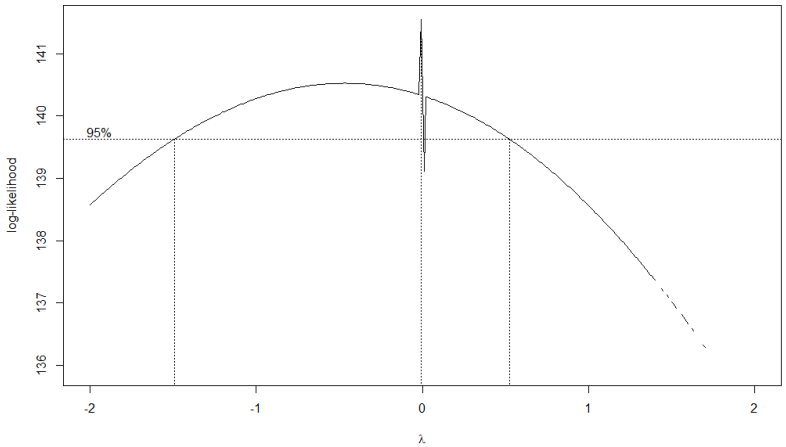



```
> SummTable_Dietary()
  Estimate Std.Error      2.5%     97.5%              unit
C0d            0.0037    0.0003    0.0031   0.00429        mgX/kgFish
k2             0.01378   0.00591   0.0022   0.02536             1/day
k2g           -0.00502   0.00591  -0.0166   0.00656             1/day
kf             0.00207   0.00024   0.0016   0.00254 kgFood/kgFish/day
alpha          0.13829   0.01567   0.1076   0.16901                 -
BMFK           0.15057   0.05089   0.0508   0.25031     kgFood/kgFish
BMFKg         -0.41348   0.52729  -1.447    0.62001     kgFood/kgFish
tHalfg     -138.13     162.67    -456.96   180.7                 day
BMFKgLipid    -1.167     1.4882    -4.0839   1.7499      kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of -0.00502 and a BMF_{KgL} of -1.167 (95% Confidence interval: -4.0839—1.7499) are estimated for $C_{14}Cl_{10}$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
   fit     conflo     confup
-0.0100000 -1.4938205  0.5249452
```

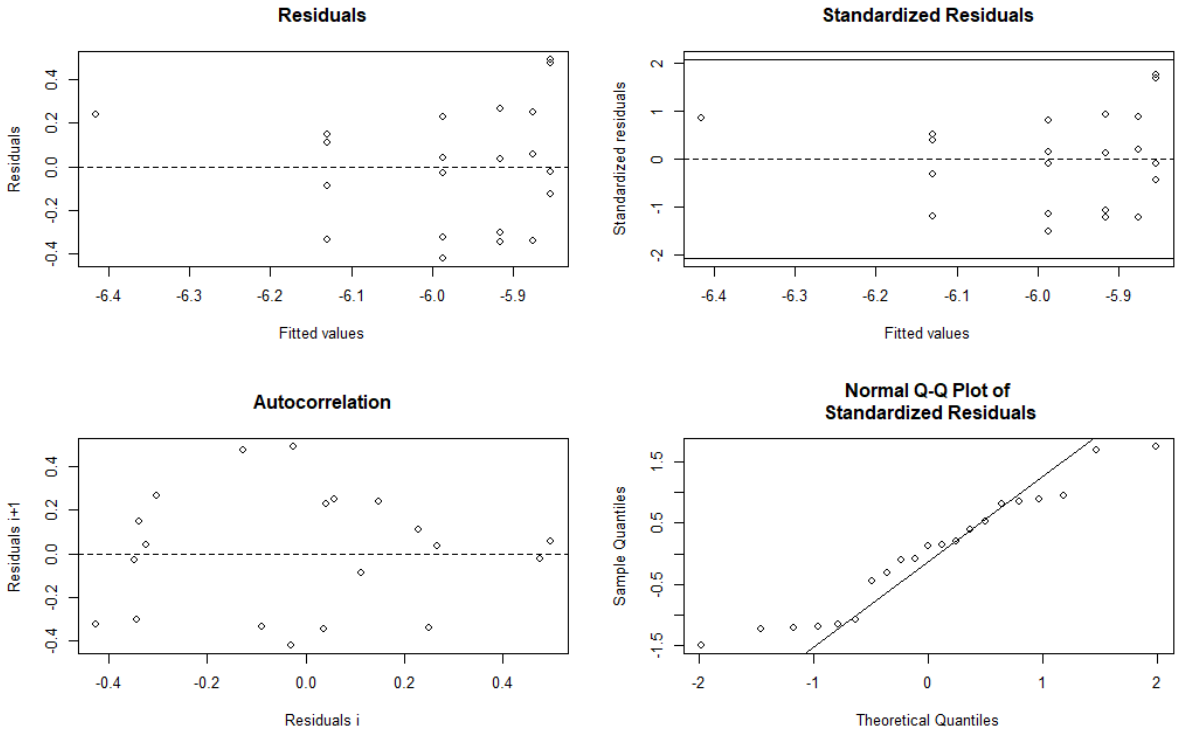


The estimated optimal λ value is -0.01 and its confidence interval is -1.4938205 up to 0.5249452. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0034122  0.0002787   12.24 1.85e-10 ***
fitk2  0.0095870  0.0043182    2.22   0.0388 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2816 on 19 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 3.935e-06
```

A k_2 value of 0.0095870 is predicted with the Box-Cox power transformation model for $C_{14}Cl_{10}$ group of congeners. This k_2 value is significantly different from zero (p=0.0388).

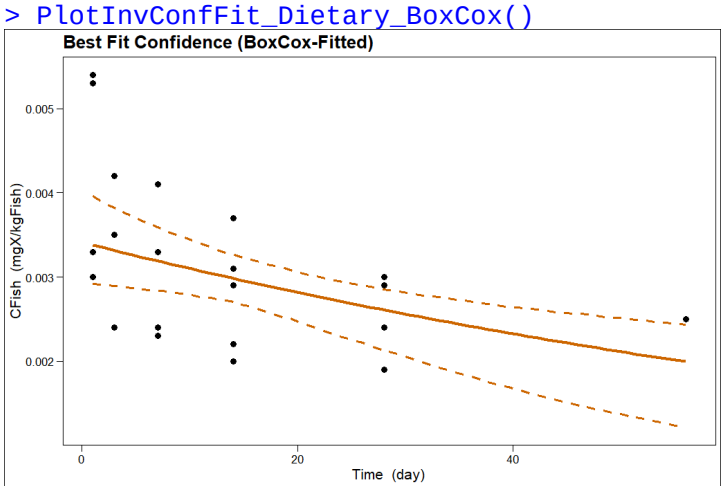
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.9455, p-value = 0.2793


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.66258, p-value = 0.5076
alternative hypothesis: two.sided
```



The Q-Q plot for the Box-Cox power transformation model is less attractive than for the untransformed model. No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.5076, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2793), the
hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is slightly higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.00341	0.00028	0.00287	0.003958	mgX/kgFish
k2	0.00959	0.00432	0.00112	0.018051	1/day
k2g	-0.00921	0.00432	-0.01767	-0.000743	1/day
kf	0.00186	0.00019	0.00148	0.002242	kgFood/kgFish/day
alpha	0.12402	0.01297	0.09859	0.14945	-
BMFK	0.19405	0.0714	0.05411	0.33399	kgFood/kgFish
BMFKg	-0.20206	0.11297	-0.42348	0.019364	kgFood/kgFish
tHalfg	-75.269	35.302	-144.46	-6.077	day
BMFKgLipid	-0.57028	0.31884	-1.1952	0.054651	kgFood/kgFish

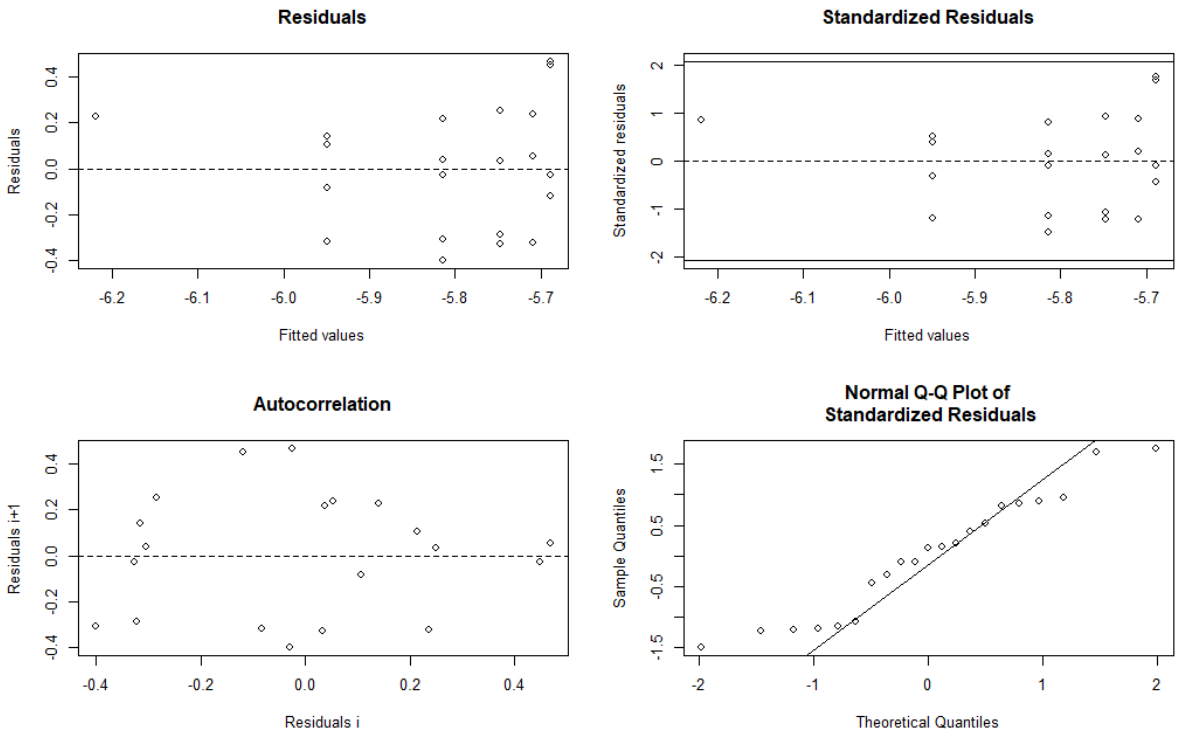
A depuration rate growth corrected (k_{2g}) of -0.00921 and a BMF_{KgL} of -0.57028 (95% Confidence interval: -1.1952–0.054651) are estimated with the Box-Cox power transformation model for $C_{14}Cl_{10}$ group of congeners.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()

Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0034146  0.0002789  12.242 1.85e-10 ***
fitk2  0.0096170  0.0043286   2.222   0.0386 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2659 on 19 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 1.343e-06
```

A k_2 value of 0.0096170 is predicted with the logarithm transformation model for $C_{14}Cl_{10}$ group of congeners. This k_2 value is significantly different from zero (p=0.0386).

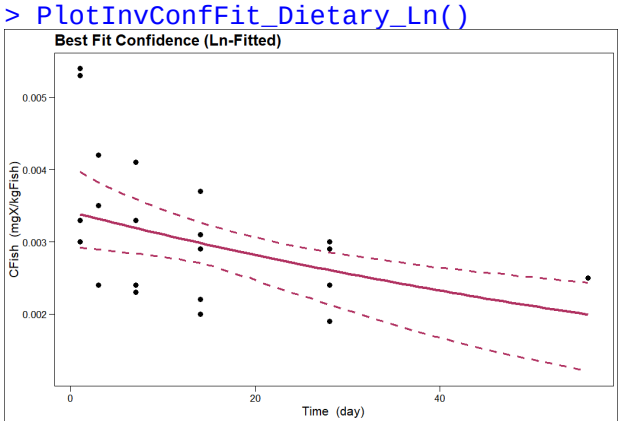
```
> ModelDiagnostics_Dietary_Ln()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.94554, p-value = 0.2798


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.66258, p-value = 0.5076
alternative hypothesis: two.sided
```



The Q-Q plot for the logarithm transformation model is less attractive than for the untransformed model. No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.5076, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2798), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model and than in the Box-cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
            Estimate Std.Error       2.5%     97.5%              unit
C0d          0.00341   0.00028    0.00287  0.003961         mgX/kgFish
k2           0.00962   0.00433    0.00113  0.018101              1/day
k2g         -0.00918   0.00433   -0.01766 -0.000693              1/day
kf           0.00186   0.00019    0.00148  0.002244 kgFood/kgFish/day
alpha        0.12414   0.01299    0.09867  0.14961                  -
BMFK         0.19362   0.07117    0.05413  0.33312      kgFood/kgFish
BMFKg       -0.20291   0.114     -0.42634  0.020525     kgFood/kgFish
tHalfg     -75.515    35.619   -145.33    -5.7017               day
BMFKgLipid  -0.57268   0.32174   -1.2033   0.057929     kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of -0.00918 and a BMF_{KgL} of -0.57268 (95% Confidence interval: -1.2033–0.057929) are estimated with the logarithm transformation model for $C_{14}Cl_{10}$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_{10}$ group of congeners, the logarithm transformation model is the best fit model to the data.

$C_{14}Cl_{10}$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

For $C_{14}Cl_{10}$ as the growth rate constant (k_g) was higher than the depuration rate constant (k_2), the corresponding depuration rate growth corrected constant (k_{2g}) was negative thus the BMFs derived from this negative k_{2g} was also negative. As the mass approach did not work in our case, the bcmfR R-package was re-run for $C_{14}Cl_{10}$ without correcting the depuration rate (k_2) for growth (k_g) and thus assuming that $k_2=k_{2g}$. This scenario ($k_g=0$ and $k_2=k_{2g}$) overestimates the depuration rate and the estimated BMF value will be underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB.

Input data for $C_{14}Cl_{10}$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

```
TEST.Dietary.Design:
           value              unit
cfood      0.140        mgX/kgFood
ingestion  0.015 kgFood/kgFish/day
tfeed     14.000               day
lipidfood 16.350           percent
lipidfish  5.793           percent
```

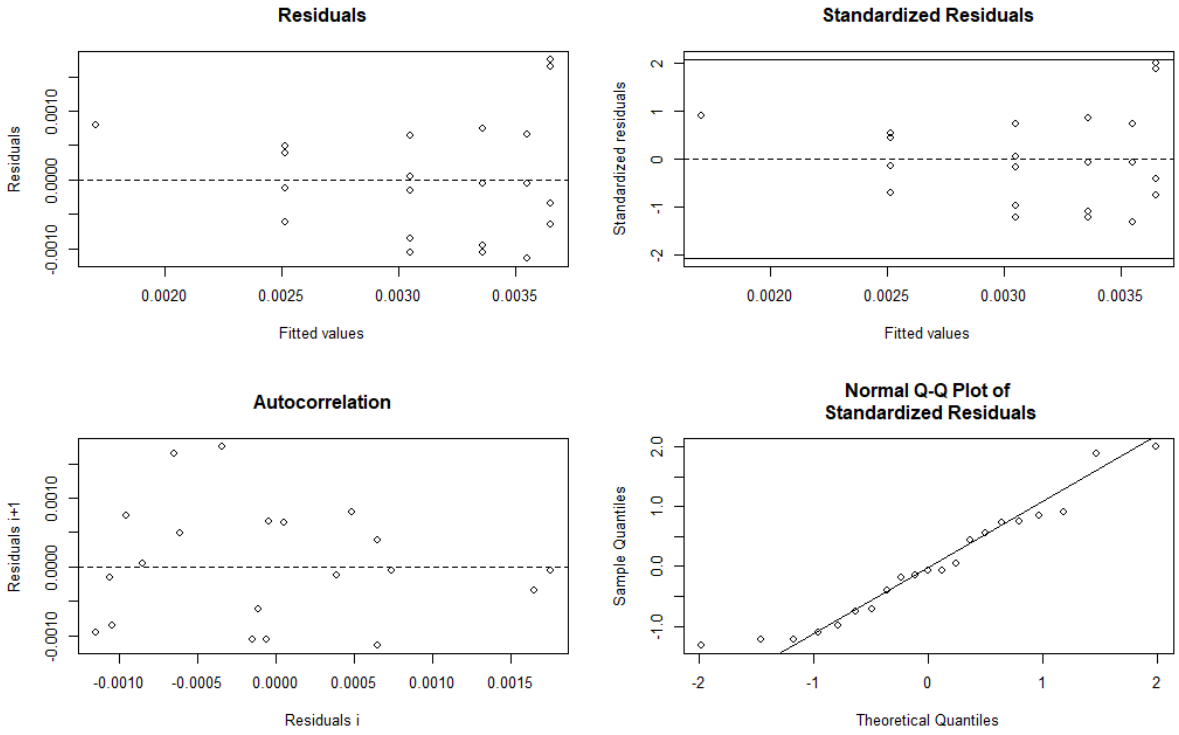
```
tdepur     0.000                day
tend      56.000                day
kgrowth    0.000              1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1     0.0030
2          1     0.0053
3          1     0.0033
4          1     0.0054
5          3     0.0035
6          3     0.0042
7          3     0.0024
8          7     0.0024
9          7     0.0041
10         7     0.0033
11         7     0.0023
12        14     0.0029
13        14     0.0020
14        14     0.0022
15        14     0.0031
16        14     0.0037
17        28     0.0029
18        28     0.0024
19        28     0.0019
20        28     0.0030
21        56     0.0025
```

UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()
Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0036978  0.0003036  12.180 2.01e-10 ***
fitk2  0.0137770  0.0059081   2.332   0.0309 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.000869 on 19 degrees of freedom

Number of iterations to convergence: 6
Achieved convergence tolerance: 2.379e-06
```

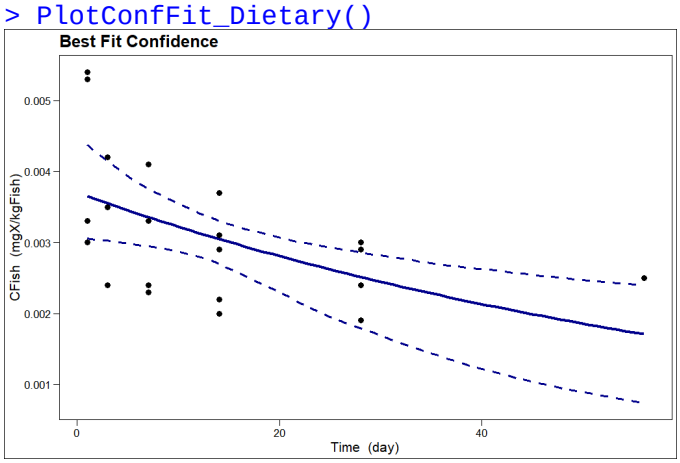
A k_2 value of 0.0137770 is predicted with the untransformation model for $C_{14}Cl_{10}$ group of congeners. This k_2 value is significantly different from zero (p=0.0309).

```
> ModelDiagnostics_Dietary()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.94216, p-value = 0.2403


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.32686, p-value = 0.7438
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates *p-value* of 0.7438, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2403) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```




```
> SummTable_Dietary()
```

A depuration rate growth corrected (k_{2g}) of -0.00502 and a BMF_{KgL} of -1.167 (95% Confidence interval: -4.0839–1.7499) are estimated for $C_{14}Cl_{10}$ group of congeners with the untransformation model.

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.0037	0.000304	0.003103	0.00429	mgX/kgFish
k2	0.01378	0.005908	0.002197	0.02536	1/day
k2g	0.01378	0.005908	0.002197	0.02536	1/day
kf	0.00207	0.000235	0.001614	0.00254	kgFood/kgFish/day
alpha	0.13829	0.015672	0.10758	0.16901	-
BMFK	0.15057	0.050887	0.050833	0.25031	kgFood/kgFish
BMFKg	0.15057	0.050887	0.050833	0.25031	kgFood/kgFish
tHalfg	50.301	21.571	8.0219	92.58	day
BMFKgLipid	0.42497	0.14362	0.14347	0.70647	kgFood/kgFish

A depuration rate growth corrected (k_{2g}) of 0.01378 (equal to k_2) and a BMF_{KgL} of 0.42497 (95% Confidence interval: 0.14347–0.70647) are estimated with the logarithm transformation model for $C_{14}Cl_{10}$ group of congeners.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

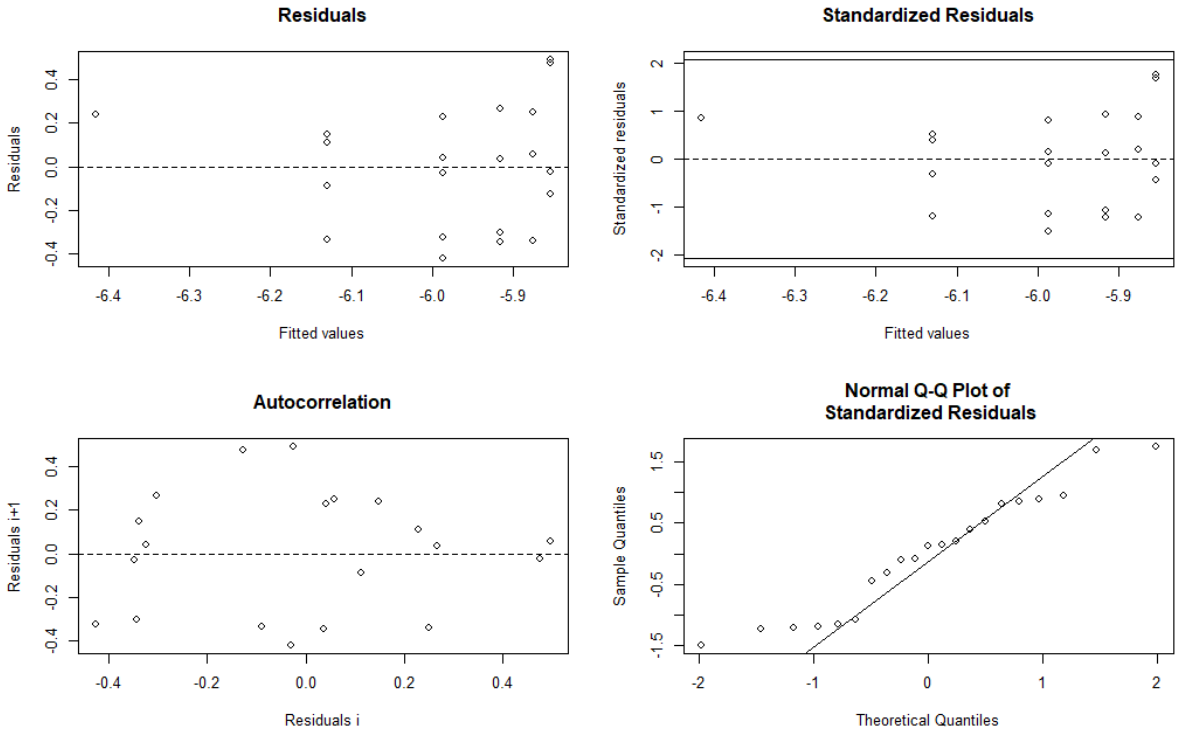
```
> ModelTrans_BoxCox_Dietary()
   fit      conflo      confup
-0.0100000 -1.4938205  0.5249452
```

The estimated optimal λ value is -0.01 and its confidence interval is -1.494 up to 0.525. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0034122  0.0002787   12.24 1.85e-10 ***
fitk2  0.0095870  0.0043182    2.22   0.0388 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2816 on 19 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 3.935e-06
```

A k_2 value of 0.0095870 is predicted with the Box-Cox power transformation model for $C_{14}Cl_{10}$ group of congeners. This k_2 value is significantly different from zero (p=0.0388).

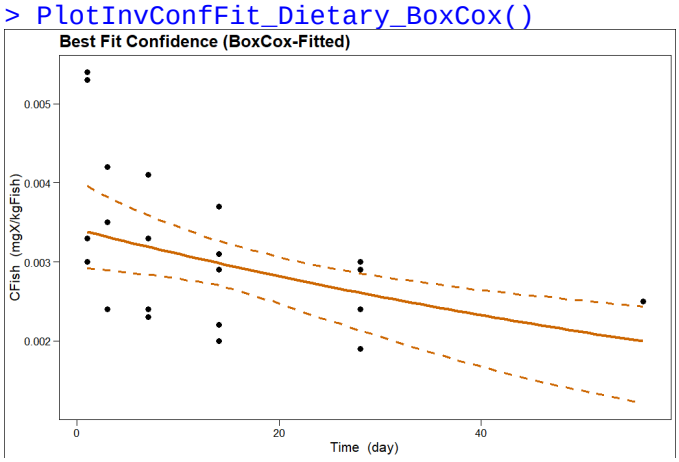
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.9455, p-value = 0.2793


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.66258, p-value = 0.5076
alternative hypothesis: two.sided
```



The Q-Q plot for the Box-Cox power transformation model is less attractive than for the untransformed model. No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.5076, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2793), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is slightly higher than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.00341	0.00028	0.002866	0.00396	mgX/kgFish
k2	0.00959	0.00432	0.001123	0.01805	1/day
k2g	0.00959	0.00432	0.001123	0.01805	1/day
kf	0.00186	0.00019	0.001479	0.00224	kgFood/kgFish/day
alpha	0.12402	0.01297	0.098593	0.14945	-
BMFK	0.19405	0.0714	0.054105	0.33399	kgFood/kgFish
BMFKg	0.19405	0.0714	0.054105	0.33399	kgFood/kgFish
tHalfg	72.285	32.559	8.4703	136.1	day
BMFKgLipid	0.54768	0.20152	0.1527	0.94265	kgFood/kgFish

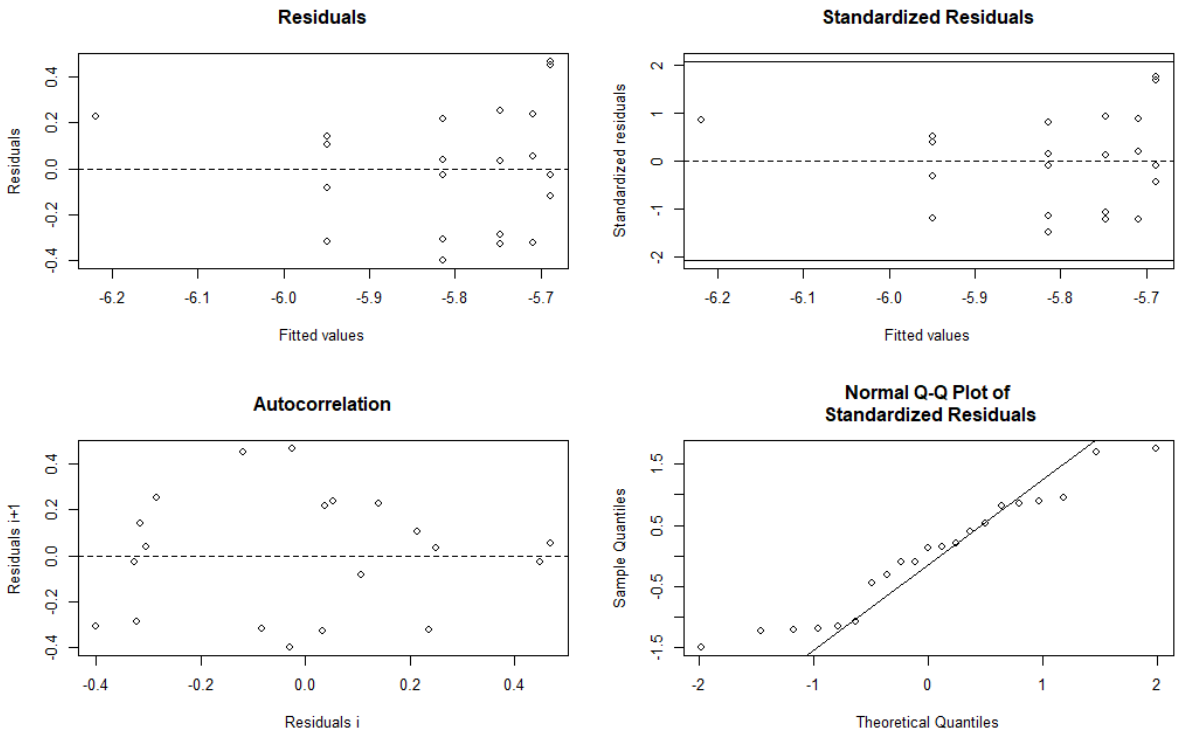
A depuration rate growth corrected (k_{2g}) of 0.00959 (equal to k_2) and a BMF_{KgL} of 0.54768 (95% Confidence interval: 0.1527–0.94265) are estimated with the Box-Cox power transformation model for $C_{14}Cl_{10}$ group of congeners.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0034146  0.0002789  12.242 1.85e-10 ***
fitk2  0.0096170  0.0043286   2.222   0.0386 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2659 on 19 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 1.343e-06
```

A k_2 value of 0.0096170 is predicted with the logarithm transformation model for $C_{14}Cl_{10}$ group of congeners. This k_2 value is significantly different from zero (p=0.0386).

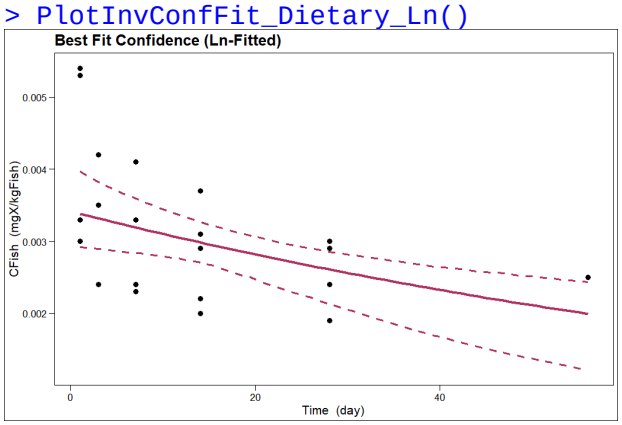
```
> ModelDiagnostics_Dietary_Ln()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.94554, p-value = 0.2798


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.66258, p-value = 0.5076
alternative hypothesis: two.sided
```



The Q-Q plot for the logarithm transformation model is less attractive than for the untransformed model. No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.5076, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.2798), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model and than in the Box-cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
            Estimate Std.Error     2.5%     97.5%              unit
C0d          0.00341   0.00028 0.002868   0.00396        mgX/kgFish
k2           0.00962   0.00433 0.001133    0.0181             1/day
k2g          0.00962   0.00433 0.001133    0.0181             1/day
kf           0.00186   0.00019  0.00148   0.00224 kgFood/kgFish/day
alpha        0.12414   0.01299 0.098669    0.14961                 -
BMFK         0.19362   0.07117 0.054127    0.33312     kgFood/kgFish
BMFKg        0.19362   0.07117 0.054127    0.33312     kgFood/kgFish
tHalfg     72.06     32.434    8.4889   135.63               day
BMFKgLipid   0.54647   0.20087 0.15277     0.94018     kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of 0.00962 (equal to k_2) and a BMF_{KgL} of 0.54647 (95% Confidence interval: 0.15277–0.94018) are estimated with the logarithm transformation model for $C_{14}Cl_{10}$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_{10}$ group of congeners, the logarithm transformation model is the best fit model to the data.

$C_{14}Cl_{11}$ group of congeners:

Input data for $C_{14}Cl_{11}$ group of congeners:

```
TEST.Dietary.Design:
              value              unit
cfood      0.060000        mgX/kgFood
ingestion  0.015000 kgFood/kgFish/day
tfeed     14.000000               day
lipidfood 16.350000           percent
lipidfish  5.793000           percent
tdepur     0.000000               day
tend      56.000000               day
kgrowth    0.018794             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1    0.00124
```

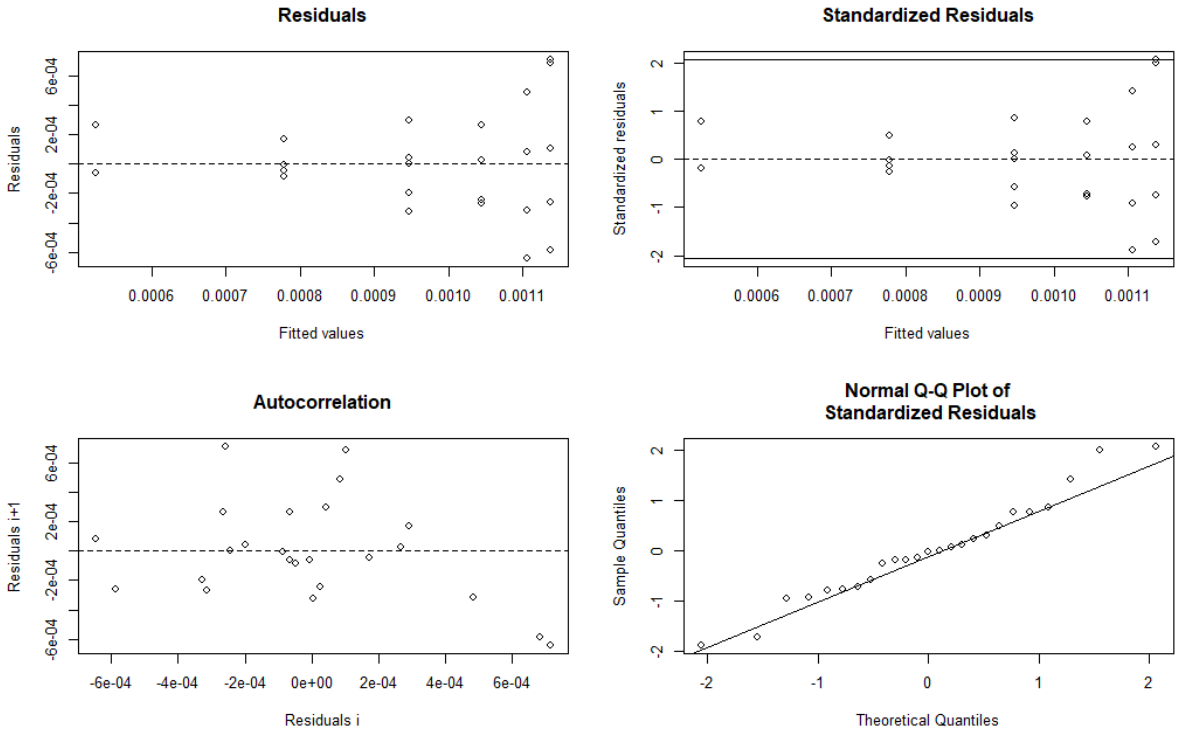
```
2          1    0.00182
3          1    0.00055
4          1    0.00088
5          1    0.00185
6          3    0.00046
7          3    0.00119
8          3    0.00159
9          3    0.00079
10         7    0.00078
11         7    0.00131
12         7    0.00107
13         7    0.00080
14        14    0.00095
15        14    0.00062
16        14    0.00075
17        14    0.00099
18        14    0.00124
19        28    0.00095
20        28    0.00073
21        28    0.00069
22        28    0.00077
23        56    0.00046
24        56    0.00046
25        56    0.00079
```

UNTRANSFORMED FIT (the untransformed model)

```
> FitModel_Dietary()
Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0011531  0.0001051  10.975 1.28e-10 ***
fitk2  0.0140605  0.0058801   2.391   0.0254 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.0003431 on 23 degrees of freedom

Number of iterations to convergence: 3
Achieved convergence tolerance: 6.522e-06
```

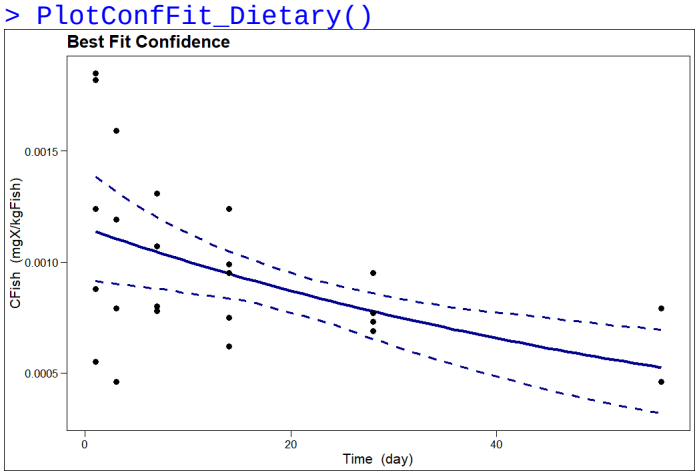
A k_2 value of 0.0140605 is predicted with the untransformation model for $C_{14}Cl_{11}$ group of congeners. This k_2 value is significantly different from zero ($p = 0.0254$).

```
> ModelDiagnostics_Dietary()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.96957, p-value = 0.6342


------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.19646, p-value = 0.8443
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates *p-value* of 0.8443, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.6342) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```



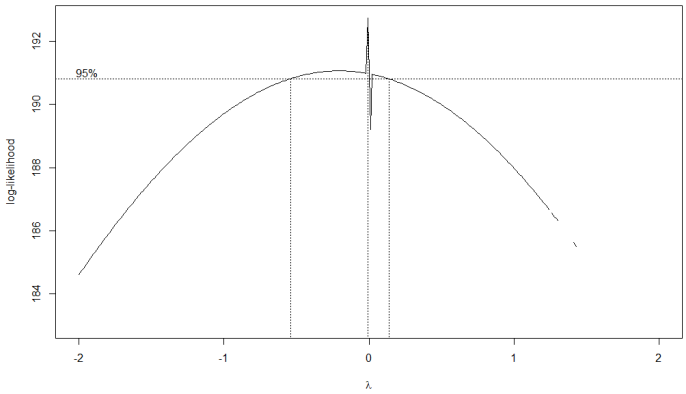

```
> SummTable_Dietary()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.00115	0.00011	0.0009	0.00136	mgX/kgFish
k2	0.01406	0.00588	0.0025	0.02559	1/day
k2g	-0.00473	0.00588	-0.0163	0.00679	1/day
kf	0.00151	0.00018	0.0012	0.00187	kgFood/kgFish/day
alpha	0.10082	0.01212	0.0771	0.12457	-
BMFK	0.10755	0.03537	0.0382	0.17687	kgFood/kgFish
BMFKg	-0.31948	0.42849	-1.1593	0.52036	kgFood/kgFish
tHalfg	-146.4	181.87	-502.86	210.06	day
BMFKgLipid	-0.90169	1.2094	-3.272	1.4686	kgFood/kgFish

A depuration rate growth corrected (k_{2g}) of -0.00473 and a BMF_{KgL} of -0.90169 (95% Confidence interval: -3.272—1.4686) are estimated for $C_{14}Cl_{11}$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
fit      conflo     confup
-0.0100000 -0.5422723  0.1366718
```

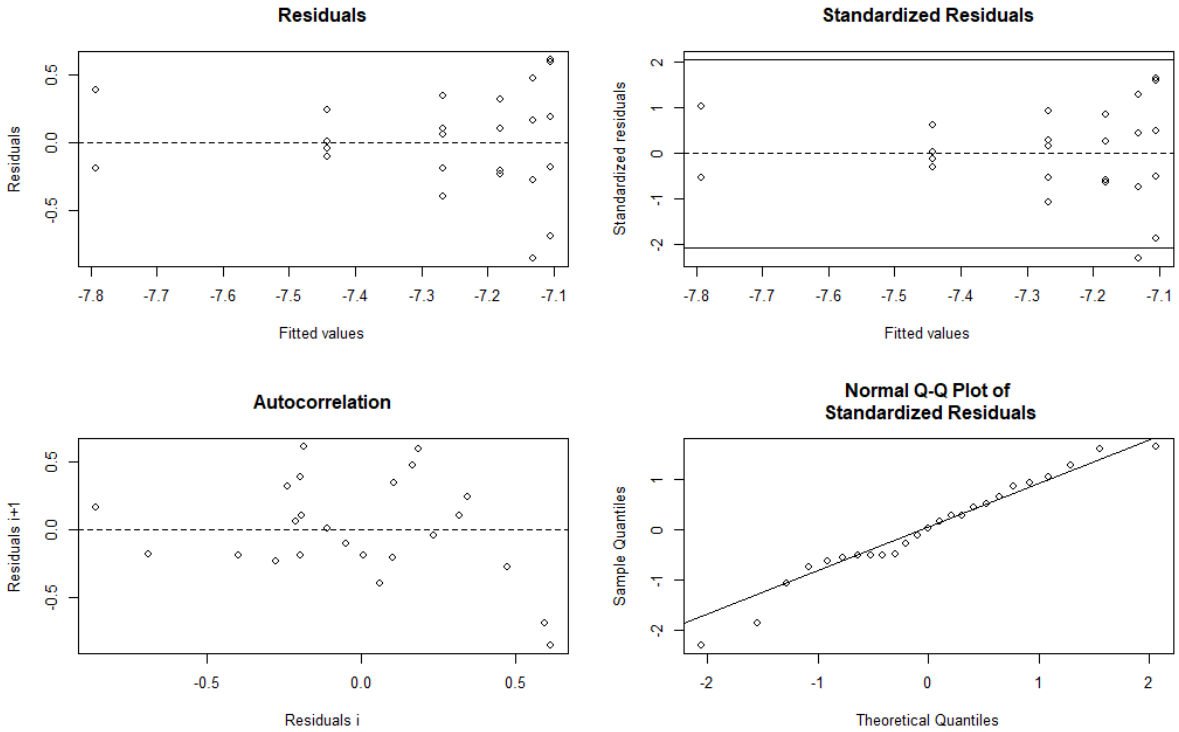


The estimated optimal λ value is -0.01 and its confidence interval is -0.5422723 up to 0.1366718. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0010562  0.0000989  10.680 2.18e-10 ***
fitk2  0.0116104  0.0039770   2.919  0.00772 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.371 on 23 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 9.861e-07
```

A k_2 value of 0.0116104 is predicted with the Box-Cox power transformation model for $C_{14}Cl_{11}$ group of congeners. This k_2 value is significantly different from zero (p=0.00772).

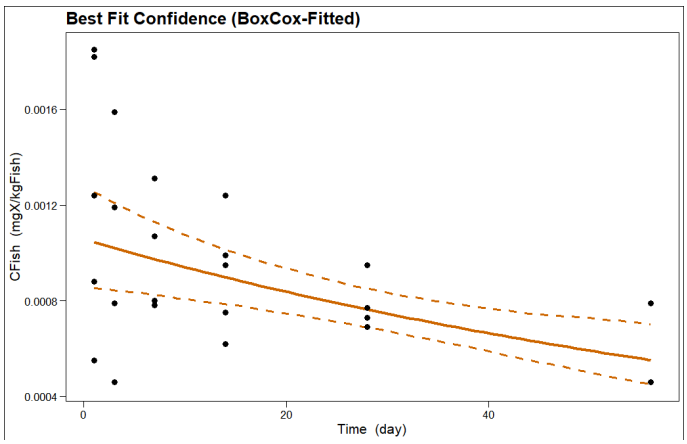
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.96957, p-value = 0.6341


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.62212, p-value = 0.5339
alternative hypothesis: two.sided
```



The Q-Q plot for the Box-Cox power transformation model is more attractive than for the untransformed model. No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.5339, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.6341), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is slightly lower than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
```

	Estimate	Std.Error	2.5%	97.5%		unit
C0d	0.00106	0.0001	0.00086	0.00125		mgX/kgFish
k2	0.01161	0.00398	0.00382	0.019405		1/day
k2g	-0.00718	0.00398	-0.01498	0.000611		1/day
kf	0.00136	0.00015	0.00106	0.001666		kgFood/kgFish/day
alpha	0.09083	0.01032	0.07059	0.11106		-
BMFK	0.11734	0.0307	0.05717	0.17752		kgFood/kgFish
BMFKg	-0.18965	0.12281	-0.43035	0.051047		kgFood/kgFish
tHalfg	-96.469	53.408	-201.15	8.2099		day
BMFKgLipid	-0.53527	0.34661	-1.2146	0.14407		kgFood/kgFish

```
>
```

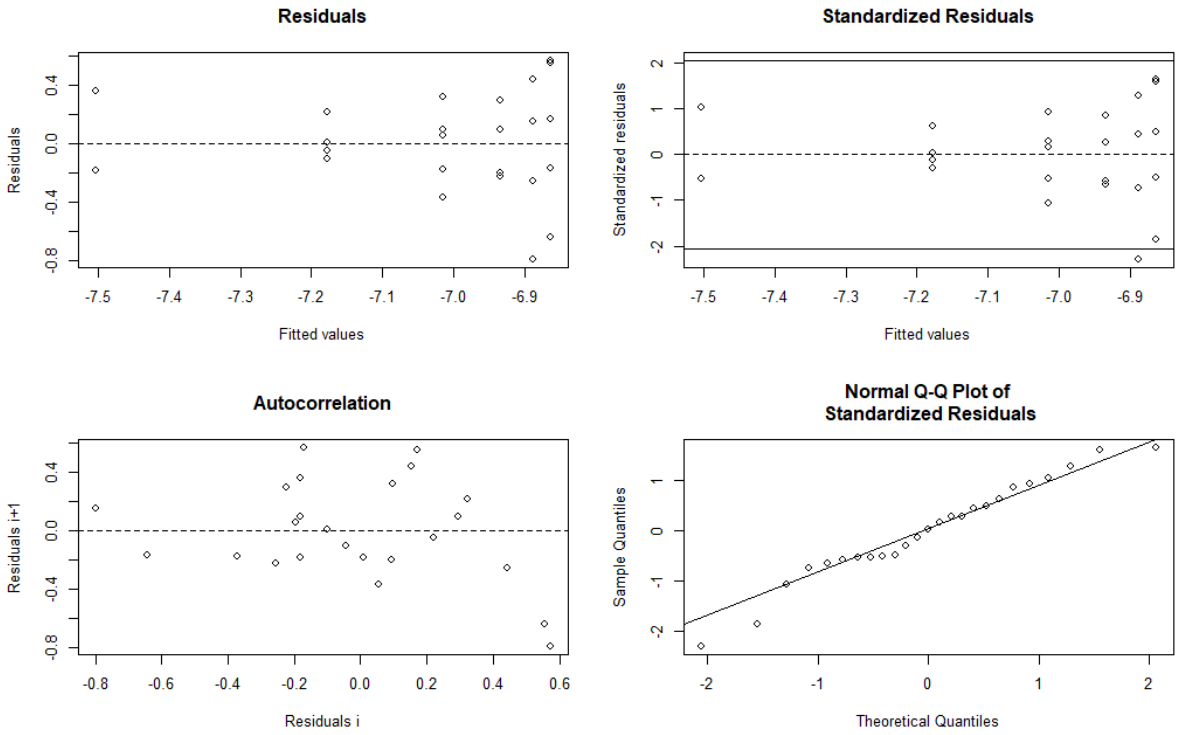
A depuration rate growth corrected (k_{2g}) of -0.00718 and a BMF_{KgL} of -0.53527 (95% Confidence interval: -1.2146–0.14407) are estimated with the Box-Cox power transformation model for $C_{14}Cl_{11}$ group of congeners.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 1.057e-03  9.894e-05  10.685 2.16e-10 ***
fitk2  1.163e-02  3.989e-03   2.914  0.00781 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3459 on 23 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 3.595e-06
```

A k_2 value of 0.01163 is predicted with the logarithm transformation model for $C_{14}Cl_{11}$ group of congeners. This k_2 value is significantly different from zero (p=0.00781).

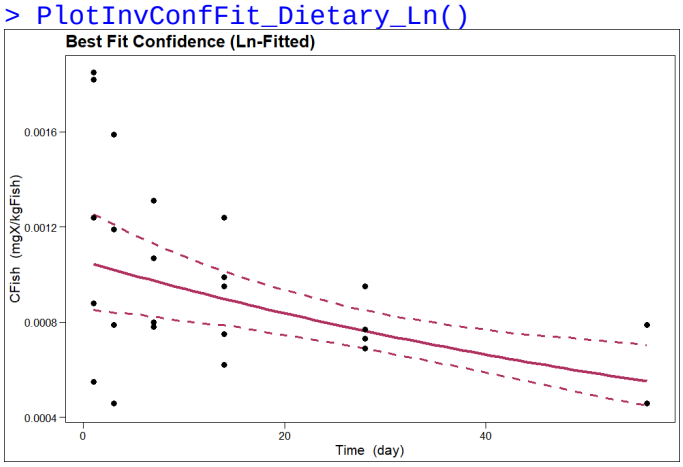
```
> ModelDiagnostics_Dietary_Ln()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.96987, p-value = 0.6418


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.62212, p-value = 0.5339
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.5339, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.6418), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model and than in the Box-cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.00106	0.0001	0.00086	0.001251	mgX/kgFish
k2	0.01163	0.00399	0.00381	0.019445	1/day
k2g	-0.00717	0.00399	-0.01499	0.000651	1/day
kf	0.00136	0.00016	0.00106	0.001667	kgFood/kgFish/day
alpha	0.09091	0.01033	0.07065	0.11116	-
BMFK	0.11729	0.03076	0.05701	0.17758	kgFood/kgFish
BMFKg	-0.19024	0.12373	-0.43275	0.052275	kgFood/kgFish
tHalfg	-96.678	53.803	-202.13	8.7756	day
BMFKgLipid	-0.53692	0.34921	-1.2214	0.14754	kgFood/kgFish

A depuration rate growth corrected (k_{2g}) of -0.00717 and a BMF_{KgL} of -0.53692 (95% Confidence interval: -1.2214–0.14754) are estimated with the logarithm transformation model for C_{14} Cl_{11} congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for $C_{14}Cl_{11}$ group of congeners, the logarithm transformation model is the best fit model to the data.

$C_{14}Cl_{11}$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

For $C_{14}Cl_{11}$ as the growth rate constant (k_g) was higher than the depuration rate constant (k_2), the corresponding depuration rate growth corrected constant (k_{2g}) was negative thus the BMF derived from this negative k_{2g} was also negative. As the mass approach did not work in our case, the bcmfR R-package was re-run for $C_{14}Cl_{11}$ without correcting the depuration rate (k_2) for growth (k_g) and thus assuming that $k_2=k_{2g}$. This scenario ($k_g=0$ and $k_2=k_{2g}$) overestimates the depuration rate and the estimated BMF value will be underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB.

Input data for $C_{14}Cl_{11}$ group of congeners (scenario $k_g=0$ and $k_2=k_{2g}$):

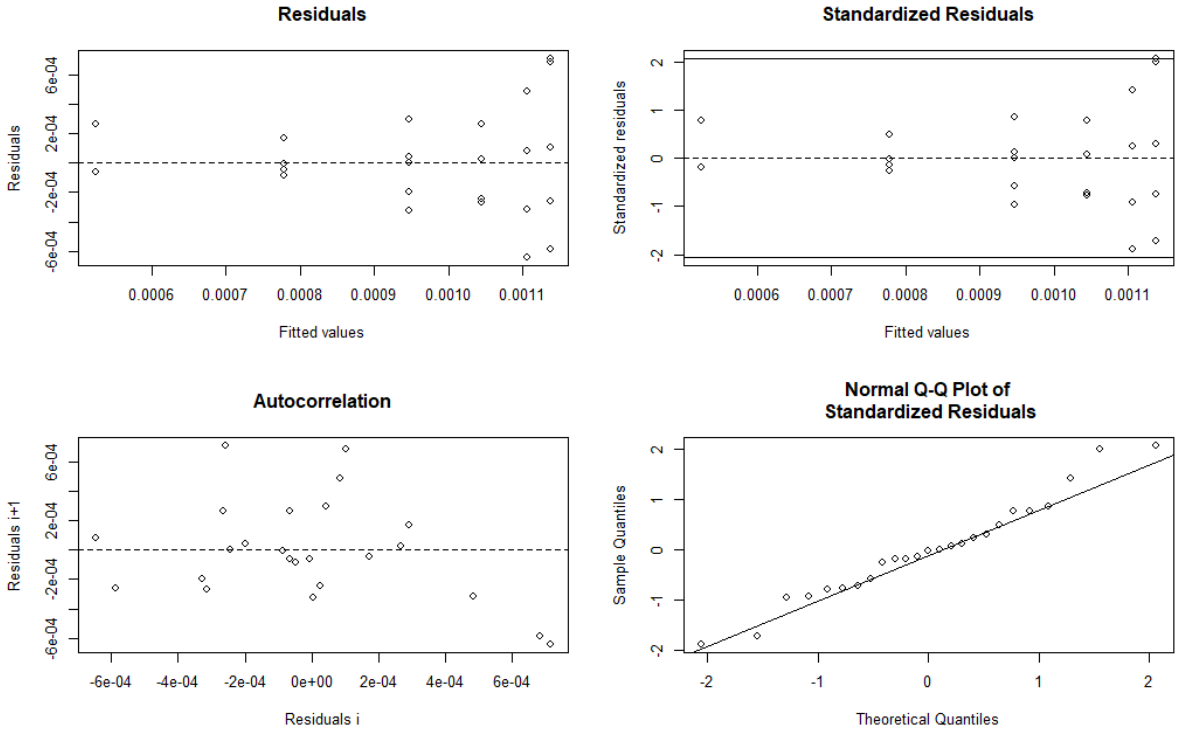
UNTRANSFORMED FIT (the untransformed model)

```
TEST.Dietary.Design:
           value              unit
cfood      0.060        mgX/kgFood
ingestion  0.015 kgFood/kgFish/day
tfeed     14.000               day
lipidfood 16.350           percent
lipidfish  5.793           percent
tdepur     0.000               day
tend      56.000               day
kgrowth    0.000             1/day

TEST.Dietary.Measured:
       name       unit
time   Time        day
cfish CFish mgX/kgFish

DATA.Dietary.Work:
   time.data cfish.data
1          1    0.00124
2          1    0.00182
3          1    0.00055
4          1    0.00088
5          1    0.00185
6          3    0.00046
7          3    0.00119
8          3    0.00159
9          3    0.00079
10         7    0.00078
11         7    0.00131
12         7    0.00107
13         7    0.00080
14        14    0.00095
15        14    0.00062
16        14    0.00075
17        14    0.00099
18        14    0.00124
19        28    0.00095
20        28    0.00073
21        28    0.00069
22        28    0.00077
23        56    0.00046
24        56    0.00046
25        56    0.00079

> FitModel_Dietary()


Formula: cfish.data ~ RunModel_Dietary(time.data, fitc0d, fitk2)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0011531  0.0001051  10.975 1.28e-10 ***
fitk2  0.0140605  0.0058801   2.391   0.0254 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.0003431 on 23 degrees of freedom

Number of iterations to convergence: 3
Achieved convergence tolerance: 6.522e-06
```

A k_2 value of 0.0140605 is predicted with the untransformation model for $C_{14}Cl_{11}$ group of congeners. This k_2 value is significantly different from zero ($p = 0.0254$).

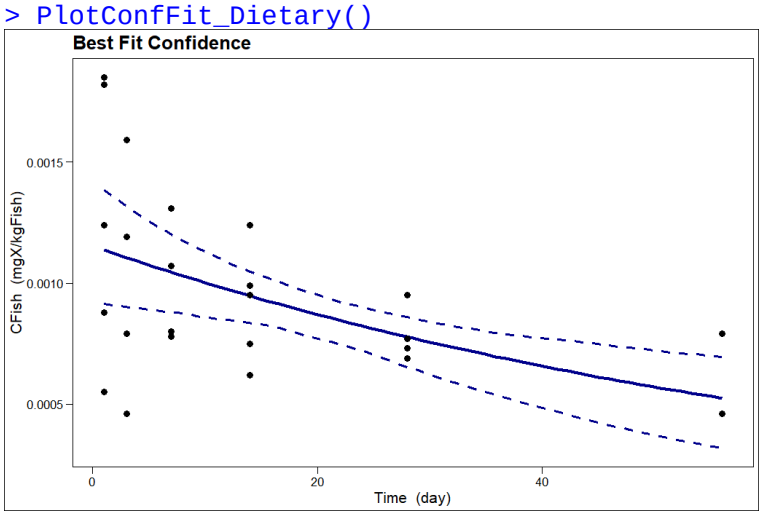
```
> ModelDiagnostics_Dietary()

------
        Shapiro-Wilk normality test

data:  stdres
W = 0.96957, p-value = 0.6342
```

```
------
        Runs Test

data:  as.factor(run)
Standard Normal = -0.19646, p-value = 0.8443
alternative hypothesis: two.sided
```



A trend over time does not seem indicated by the autocorrelation plot.
The run test indicates *p-value* of 0.8443, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.6342) so that the hypothesis that the error distribution is normal is not rejected.

```
> PlotConfFit_Dietary()
```




```
> SummTable_Dietary()
```

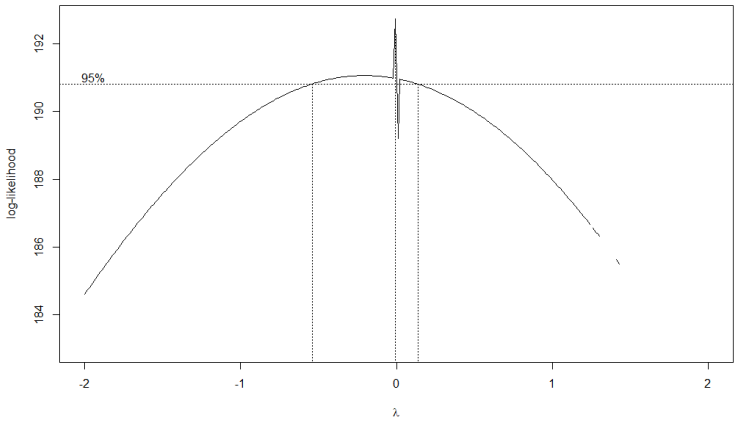
	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.00115	0.000105	0.000947	0.00136	mgX/kgFish
k2	0.01406	0.00588	0.002536	0.02559	1/day
k2g	0.01406	0.00588	0.002536	0.02559	1/day
kf	0.00151	0.000182	0.001156	0.00187	kgFood/kgFish/day
alpha	0.10082	0.012119	0.077065	0.12457	-
BMFK	0.10755	0.035365	0.038238	0.17687	kgFood/kgFish
BMFKg	0.10755	0.035365	0.038238	0.17687	kgFood/kgFish
tHalfg	49.287	20.612	8.8881	89.686	day

```
BMFKgLipid  0.30356  0.099813 0.10792   0.49919      kgFood/kgFish
```

A depuration rate growth corrected (k_{2g}) of 0.01406 (equal to k_2) and a BMF_{KgL} of 0.30356 (95% Confidence interval: 0.10792–0.49919) are estimated for $C_{14}Cl_{11}$ group of congeners with the untransformation model.

BOX-COX TRANSFORMED FIT (the Box-Cox power transformation model)

```
> ModelTrans_BoxCox_Dietary()
      fit     conflo     confup
-0.0100000 -0.5422723  0.1366718
```

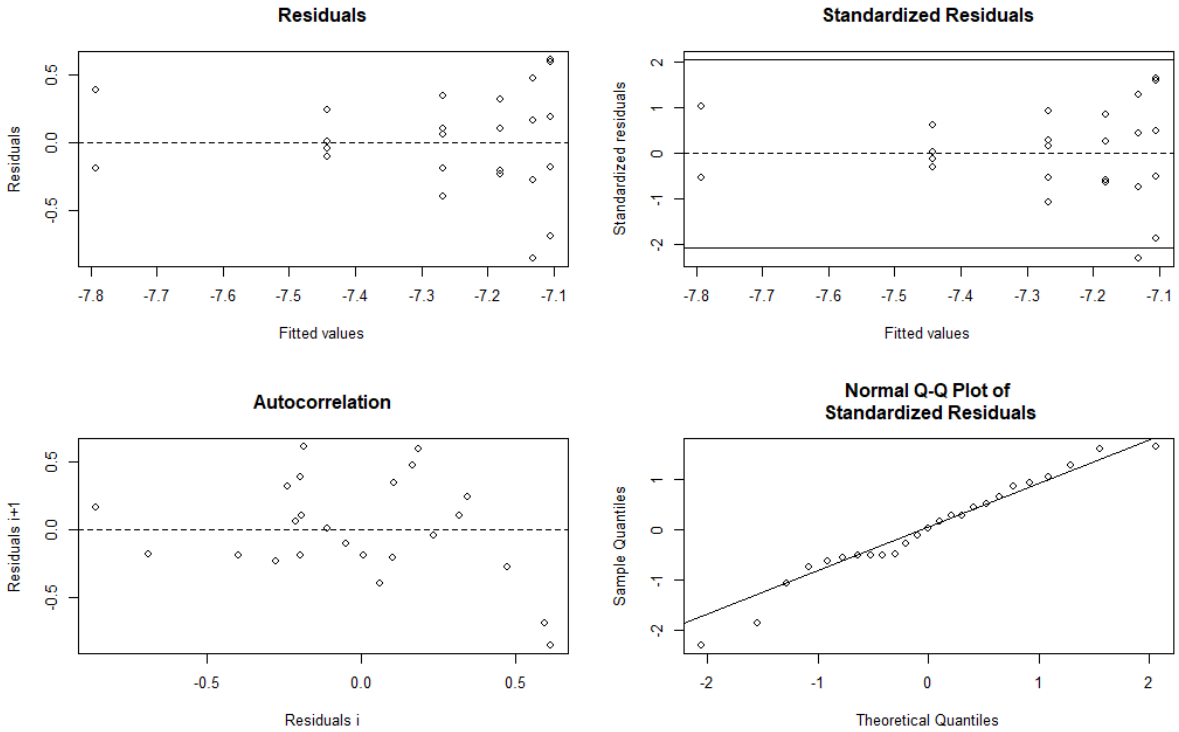


The estimated optimal λ value is -0.01 and its confidence interval is -0.5422723 up to 0.1366718. The most likely value (-0.01) is near the logarithm transformation (0).

```
> FitModel_Dietary_BoxCox()
Formula: bc.cfish.data ~ car::bcPower(RunModel_Dietary(time.data, fitc0d,
    fitk2) + lnstarter, lambda)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 0.0010562  0.0000989  10.680 2.18e-10 ***
fitk2  0.0116104  0.0039770   2.919  0.00772 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.371 on 23 degrees of freedom

Number of iterations to convergence: 1
Achieved convergence tolerance: 9.861e-07
```

A k_2 value of 0.0116104 is predicted with the Box-Cox power transformation model for $C_{14}Cl_{11}$ group of congeners. This k_2 value is significantly different from zero (p=0.00772).

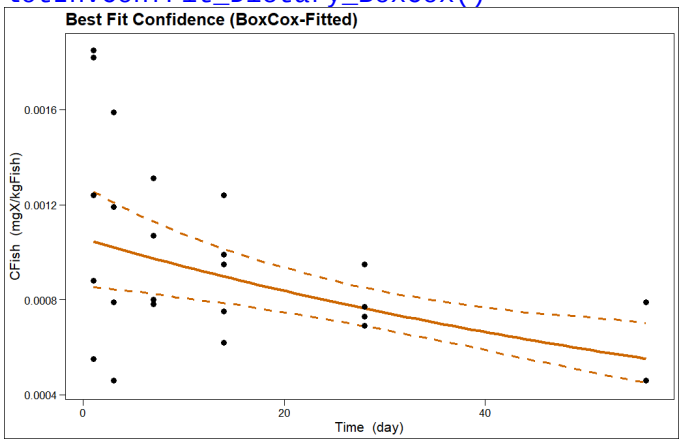
```
> ModelDiagnostics_Dietary_BoxCox()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.96957, p-value = 0.6341


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.62212, p-value = 0.5339
alternative hypothesis: two.sided
```



The Q-Q plot for the Box-Cox power transformation model is more attractive than for the untransformed model. No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.5339, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.6341), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is slightly lower than in the untransformed model.

```
> PlotInvConfFit_Dietary_BoxCox()
```




```
> SummTable_Dietary_BoxCox()
  Estimate Std.Error      2.5%    97.5%              unit
C0d           0.00106  0.000099  0.000862  0.00125        mgX/kgFish
k2            0.01161  0.003977  0.003815  0.01941             1/day
k2g           0.01161  0.003977  0.003815  0.01941             1/day
kf            0.00136  0.000155  0.001059  0.00167 kgFood/kgFish/day
alpha         0.09083  0.010324  0.070592  0.11106                 -
BMFK          0.11734  0.030703  0.057167  0.17752     kgFood/kgFish
BMFKg         0.11734  0.030703  0.057167  0.17752     kgFood/kgFish
tHalfg       59.688   20.446    19.615    99.761               day
BMFKgLipid    0.33119  0.086654  0.16134   0.50103     kgFood/kgFish
```

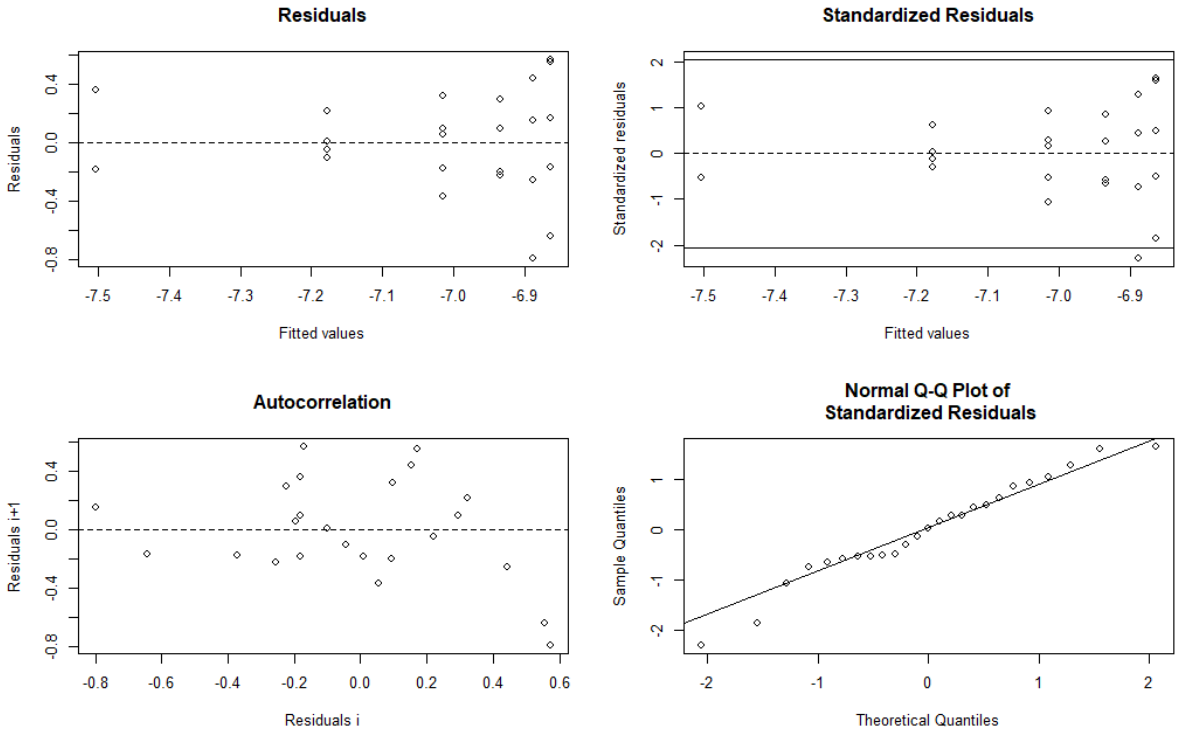
A depuration rate growth corrected (k_{2g}) of 0.01161 (equal to k_2) and a BMF_{KgL} of 0.33119 (95% Confidence interval: 0.16134–0.50103) are estimated with the Box-Cox power transformation model for $C_{14}Cl_{11}$ group of congeners.

LN- TRANSFORMED FIT (the natural logarithm transformation model)

```
> FitModel_Dietary_Ln()
Formula: ln.cfish.data ~ log(RunModel_Dietary(time.data, fitc0d, fitk2) +
    lnstarter)

Parameters:
        Estimate Std. Error t value Pr(>|t|)
fitc0d 1.057e-03  9.894e-05  10.685 2.16e-10 ***
fitk2  1.163e-02  3.989e-03   2.914  0.00781 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.3459 on 23 degrees of freedom

Number of iterations to convergence: 0
Achieved convergence tolerance: 3.595e-06
```

A k_2 value of 0.01163 is predicted with the logarithm transformation model for $C_{14}Cl_{11}$ group of congeners. This k_2 value is significantly different from zero (p=0.00781).

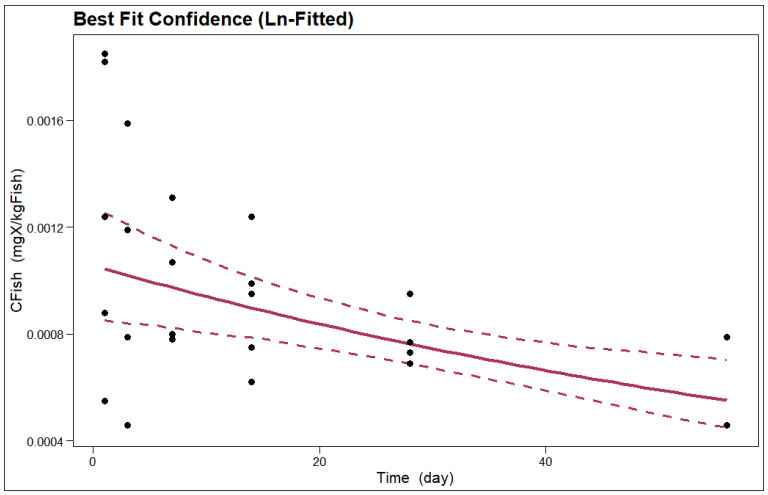
```
> ModelDiagnostics_Dietary_Ln()
------
        Shapiro-Wilk normality test

data:  stdres
W = 0.96987, p-value = 0.6418


------
        Runs Test

data:  as.factor(run)
Standard Normal = 0.62212, p-value = 0.5339
alternative hypothesis: two.sided
```



No trend over time is indicated by the autocorrelation plot.

The run test indicates a *p-value* of 0.5339, confirming the interpretation of independent errors in the autocorrelation plot. The Shapiro-Wilk test *p-value* for normality is high (0.6418), the hypothesis that the error distribution is normal is not rejected. The Shapiro-wilk *p-value* with this model is higher than in the untransformed model and than in the Box-cox power transformation model.

```
> PlotInvConfFit_Dietary_Ln()
```




```
> SummTable_Dietary_Ln()
```

	Estimate	Std.Error	2.5%	97.5%	unit
C0d	0.00106	0.000099	0.000863	0.00125	mgX/kgFish
k2	0.01163	0.003989	0.003807	0.01944	1/day
k2g	0.01163	0.003989	0.003807	0.01944	1/day
kf	0.00136	0.000155	0.00106	0.00167	kgFood/kgFish/day
alpha	0.09091	0.010334	0.070654	0.11116	-
BMFK	0.11729	0.030757	0.057009	0.17758	kgFood/kgFish
BMFKg	0.11729	0.030757	0.057009	0.17758	kgFood/kgFish
tHalfg	59.608	20.453	19.52	99.697	day
BMFKgLipid	0.33104	0.086808	0.1609	0.50119	kgFood/kgFish

A depuration rate growth corrected (k_{2g}) of 0.01163 (equal to k_2) and a BMF_{KgL} of 0.33104 (95% Confidence interval: 0.1609–0.50119) are estimated with the logarithm transformation model for $C_{14}Cl_{11}$ group of congeners.

The combined results, followed by graphical inspection model diagnostics and statistical testing provides confidence that for C_{14} Cl_{11} group of congeners, the logarithm transformation model is the best fit model to the data.

Derivation of BCFs using the spreadsheet 'BCF estimation tool (version 2)', available on the OECD website

Table 68: Summary Table of the BCFs estimated with 15 models within the OECD TG 305 BCF estimation tool (Excel® spread sheet Version 2)

	$C_{14}Cl_5$	$C_{14}Cl_6$	$C_{14}Cl_7$	$C_{14}Cl_8$	$C_{14}Cl_9$	$C_{14}Cl_{10}$	$C_{14}Cl_{11}$	C_{14} chlorinated n-alkane, 50% Cl wt.
BCFs (15 models)	All BCFs > 5000 (using the less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	All BCFs > 5000	All BCFs > 5000 Or All BCFs > 2 000 and BCFs > 5 000 (11 out of 15 models) (using the less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	All BCFs > 5000 (using the less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	All BCFs > 2 000 and BCFs > 5 000 (14 out of 15 models) (using the less conservative scenario with $k_g=0$ and $k_2=k_{2g;}$ and a log Kow of 6.86 for the consituent)	All BCFs > 5000 (using the less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	All BCFs > 5000 (using the less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)	All BCFs > 5000

C_{14} chlorinated n-alkane, 50% Cl wt. The results indicate a BCF for C_{14} chlorinated n-alkane, 50% Cl wt. above 5 000 L/kg for all of the models. That is why C_{14} chlorinated n-alkane, 50% Cl wt. is concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0.018794
Log K_{OW}	6.58
$K_{2\,g}$ (K_2 - K_g)	0.00861
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
$BMF_{g\,l}$	0.33303

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.095
Mean lipid content midpoint depuration phase	0.058
$K_{2\,g\,l}$	0.010

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	435.73	43679.9	Hayton and Barron (1990)
weight	598.77	60023.4	Erickson and McKim (1990a)
weight	594.89	59635.1	Barber et al. (1991)
weight	384.66	38560.3	Barber (2003) - observed
weight	615.18	61668.7	Barber (2001)
weight	116.51	11679.3	Streit and Sire (1993)
weight	481.23	48241.5	Erickson and McKim (1990b)
weight	410.40	41140.7	Sijm et al. (1995)
weight	496.83	49804.8	Barber (2003) - calibrated
log Kow	988.01	99042.9	Tolls and Sijm (1995)
log Kow	885.65	88781.7	Spacie and Hamelink (1982)
weight, log Kow	106.32	10657.7	Hendriks et al. (2001)
weight, log Kow	81.48	8167.6	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
$K_{2\,g\,l}$	688.23	68992.1	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
$BMF_{g\,l}$	52.91	5304.2	Inoue et al (2012)

C_{14} chlorinated n-alkane, 50 % Cl wt. (scenario k_g=0 for the bioaccumulation discussion on Fisk *et al.* studies; see section 0 3.4.2.2 Dietary studies)

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.58
K_{2g} (K_2 - K_g)	0.02741
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.33303

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.032

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	13819.4	Hayton and Barron (1990)
weight	602.21	18963.1	Erickson and McKim (1990a)
weight	598.87	18857.6	Barber et al. (1991)
weight	387.44	12200.1	Barber (2003) - observed
weight	618.81	19485.7	Barber (2001)
weight	117.21	3690.9	Streit and Sire (1993)
weight	485.26	15280.4	Erickson and McKim (1990b)
weight	415.23	13075.2	Sijm et al. (1995)
weight	504.34	15881.0	Barber (2003) - calibrated
log Kow	988.01	31111.2	Tolls and Sijm (1995)
log Kow	885.65	27888.0	Spacie and Hamelink (1982)
weight, log Kow	107.29	3378.5	Hendriks et al. (2001)
weight, log Kow	81.48	2565.6	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	532.22	16759.0	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	168.45	5304.2	Inoue et al (2012)

$C_{14}Cl_5$ group of congeners (less conservative scenario with $k_g = 0$ and $k_2 = k_{2g}$)

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.58
K_{2g} (K_2 - K_g)	0.0021
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.6673

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.002

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	180375.9	Hayton and Barron (1990)
weight	602.21	247513.2	Erickson and McKim (1990a)
weight	598.87	246136.6	Barber et al. (1991)
weight	387.44	159240.3	Barber (2003) - observed
weight	618.81	254334.8	Barber (2001)
weight	117.21	48175.0	Streit and Sire (1993)
weight	485.26	199446.1	Erickson and McKim (1990b)
weight	415.23	170662.5	Sijm et al. (1995)
weight	504.34	207284.6	Barber (2003) - calibrated
log Kow	988.01	406075.9	Tolls and Sijm (1995)
log Kow	885.65	364004.9	Spacie and Hamelink (1982)
weight, log Kow	107.29	44098.1	Hendriks et al. (2001)
weight, log Kow	81.48	33487.1	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	941.40	386920.1	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.

BMF_{gl}	22.95	9430.6	Inoue et al (2012)

As previously explained, the scenario used for $C_{14}Cl_5$ (k_g=0 and k_2=k_{2g}) overestimates the depuration rate and the estimated BMF value of 0.6673 is underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB. The results indicate a BCF for $C_{14}Cl_5$ above 5 000 L/kg for all of the models. That is why $C_{14}Cl_5$ are concluded B/vB.

The log Kow of 6.58 used as input parameter refers to the experimental log Kow for C_{14} chlorinated n-alkane 50% Cl wt. from Unpublished (2019b). The OECD spreadsheet was also run with a log Kow of 6.32 which refers to an experimental value for the gourp of congeners $C_{14}Cl_5$ (Unpublished, 2019b). With a log Kow of 6.32, the results indicate a BCF for $C_{14}Cl_5$ group of congeners well above 5 000 L/kg for all of the models (see below). That is why $C_{14}Cl_5$ are concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.32
K_{2g} (K_2 - K_g)	0.0021
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.6673

Interim Outputs

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	180375.9	Hayton and Barron (1990)
weight	602.21	247513.2	Erickson and McKim (1990a)
weight	598.87	246136.6	Barber et al. (1991)
weight	387.44	159240.3	Barber (2003) - observed
weight	618.81	254334.8	Barber (2001)
weight	117.21	48175.0	Streit and Sire (1993)
weight	485.26	199446.1	Erickson and McKim (1990b)
weight	415.23	170662.5	Sijm et al. (1995)
weight	504.32	207280.0	Barber (2003) - calibrated
log Kow	918.42	377474.1	Tolls and Sijm (1995)
log Kow	811.04	333339.8	Spacie and Hamelink (1982)

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.002

weight, log Kow	107.09	44015.6	Hendriks et al. (2001)
weight, log Kow	109.91	45172.8	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	941.40	386920.1	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	22.95	9430.6	Inoue et al (2012)

$C_{14}Cl_6$ group of congeners

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0.018794
Log K_{OW}	6.58
$K_{2\,g}$ (K_2 - K_g)	0.00422
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
$BMF_{g\,l}$	0.47292

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.095
Mean lipid content midpoint depuration phase	0.058
$K_{2\,g\,l}$	0.005

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	435.73	89119.4	Hayton and Barron (1990)
weight	598.77	122464.9	Erickson and McKim (1990a)
weight	594.89	121672.5	Barber et al. (1991)
weight	384.66	78673.9	Barber (2003) - observed
weight	615.18	125821.7	Barber (2001)
weight	116.51	23829.1	Streit and Sire (1993)
weight	481.23	98426.3	Erickson and McKim (1990b)
weight	410.40	83938.7	Sijm et al. (1995)
weight	496.83	101616.0	Barber (2003) - calibrated
log Kow	988.01	202075.7	Tolls and Sijm (1995)
log Kow	885.65	181139.9	Spacie and Hamelink (1982)
weight, log Kow	106.32	21744.8	Hendriks et al. (2001)
weight, log Kow	81.48	16664.2	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
$K_{2\,g\,l}$	806.28	164907.9	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.

	$BMF_{g\,I}$	34.67	7091.3	Inoue et al (2012)

The results indicate a BCF for $C_{14}Cl_6$ group of congeners well above 5 000 L/kg for all of the models. That is why $C_{14}Cl_6$ are concluded B/vB.

The log Kow of 6.58 used as input parameter refers to the experimental log Kow for C_{14} chlorinated n-alkane 50% Cl wt. from Unpublished (2019b). The OECD spreadsheet was also run with a log Kow of 6.66 which refers to an experimental value for the congeners $C_{14}Cl_6$ (Unpublished, 2019b). With a log Kow of 6.66, the results indicate a BCF for $C_{14}Cl_6$ group of congeners well above 5 000 L/kg for all of the models (see below). That is why $C_{14}Cl_6$ are concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0.018794
Log K_{OW}	6.66
$K_{2\,g}$ (K_2 - K_g)	0.00422
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
$BMF_{g\,I}$	0.47292

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.095
Mean lipid content midpoint depuration phase	0.058
$K_{2\,g\,I}$	0.005

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	435.73	89119.4	Hayton and Barron (1990)
weight	598.77	122464.9	Erickson and McKim (1990a)
weight	594.89	121672.5	Barber et al. (1991)
weight	384.66	78673.9	Barber (2003) - observed
weight	615.18	125821.7	Barber (2001)
weight	116.51	23829.1	Streit and Sire (1993)
weight	481.23	98426.3	Erickson and McKim (1990b)
weight	410.40	83938.7	Sijm et al. (1995)
weight	496.83	101616.4	Barber (2003) - calibrated
log Kow	1010.46	206668.4	Tolls and Sijm (1995)
log Kow	909.96	186111.8	Spacie and Hamelink (1982)
weight, log Kow	106.36	21753.2	Hendriks et al. (2001)
weight, log Kow	74.31	15197.9	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.

K_{2gl}	806.28	164907.9	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	34.67	7091.3	Inoue et al (2012)

$C_{14}Cl_7$ group of congeners

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0.018794
Log K_{OW}	6.58
$K_{2\,g}$ (K_2 - K_g)	0.00799
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
$BMF_{g\,l}$	0.42977

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.095
Mean lipid content midpoint depuration phase	0.058
$K_{2\,g\,l}$	0.009

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	435.73	47069.3	Hayton and Barron (1990)
weight	598.77	64681.1	Erickson and McKim (1990a)
weight	594.89	64262.6	Barber et al. (1991)
weight	384.66	41552.4	Barber (2003) - observed
weight	615.18	66454.0	Barber (2001)
weight	116.51	12585.6	Streit and Sire (1993)
weight	481.23	51984.9	Erickson and McKim (1990b)
weight	410.40	44333.1	Sijm et al. (1995)
weight	496.83	53669.5	Barber (2003) - calibrated
log Kow	988.01	106728.3	Tolls and Sijm (1995)
log Kow	885.65	95670.9	Spacie and Hamelink (1982)
weight, log Kow	106.32	11484.8	Hendriks et al. (2001)
weight, log Kow	81.48	8801.4	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
$K_{2\,g\,l}$	699.75	75589.4	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
$BMF_{g\,l}$	60.65	6551.2	Inoue et al (2012)

The results indicate a BCF for $C_{14}Cl_7$ congeners well above 5 000 L/kg for all of the models. That is why $C_{14}Cl_7$ are concluded B/vB.

The log Kow of 6.58 used as input parameter refers to the experimental log Kow for C_{14} chlorinated n-alkane 50% Cl wt. from Unpublished (2019b). The OECD spreadsheet was also run with a log Kow of 6.59 which refers to an experimental value for the group of congeners $C_{14}Cl_7$ (Unpublished, 2019b). With a log Kow of 6.59, the results indicate a BCF for $C_{14}Cl_7$ group of congeners well above 5 000 L/kg for all of the models (see below). That is why $C_{14}Cl_7$ are concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0.018794
Log K_{OW}	6.59
K_{2g} (K_2 - K_g)	0.00799
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.42977

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.095
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.009

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	435.73	47069.3	Hayton and Barron (1990)
weight	598.77	64681.1	Erickson and McKim (1990a)
weight	594.89	64262.6	Barber et al. (1991)
weight	384.66	41552.4	Barber (2003) - observed
weight	615.18	66454.0	Barber (2001)
weight	116.51	12585.6	Streit and Sire (1993)
weight	481.23	51984.9	Erickson and McKim (1990b)
weight	410.40	44333.1	Sijm et al. (1995)
weight	496.83	53669.5	Barber (2003) - calibrated
log Kow	990.79	107028.6	Tolls and Sijm (1995)
log Kow	888.65	95995.2	Spacie and Hamelink (1982)
weight, log Kow	106.32	11485.4	Hendriks et al. (2001)
weight, log Kow	80.54	8700.6	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	699.75	75589.4	Brookes and Crooke (2012)

	Method 3		
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	60.65	6551.2	Inoue et al (2012)

$C_{14}Cl_7$ group of congeners(less conservative scenario with $k_g=0$ and $k_2=k_{2g}$)

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.58
K_{2g} (K_2 - K_g)	0.026786
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.12823

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.031

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	14141.3	Hayton and Barron (1990)
weight	602.21	19404.8	Erickson and McKim (1990a)
weight	598.87	19296.9	Barber et al. (1991)
weight	387.44	12484.3	Barber (2003) - observed
weight	618.81	19939.6	Barber (2001)
weight	117.21	3776.9	Streit and Sire (1993)
weight	485.26	15636.4	Erickson and McKim (1990b)
weight	415.23	13379.8	Sijm et al. (1995)
weight	504.34	16250.9	Barber (2003) - calibrated
log Kow	988.01	31836.0	Tolls and Sijm (1995)
log Kow	885.65	28537.7	Spacie and Hamelink (1982)
weight, log Kow	107.29	3457.3	Hendriks et al. (2001)
weight, log Kow	81.48	2625.4	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	534.95	17237.3	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.

$BMF_{g\,l}$	74.69	2406.7	Inoue et al (2012)

As previously explained, the scenario used for $C_{14}Cl_7$ (k_g=0 and k_2=k_{2g}) overestimates the depuration rate and the estimated BMF value of 0.12823 is underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB. The results indicate a BCF for $C_{14}Cl_7$ above 2 000 for all of the models and above 5 000 L/kg for 11 out of 15 models. That is why, based on a weight-of-evidence approach, $C_{14}Cl_7$ are concluded B/vB.

The log Kow of 6.58 used as input parameter refers to the experimental log Kow for C_{14} chlorinated n-alkane 50% Cl wt. from Unpublished (2019b). The OECD spreadsheet was also run with a log Kow of 6.59 which refers to an experimental value for the group of congeners $C_{14}Cl_7$ (Unpublished, 2019b) and using the less conservative scenario. With a log Kow of 6.59, the results indicate a BCF for $C_{14}Cl_7$ above 2 000 L/kg for all of the models and above 5 000 L/kg for 11 out of 15 models. That is why, based on a weight-of-evidence approach and using the less conservative scenario, $C_{14}Cl_7$ are concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.59
$K_{2\,g}$ (K_2 - K_g)	0.026786
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
$BMF_{g\,l}$	0.12823

Interim Outputs

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	14141.3	Hayton and Barron (1990)
weight	602.21	19404.8	Erickson and McKim (1990a)
weight	598.87	19296.9	Barber et al. (1991)
weight	387.44	12484.3	Barber (2003) - observed
weight	618.81	19939.6	Barber (2001)
weight	117.21	3776.9	Streit and Sire (1993)
weight	485.26	15636.4	Erickson and McKim (1990b)
weight	415.23	13379.8	Sijm et al. (1995)
weight	504.34	16250.9	Barber (2003) - calibrated
log Kow	990.79	31925.6	Tolls and Sijm (1995)
log Kow	888.65	28634.4	Spacie and Hamelink (1982)
weight, log Kow	107.30	3457.4	Hendriks et al. (2001)

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.031

weight, log Kow	80.54	2595.3	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	534.95	17237.3	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	74.69	2406.7	Inoue et al (2012)

$C_{14}Cl_8$ group of congeners (less conservative scenario with $k_g = 0$ and $k_2 = k_{2g}$)

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.58
K_{2g} (K_2 - K_g)	0.01244
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.31626

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.014

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	30449.3	Hayton and Barron (1990)
weight	602.21	41782.8	Erickson and McKim (1990a)
weight	598.87	41550.4	Barber et al. (1991)
weight	387.44	26881.4	Barber (2003) - observed
weight	618.81	42934.3	Barber (2001)
weight	117.21	8132.4	Streit and Sire (1993)
weight	485.26	33668.6	Erickson and McKim (1990b)
weight	415.23	28809.6	Sijm et al. (1995)
weight	504.34	34991.8	Barber (2003) - calibrated
log Kow	988.01	68549.8	Tolls and Sijm (1995)
log Kow	885.65	61447.8	Spacie and Hamelink (1982)
weight, log Kow	107.29	7444.2	Hendriks et al. (2001)
weight, log Kow	81.48	5653.0	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	634.24	44005.1	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.

BMF_{gl}	73.25	5082.0	Inoue et al (2012)

As previously explained, the scenario used for $C_{14}Cl_8$ (k_g=0 and k_2=k_{2g}) overestimates the depuration rate and the estimated BMF value of 0.31626 is underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB. The results indicate a BCF for $C_{14}Cl_8$ above 5 000 L/kg for all of the models. That is why $C_{14}Cl_8$ are concluded B/vB.

The log Kow of 6.58 used as input parameter refers to the experimental log Kow for C_{14} chlorinated n-alkane 50% Cl wt. from Unpublished (2019b). The OECD spreadsheet was also run with a log Kow of 6.66 which refers to an experimental value for the group of congeners $C_{14}Cl_8$ (Unpublished, 2019b) and using the less conservative scenario. With a log Kow of 6.66, the results indicate a BCF for $C_{14}Cl_8$ above 5 000 L/kg for all of the models. That is why $C_{14}Cl_8$ are concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.66
K_{2g} (K_2 - K_g)	0.01244
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.31626

Interim Outputs

Variable	Value

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	30449.3	Hayton and Barron (1990)
weight	602.21	41782.8	Erickson and McKim (1990a)
weight	598.87	41550.4	Barber et al. (1991)
weight	387.44	26881.4	Barber (2003) - observed
weight	618.81	42934.3	Barber (2001)
weight	117.21	8132.4	Streit and Sire (1993)
weight	485.26	33668.6	Erickson and McKim (1990b)
weight	415.23	28809.6	Sijm et al. (1995)
weight	504.34	34991.9	Barber (2003) - calibrated
log Kow	1010.46	70107.8	Tolls and Sijm (1995)
log Kow	909.96	63134.4	Spacie and Hamelink (1982)
weight, log Kow	107.33	7447.1	Hendriks et al. (2001)
weight, log Kow	74.31	5155.6	Thomann (1989)

Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.014

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	634.24	44005.1	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	73.25	5082.0	Inoue et al (2012)

$C_{14}Cl_9$ group of congeners (less conservative scenario with $k_g = 0$ and $k_2 = k_{2g}$)

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.58
K_{2g} (K_2 - K_g)	0.01044
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.47684

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.012

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	36282.5	Hayton and Barron (1990)
weight	602.21	49787.1	Erickson and McKim (1990a)
weight	598.87	49510.2	Barber et al. (1991)
weight	387.44	32031.1	Barber (2003) - observed
weight	618.81	51159.3	Barber (2001)
weight	117.21	9690.4	Streit and Sire (1993)
weight	485.26	40118.5	Erickson and McKim (1990b)
weight	415.23	34328.7	Sijm et al. (1995)
weight	504.34	41695.2	Barber (2003) - calibrated
log Kow	988.01	81681.9	Tolls and Sijm (1995)
log Kow	885.65	73219.4	Spacie and Hamelink (1982)
weight, log Kow	107.29	8870.3	Hendriks et al. (2001)
weight, log Kow	81.48	6735.9	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	659.41	54515.7	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	86.36	7139.9	Inoue et al (2012)

As previously explained, the scenario used for $C_{14}Cl_9$ (k_g=0 and k_2=k_{2g}) overestimates the depuration rate and the estimated BMF value of 0.47684 is underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB. The results indicate a BCF for $C_{14}Cl_9$ above 5 000 L/kg for all of the models. That is why $C_{14}Cl_9$ are concluded B/vB.

The log Kow of 6.58 used as input parameter refers to the experimental log Kow for C_{14} chlorinated n-alkane 50% Cl wt. from Unpublished (2019b). The OECD spreadsheet was also run with a log Kow of 6.86 which refers to an experimental value for the group of congeners $C_{14}Cl_9$ (Unpublished, 2019b) and using the less conservative scenario. With a log Kow of 6.86, the results indicate a BCF for $C_{14}Cl_9$ above 2 000 L/kg for all of the models and above 5 000 L/kg for 14 out of 15 models (see below). That is why, based on a weight-of-evidence approach and using the less conservative scenario, $C_{14}Cl_9$ are concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.86
K_{2g} (K_2 - K_g)	0.01044
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.47684

Interim Outputs

Variable	Value

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	36282.5	Hayton and Barron (1990)
weight	602.21	49787.1	Erickson and McKim (1990a)
weight	598.87	49510.2	Barber et al. (1991)
weight	387.44	32031.1	Barber (2003) - observed
weight	618.81	51159.3	Barber (2001)
weight	117.21	9690.4	Streit and Sire (1993)
weight	485.26	40118.5	Erickson and McKim (1990b)
weight	415.23	34328.7	Sijm et al. (1995)
weight	504.34	41695.7	Barber (2003) - calibrated
log Kow	1068.86	88366.2	Tolls and Sijm (1995)
log Kow	973.69	80498.2	Spacie and Hamelink (1982)
weight, log Kow	107.41	8880.0	Hendriks et al. (2001)
weight, log Kow	59.02	4879.7	Thomann (1989)

Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.012

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	659.41	54515.7	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	86.36	7139.9	Inoue et al (2012)

$C_{14}Cl_{10}$ group of congeners (less conservative scenario with $k_g = 0$ and $k_2 = k_{2g}$)

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.58
K_{2g} (K_2 - K_g)	0.00962
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gI}	0.54647

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gI}	0.011

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	39375.2	Hayton and Barron (1990)
weight	602.21	54031.0	Erickson and McKim (1990a)
weight	598.87	53730.4	Barber et al. (1991)
weight	387.44	34761.4	Barber (2003) - observed
weight	618.81	55520.1	Barber (2001)
weight	117.21	10516.4	Streit and Sire (1993)
weight	485.26	43538.1	Erickson and McKim (1990b)
weight	415.23	37254.8	Sijm et al. (1995)
weight	504.34	45249.2	Barber (2003) - calibrated
log Kow	988.01	88644.4	Tolls and Sijm (1995)
log Kow	885.65	79460.5	Spacie and Hamelink (1982)
weight, log Kow	107.29	9626.4	Hendriks et al. (2001)
weight, log Kow	81.48	7310.1	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gI}	671.49	60246.7	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gI}	89.09	7992.9	Inoue et al (2012)

As previously explained, the scenario used for $C_{14}Cl_{10}$ (k_g=0 and k_2=k_{2g}) overestimates the depuration rate and the estimated BMF value of 0.54647 is underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB. The results indicate a BCF for $C_{14}Cl_{10}$ above 5 000 L/kg for all of the models. That is why $C_{14}Cl_{10}$ are concluded B/vB.

The log Kow of 6.58 used as input parameter refers to the experimental log Kow for C_{14} chlorinated n-alkane 50% Cl wt. from Unpublished (2019b). The OECD spreadsheet was also run with a log Kow of 5.98 which refers to an experimental value for the group of congeners $C_{14}Cl_{10}$ (Unpublished, 2019b) and using the less conservative scenario. With a log Kow of 5.98, the results indicate a BCF for $C_{14}Cl_{10}$ above 5 000 L/kg for all of the models. That is why $C_{14}Cl_{10}$ are concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	5.98
K_{2g} (K_2 - K_g)	0.00962
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.54647

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	39375.2	Hayton and Barron (1990)
weight	602.21	54031.0	Erickson and McKim (1990a)
weight	598.87	53730.4	Barber et al. (1991)
weight	387.44	34761.4	Barber (2003) - observed
weight	618.81	55520.1	Barber (2001)
weight	117.21	10516.4	Streit and Sire (1993)
weight	485.26	43538.1	Erickson and McKim (1990b)
weight	415.23	37254.8	Sijm et al. (1995)
weight	504.30	45245.6	Barber (2003) - calibrated
log Kow	834.76	74894.8	Tolls and Sijm (1995)
log Kow	722.87	64856.2	Spacie and Hamelink (1982)
weight, log Kow	106.57	9561.2	Hendriks et al. (2001)
weight, log Kow	160.00	14355.3	Thomann (1989)

Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.011

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	671.49	60246.7	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	89.09	7992.9	Inoue et al (2012)

$C_{14}Cl_{11}$ group of congeners (less conservative scenario with $k_g = 0$ and $k_2 = k_{2g}$)

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.58
K_{2g} (K_2 - K_g)	0.01163
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.33104

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020
Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.013

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	32570.0	Hayton and Barron (1990)
weight	602.21	44692.8	Erickson and McKim (1990a)
weight	598.87	44444.3	Barber et al. (1991)
weight	387.44	28753.6	Barber (2003) - observed
weight	618.81	45924.6	Barber (2001)
weight	117.21	8698.8	Streit and Sire (1993)
weight	485.26	36013.5	Erickson and McKim (1990b)
weight	415.23	30816.1	Sijm et al. (1995)
weight	504.34	37428.9	Barber (2003) - calibrated
log Kow	988.01	73324.1	Tolls and Sijm (1995)
log Kow	885.65	65727.4	Spacie and Hamelink (1982)
weight, log Kow	107.29	7962.7	Hendriks et al. (2001)
weight, log Kow	81.48	6046.7	Thomann (1989)

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	643.80	47778.8	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	71.12	5277.9	Inoue et al (2012)

As previously explained, the scenario used for $C_{14}Cl_{11}$ (k_g=0 and k_2=k_{2g}) overestimates the depuration rate and the estimated BMF value of 0.33104 is underestimated (corresponding to the less conservative scenario). The assumption is that if the BCF values calculated on the basis of such an underestimated BMF indicate B and/or vB for a group of congeners, then this group of congeners can be concluded as B and/or vB. The results indicate a BCF for $C_{14}Cl_{11}$ above 5 000 L/kg for all of the models. That is why $C_{14}Cl_{11}$ are concluded B/vB.

The log Kow of 6.58 used as input parameter refers to the experimental log Kow for C_{14} chlorinated n-alkane 50% Cl wt. from Unpublished (2019b). The OECD spreadsheet was also run with a log Kow of 6.34 which refers to an experimental value for the group of congeners $C_{14}Cl_{11}$ (Unpublished, 2019b) and using the less conservative scenario. With a log Kow of 6.34, the results indicate a BCF for $C_{14}Cl_{11}$ above 5 000 L/kg for all of the models. That is why $C_{14}Cl_{11}$ are concluded B/vB.

Inputs

Variable	Value
Mean weight at test start (g)	2.02
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0
Log K_{OW}	6.34
K_{2g} (K_2 - K_g)	0.01163
Mean fish lipid uptake end or depuration start (fraction)	0.05068
Mean fish lipid depuration end (fraction)	0.06518
Depuration phase duration (days)	56
BMF_{gl}	0.33104

Interim Outputs

Variable	Value
Mean weight midpoint uptake phase (g)	2.020

Outputs

Method 1			
inputs for K1	K1	BCF Est.	Ref.
weight	438.87	32570.0	Hayton and Barron (1990)
weight	602.21	44692.8	Erickson and McKim (1990a)
weight	598.87	44444.3	Barber et al. (1991)
weight	387.44	28753.6	Barber (2003) - observed
weight	618.81	45924.6	Barber (2001)
weight	117.21	8698.8	Streit and Sire (1993)
weight	485.26	36013.5	Erickson and McKim (1990b)
weight	415.23	30816.1	Sijm et al. (1995)
weight	504.33	37428.1	Barber (2003) - calibrated
log Kow	923.59	68543.6	Tolls and Sijm (1995)
log Kow	816.54	60599.2	Spacie and Hamelink (1982)
weight, log Kow	107.11	7949.3	Hendriks et al. (2001)
weight, log Kow	107.41	7971.1	Thomann (1989)

Mean lipid content midpoint depuration phase	0.058
K_{2gl}	0.013

Method 2			
input	Estimated K1	BCF Est.	Ref.
K_{2gl}	643.80	47778.8	Brookes and Crooke (2012)

Method 3			
input	Estimated K1	BCF Est.	Ref.
BMF_{gl}	71.12	5277.9	Inoue et al (2012)

Annex IX – 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 fish BCFs have been calculated using this tool based on relevant data from the Fisk *et al.* (1996), Fisk *et al.* (1998b) and Fisk *et al.* (2000). The data are provided in the following tables. Specific data for C_{14} 50% Cl wt. can be found in 'Annex VIII – Calculations performed on the dietary BMF study (Unpublished, 2019e) .

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

Substance[a]				Fish weights (g)			Estimated uptake rate constant (L/kg/day)[c]												
C	H	Cl	Cl content (% wt.)	Range at start of study	Est. at day 40[b]	Ref.	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

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

Substance[a]				Fish weights (g)			Estimated uptake rate constant (L/kg/day)[c]												
C	H	Cl	Cl content (% wt.)	Range at start of study	Est. at day 40[b]	Ref.	1	2	3	4	5	6	7	8	9	10	11	12	13
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

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

Substance[a]				Fish weights (g)			Estimated uptake rate constant (L/kg/day)[c]												
C	H	Cl	Cl content (% wt.)	Range at start of study	Est. at day 40[b]	Ref.	1	2	3	4	5	6	7	8	9	10	11	12	13
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

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 Kow 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

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
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

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
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

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	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

ESTIMATION OF NON-GROWTH CORRECTED BCF VALUES FROM DIETARY ACCUMULATION STUDIES WITH FISH																	
Substance[a]				Overall depuration rate	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
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

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

Annex X – Experimental and modelling data used as part of a weight-of-evidence (WoE) approach in order to conclude on the bioaccumulation potential of the congener groups of MCCP

It is important to note that all studies reported below and used in a weight-of-evidence approach have been assessed as reliable (with or without restrictions), relevant and adequate for the assessment.

Testing material/Species tested/Test guidelines (when available) and test duration or sampling date	Results	Conclusion on the B/vB criteria	Deviations from the OECD guidelines (when available)	Comments	Reliability of the study	Weight given in the WoE or Confidence level	Reference
C_{15} chlorinated n-alkane, 51% Cl wt. ($C_{15}Cl_{5-8}$) Rainbow Trout (*Oncorhynchus mykiss*) OECD TG 305 (aqueous exposure) 35 days for uptake phase, 42 days for the depuration phase	Growth-corrected kinetic BCF ~ 1 833 – 2 072 L/kg Depuration half-lives = 28 to 36 days	B	No lipid data were presented in the original study report, so it was not possible to lipid normalise the BCF. Measurement based on total radioactivity (so may represent accumulation of metabolites as well as the chlorinated paraffin, so the BCF determined may overestimate the actual accumulation potential of the substance).	Given the low water solubility of MCCP 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 underestimate steady-state BCFs.	Reliable with restrictions. Due to the study limitations, it is used as supporting information in a WoE.	Medium	Thompson *et al.*, 2000
^{14}C-labelled C_{14} chlorinated n-alkane, 45% Cl wt. ($C_{14}Cl_{3-6}$) Rainbow Trout (*Oncorhynchus mykiss*) OECD TG 305 (aqueous exposure)	Lipid-normalised and growth-corrected kinetic BCF of ~ 11 530 L/kg	B/vB		BCF value corrected based on the assumption that the parent substance was present in the fish samples at around 79% of the total radioactivity at the end of the uptake phase.	Reliable with restrictions. The results of this study are considered to be enough evidence in itself to conclude the congeners of MCCP as B/vB.	High	Unpublished, 2010h

35 days for the uptake phase, 42 days for the depuration phase							
C_{14} chlorinated n-alkane, 50% Cl wt. ($C_{14}Cl_{3-14}$) Rainbow Trout (*Oncorhynchus mykiss*) OECD TG 305 (Dietary exposure) 14 days for the uptake phase, 56 days for the depuration phase	BCF values for $C_{14}Cl_{5-11}$ congeners of MCCP and C_{14} chlorinated n-alkane, 50% Cl wt. > 5 000 L/kg A benchmark exercise confirms that the above congeners and MCCP have comparable BMF values with BMFs of SVHC substances having vPvB properties It is worth noting, that BMF value could not be derived for $C_{14}Cl_3$, $C_{14}Cl_4$, $C_{14}Cl_{12}$, $C_{14}Cl_{13}$ and $C_{14}Cl_{14}$ as these congeners either were not detected	B/vB	The fish in the test vessels were kept at a temperature of 11.8 to 12.5°C which is slightly lower than the range 13-17 °C recommended in the OECD TG for this species.	Results for the fish group dosed with a nominal 15 µg/g of test substance are not provided. The effects of freeze-drying are not considered in the study report. The freeze drying could have led to removal of volatile components but the vapour pressure of 2.7 x 10^{-4} Pa at 20 °C indicates that volatile losses would not be significant.	Reliable without restrictions. The results of this study are considered to be enough evidence in itself to conclude the congeners of MCCP as B/vB.	High	Unpublished, 2019e

	and/or not enough frequently detected during the depuration phase.						
$C_{14}H_{26}Cl_4$ $C_{14}H_{25}Cl_5$ $C_{14}H_{24}Cl_6$ $C_{14}H_{23.3}Cl_{6.7}$ with ($C_{14}Cl_{5-8}$) $C_{16}H_{31}Cl_3$ with ($C_{16}Cl_{2-5}$) $C_{16}H_{21}Cl_{13}$ with ($C_{16}Cl_{12-15}$) Rainbow Trout (*Oncorhynchus mykiss*) Dietary accumulation studies equivalent to OECD TG 305 40 days for the uptake phase, 80 to 173 days for the depuration phase (depending on the testing material)	Growth corrected depuration rate constants =0.009 to 0.024 day^{-1}, equivalent to a growth-corrected depuration half-life of 29 to 77 days	B/vB	Measurement based on total radioactivity (Fisk et al. 1996 and 2000), this means that although radioactivity was found in the organisms, the concentrations do not necessarily represent the parent compound but might also include metabolites. The method used for calculating the assimilation efficiencies in these studies is not comparable with the method currently recommended in OECD TG 305. Furthermore, for two of the studies (Fisk *et al.*, 1998b; and Fisk *et al.*, 2000), it is important to note that the measured concentration of test substance in the fish only considers concentration in the carcass (whole fish minus liver and gastrointestinal tract). Monitoring data in biota indicate that MCCP can be found in the liver of snakes, frogs, seabirds and cod (Du *et al.,* 2019 and 2020; Green *et al.*, 2019; Reth *et al.,* 2006 and Herzke *et al.,* 2019), that is why, it is most likely that the concentrations measured in the carcass only lead to an	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 congeners likely to be present in MCCP. The estimation of the growth-corrected depuration rate constant/half-life is consistent with OECD TG 305.	Reliable with restrictions. As recommended by the PBT guidance (REACH chapter R.11, ECHA, 2017b), conclusions from depuration rate constants can only be used as part of a WoE.	Medium	Fisk *et al.*, 1996; Fisk *et al.*, 1998b; and Fisk *et al.*, 2000

			underestimation of the concentration in the fish tissues, subsequently an underestimation of the BMF values.				
C_{13}-C_{18} 45% Cl wt. product (Cereclor S45; which contains $C_{14}Cl_{4-9}$, $C_{15}Cl_{3-9}$, $C_{16}Cl_{2-8}$ and $C_{17}Cl_{2-9}$ congener groups (including congeners found in Daphnia upon exposure even if not detected in the original substance tested)) *Daphnia magna* Bioaccumulation study (aqueous and dietary exposure) 48h for the uptake phase, 24h for the depuration phase	Lipid-normalised steady-state BCF of 10 000 000 L/kg lipid (or ca. 50 119 L/kg ww)	B/vB	There is no standard internationally recognised test guideline for *Daphnia* bioaccumulation. The study followed an adapted version of OECD TG 305 for fish bioaccumulation, but in the absence of a ring-test with *Daphnia*, the reliability and reproducibility of the method is unknown. Only a single water concentration value is presented, which was measured in the absence of test organisms. It is not clear how this differs from the actual exposure concentration in the presence of organisms or how variable this might have been over the duration of the test. It is not clear 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 amount of MCCP adsorbed to the Daphnia 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).	Reliable with restrictions. As recommended in REACH guidance Chapter R.7c (ECHA, 2017c), 'reliable measured BCF/BAF data from aquatic invertebrates can be used, if available, as part of a weight of evidence assessment'. This study is used as supporting information in a WoE approach as there is no standard test guideline for Daphnia bioaccumulation.	Medium	Castro *et al.*, 2019; Castro, 2020
C_{16} chlorinated n-alkane, 34.1% Cl wt. ($C_{16}Cl_{2-5}$)	BAF values = 7 031 L/kg (steady-state value) and 7	B/vB	The radioactivity measurements does not distinguish between parent compound and possible	BAF values corrected for a lipid content of 1.9%.	Reliable with restrictions. Due to the study	Medium	Renberg *et al.,* 1986

Mytilus edulis 28 days for the uptake phase (depuration was not studied)	204 L/kg (statistically determined) with confidence limits of 4 694–9 723 L/kg		metabolites and tissue-bound residues. Therefore, the results could indicate uptake, accumulation and elimination of metabolites rather than the parent compound.		limitations, it is used as supporting information in a WoE.		
n-pentadecane-8-^{14}C, 51% Cl wt. substance (C_{15} Cl_{5-8}) Earthworms (*Eisenia fetida*) 28 days for the uptake (adult worms), 56 days for the uptake (juvenile worms) (depuration was not studied)	BAF = 2.4 (based on ww concentrations) for adults BAF= 2.3 (based on ww concentrations) for juveniles	B	The interpretation of these results is complicated by the fact that the measurements are based on ^{14}C-determinations that could include metabolites of the test substance in addition to the parent compound. It was not possible to calculate the BSAFs of the worms (corresponding to the BAFs normalised for the worm lipid content and the soil total organic carbon content) as the worm lipid content was not reported in the study. In addition, it is unclear if the steady-state was reached at the end of the test.	Before radiochemical analysis, the adult and juvenile worms were purged for their gut content.	Reliable with restrictions. Due to the study limitations, it is used as supporting information in a WoE.	Low	Thompson *et al.,* 2001
$C_{14}Cl_{3-11}$, $C_{15}Cl_{3-11}$, $C_{16}Cl_{3-11}$, $C_{17}Cl_{4-10,}$ $C_{17}Cl_{12}$ Biomagnification in the muscles and livers of a snake-frog predator-prey relationship Red-backed rat snake (*Elaphe rufodorsata*;	BMFs >1 for $C_{14}Cl_{3-11}$, $C_{15}Cl_{3-11}$, $C_{16}Cl_{3-10}$ and $C_{17}Cl_{5-10}$	B/vB	No standard guidelines exist for BMF studies. It is worth noting that the BMF values reported in this study are based on the muscle and the liver tissues and as a consequence, they do not refer to the whole body weight of the snakes and frogs. It is noted that the sample size of the snakes is small compared to the one for the		Reliable with restrictions. Due to the study limitations, it is used as supporting information in a WoE.	Low	Du *et al.,* 2020

n=9) and Black-spotted frog *(Pelophylax nigromaculatus;* n=45 Samples collected in September-October 2011			frogs.				
QSAR predictions using the BCF Baseline model of CATALOGIC	BCF predictions for $C_{14}Cl_{2-11}$, $C_{15}Cl_{3-10}$ and $C_{16}Cl_{5-10}$ are over the threshold of log BCF 3.3 (BCF ~ 2000 L/kg) and/or log BCF 3.69 (BCF ~ 5000 L/kg)	B and/or vB			QSAR predictions are only used as supporting information to the experimental data. In case QSAR predictions are contradicting experimental data, a higher weight is given to the experimental data.	Low	The BCF Baseline model (v. 03.10) of CATALO-GIC (v.5.13.1.156) (LMC, 2018)

Annex XI – Brief summary of Human health hazard assessment

In the following, a brief summary of relevant information from the the human health risk assessment report produced under the Existing Substances Regulation EC (No.) 793/93 (HSE, 2008b) is provided. The cited risk assessment may 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 $BMDL_{10}$[28] of 36 mg/kg bw/day from this study.

- *Carcinogenicity*: No carcinogenicity studies have been conducted. MCCP are generally unreactive and not mutagenic. The carcinogenic potential of MCCP are expected to be similar – at least in qualitative terms – to that of SCCP, although direct read across is not appropriate. SCCP 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 MCCP might lead to kidney cancer in rats through a non-genotoxic mode of action. However, MCCP are not classified for this end point under Regulation EC No. 1272/2008.

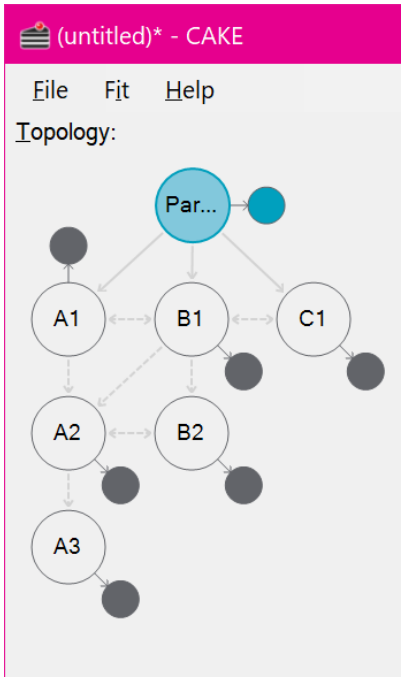
- *Toxicity to reproduction*: MCCP have no apparent effect upon fertility in rats up to approximately 400 mg/kg/day in the diet. No adverse developmental effects occurred during gestation in rats or rabbits in two conventional developmental studies using maternal doses up to 5 000 and 100 mg/kg/day, 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 MCCP 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 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 MCCP 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.

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

Annex XII – Outcome of the degradation kinetics performed on the OECD TG 308 study (Unpublished, 2019c)

The degradation kinetics of the OECD TG 308 study (Unpublished, 2019c) were performed using the CAKE software version 3.4. The model topology (see below figure) consisted in one compartment system which includes a parent substance and a sink.



The degradation rates for the testing material C_{14} chlorinated n-alkane, 50% Cl wt. (or Total C_{14}) and its constituting congener groups ($C_{14}Cl_{3\text{-}14}$) were derived using kinetic models such as the single first-order model (SFO) or bi-phasic models (the Gustafson & Holden model (FOMC), the Bi-exponential model or Double-First-Order in Parallel model (DFOP) and the Hockey-Stick Model (HS)). For C_{14} chlorinated n-alkane, 50% Cl wt. (or Total C_{14}) and each congener group of MCCP, the best fit kinetic model was used to derive a DT_{50} value. According to FOCUS (2014), the DT_{50} does not differentiate between transfer processes and degradation processes. Detailed information on degradation models (SFO, FOMC, DFOP and HS) can be found in the Generic Guidance Document for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration (FOCUS, 2014).

The OECD TG 308 study (Unpublished, 2019c) included a total of four datasets using two aerobic sediments and their associated waters: Brandywine Creek (Chadds Ford, Pennsylvania, USA) and Choptank River (Denton, Maryland, USA). As the FOCUS guidance (2014) recommends that for water-sediment studies a minimum of 6 sampling points are included, only two of the four datasets were used for deriving degradation rates (cf. datasets having measurements at days 0, 15, 30, 45, 60, 91 and 120). Furthermore, in accordance with FOCUS (2014), all samples below the limit of detection (LOD) were set to ½ LOD. No information on the limit of quantification is available in the study report. At each sampling point, true and independent replicates were available. The replicate values were used individually, and the degradation models were then fitted to all individual data points at the same time.

In order to decide if a model is acceptable, a visual assessment of the goodness of fit was performed. A visual evaluation was made for a plot of observed and calculated

concentrations vs. time and a plot of the residuals.

Furthermore, the χ^2-test was used as a tool to compare the goodness of fit of the four models (SFO, FOMC, DFOP and HS). The χ^2-test considers the deviations between measured and predicted values for each individual model relative to the uncertainty of the measurements. The measurement uncertainty is expressed as a % error that is used to scale the observed mean. The true error is unknown. The use of the test is to determine the smallest error value at which the test is passed at the 5% significance level. This error value is calculated for each model and the model with the smallest error is considered the most appropriate. The χ^2-test is particularly sensitive to replicates, so the mean of the observed replicate values was used for this statistical analysis and as recommended by FOCUS (2014). Ideally, the error value at which the χ^2-test is passed by the best-fit model (SFO, FOMC or DFOP) should be below 15% and the fit must be visually acceptable. However, this value should not be considered as an absolute cut-off criterion (FOCUS, 2014). There will be cases where the error value to pass the χ^2-test is higher, but the fit still represents a reasonable description of the degradation behaviour.

Furthermore, the FOCUS guidance (2014) recommends that a t-test (or examination of the confidence intervals) is used in order to assess the reliability of the individual rate parameter estimates of each model. If a parameter is not significantly different from zero, then the parameter is either very uncertain due to variability in the data or the model is not adequate with respect to the data. The parameter is considered significantly different from zero if the probability is smaller than 0.1 (i.e. considering a 10% significance level for water-sediment studies; FOCUS, 2014). Similarly, if zero is not included in the confidence interval, the parameter is significantly different from zero. Both, the t-test and the confidence interval give the same answer.

It is important to note that the DT_{50} values derived from the kinetic models were extrapolated beyond the experiment period of 120 days.

Table 69: Summary Table – Outcome of the calculations of the degradation kinetics of the OECD TG 308 study (Unpublished, 2019c) with the CAKE software for C14 chlorinated n-alkane, 50% Cl wt. testing material (or Total C14) and its constituting congener groups ($C_{14}Cl_{3-14}$)

	DT_{50} values in days from the best fit model												
Water-sediment system	$C_{14}Cl_3$	$C_{14}Cl_4$	$C_{14}Cl_5$	$C_{14}Cl_6$	$C_{14}Cl_7$	$C_{14}Cl_8$	$C_{14}Cl_9$	$C_{14}Cl_{10}$	$C_{14}Cl_{11}$	$C_{14}Cl_{12}$	$C_{14}Cl_{13}$	$C_{14}Cl_{14}$	Total C_{14}
Brandywine Creek	412 (SFO)	1760 (SFO)	3760 (SFO)	> 10,000 (SFO)	1110 (SFO)	590 (SFO)	3130 (SFO)	>120*	> 10,000 (HS)	>120*	> 10,000 (SFO)	> 10,000 (HS)	> 10,000 (SFO)
Choptank River	> 10,000 (SFO)	> 10,000 (DFOP)	> 10,000 (DFOP and HS)	> 10,000 (DFOP)	> 10,000 (SFO)	> 10,000 (SFO)	>120*		>120*		> 10,000 (SFO)	> 10,000 (SFO)	

*No decrease or no variation in the concentration was observed during the test duration of 120 days.

It is worth noting that the above DT_{50} values as reported in Table 69 should be interpreted with caution as these predictions were derived from parameters which are uncertain. For the DT_{50} values derived from kinetic models, it was found that parameters k, k_1 and/or k_2 do not differ significantly from zero, thus an absence of degradation for C_{14} chlorinated n-alkane, 50% Cl wt. and its constituting congener groups cannot be ruled out.

As an overall conclusion, the outcome of the degradation kinetics indicates that the testing material C_{14} chlorinated n-alkane, 50% Cl wt. (or Total C_{14}) and $C_{14}Cl_{3-14}$ congener groups of MCCP have DT_{50} values > 120 and/or 180 days in the water-sediment system at 12°C.

All the results for the different group of congeners of MCCP and C_{14} chlorinated n-alkane, 50% Cl wt. using the CAKE software are reported below:

C_{14} chlorinated n-alkane, 50 % Cl wt. (or Total C_{14}):

Results for the Water-Sediment system: Brandywine Creek

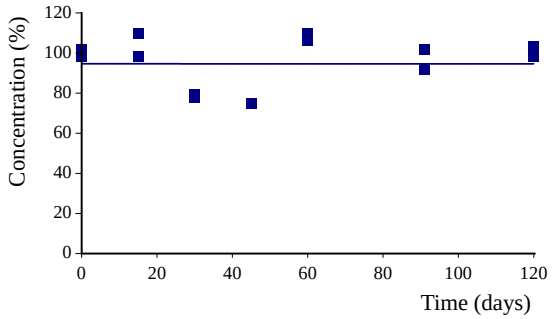
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obsved versus Predicted)	DT_{50} (days)	DT_{90} (days)
SFO	k =8.99E-014	0.5	-0.00208 — 0.002	10	5	0.02011	>10,000	>10,000
FOMC	α = 0.002272; β = 2.00E-011	NA* NA*	Nd — nd* Nd — nd*	10.7	4	0.02803	>10,000	>10,000
DFOP	k_1 =0.0992; k_2 =1.49E-011; g =0.07776	0.2612 ; 0.5; NA	-0.2342— 0.433 -0.00311— 0.003 -0.2333— 0.389	11.6	3	0.04755	>10,000 (overall DT_{50}); 6.99 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 =0; k_2 =0.007; t_b = 147.4	Nd* Nd* NA*	Nd — nd* Nd — nd* Nd — nd*	11.9	3	nd	251 (overall DT_{50}); >10,000 (k_1 DT_{50}); 104 (k_2 DT_{50})	493

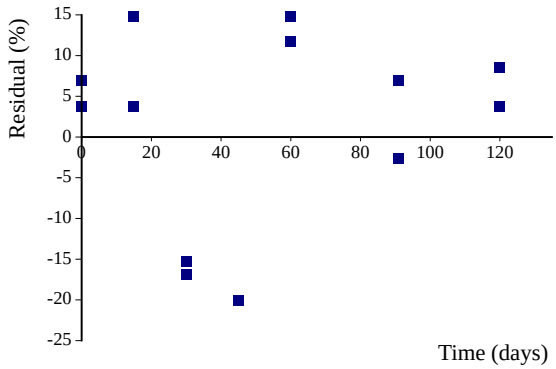
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

The SFO model is the best fit model (lowest χ^2-test value which is below 15%).

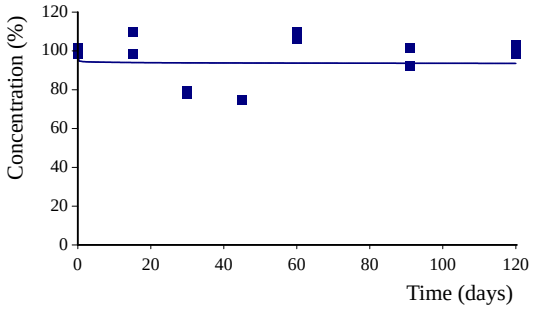
For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for C_{14} chlorinated n-alkane, 50% Cl wt. cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this testing material. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that C_{14} chlorinated n-alkane, 50% Cl wt. does not degrade significantly in the water-sediment system (DT_{50} >180 days).

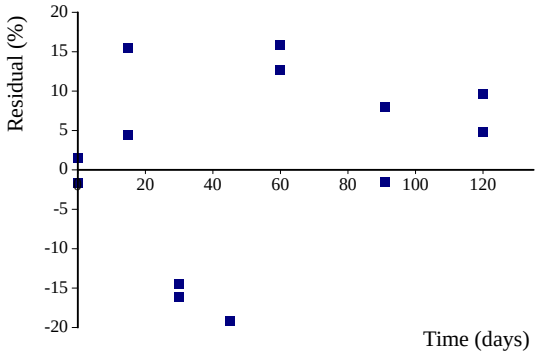
SFO model – Total C_{14}



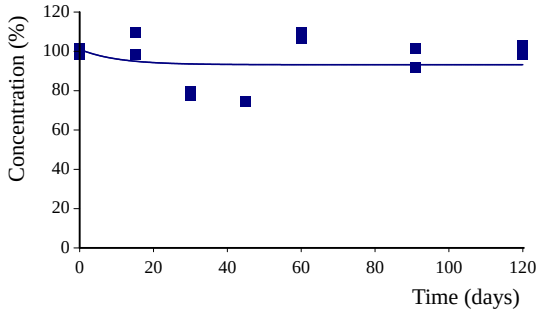


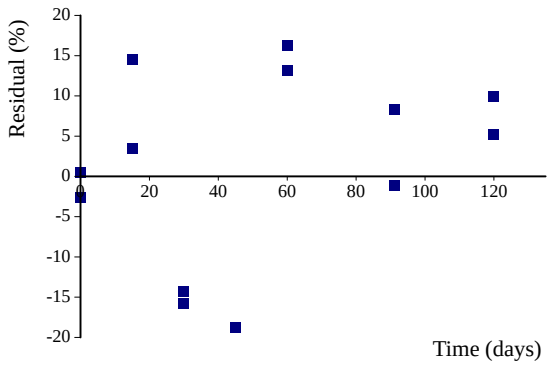
FOMC model – Total C_{14}



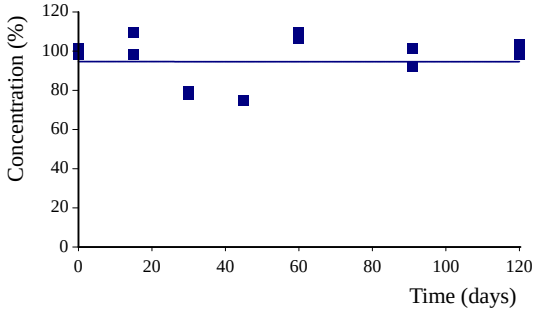


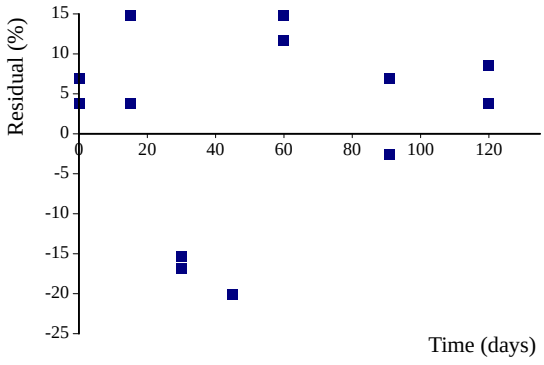
DFOP model– Total C_{14}





HS model – Total C_{14}





Results for the Water-Sediment system: Choptank River

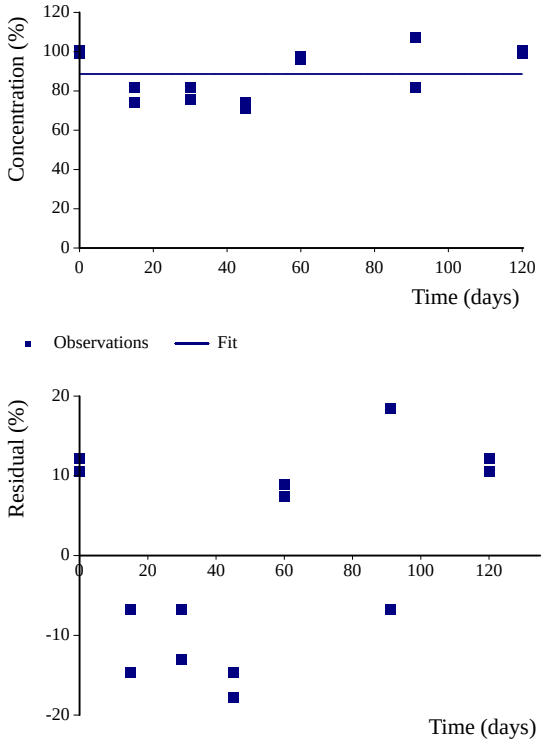
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obsved versus Predicted)	DT_{50} (days)	DT_{90} (days)
SFO	k =2.65E-013	0.5	-0.002182 — 0.002	9.79	5	0.1307	>10,000	>10,000
FOMC	α = 0.005076; β = 3.92E-010	NA* NA*	Nd — nd* Nd — nd*	9.84	4	0.1159	>10,000	>10,000
DFOP	k_1 =0.6727; k_2 = 0; g =0.1325	0.4711; 0.5; NA	-19.48 — 20.82; -0.002744 — 0.003; -0.1088 — 0.374	10.6	3	0.1472	>10,000 (overall DT_{50}); 1.03 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 =0; k_2 =0; t_b = 90.6	0.5 0.5 NA*	-0.002577 — 0.003; -0.00227 — 0.002; nd — nd*	11.7	3	Nd	>10,000 (overall DT_{50}); >10,000 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

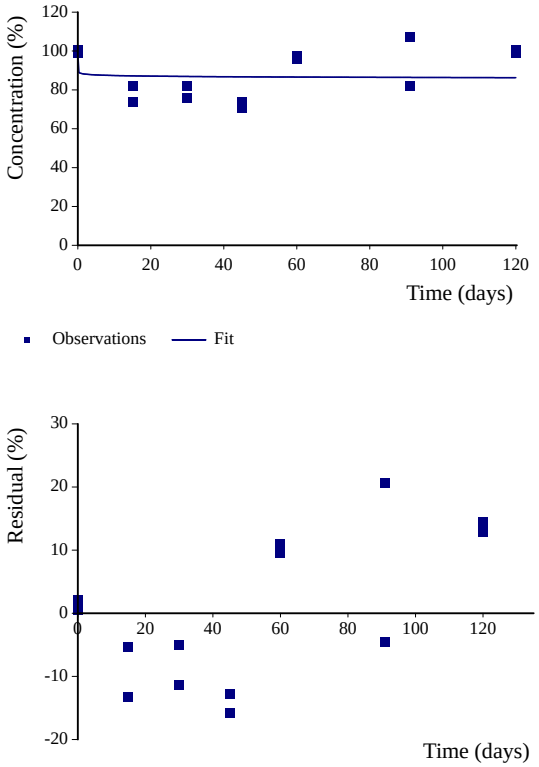
The SFO model is the best fit model (lowest χ^2-test value which is below 15%).

For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for C_{14} chlorinated n-alkane, 50% Cl wt. cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this testing material. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that C_{14} chlorinated n-alkane, 50% Cl wt. does not degrade significantly in the water-sediment system (DT_{50} >180 days).

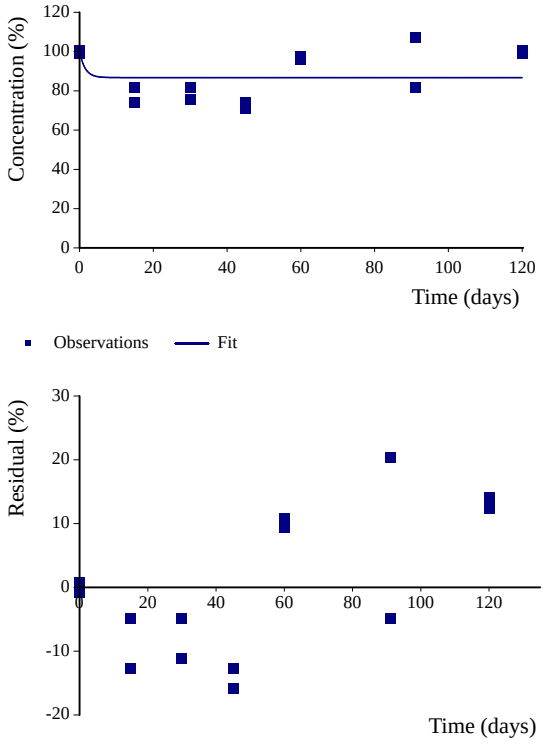
SFO model – Total C_{14}



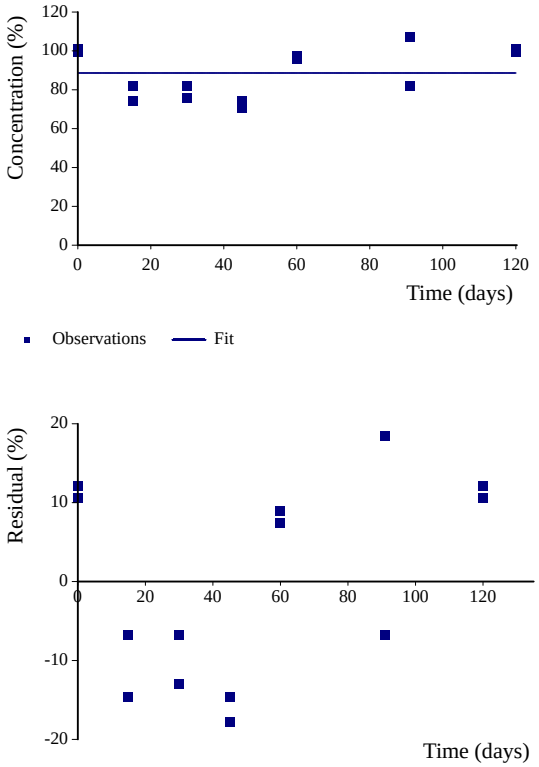
FOMC model – Total C_{14}



DFOP model– Total C_{14}



HS model – Total C_{14}



$C_{14}Cl_3$ congener group:

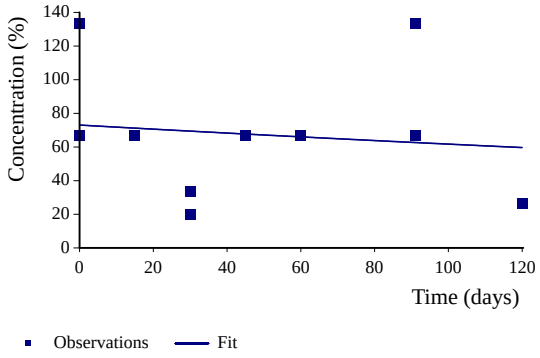
Results for the Water-Sediment system: Brandywine Creek

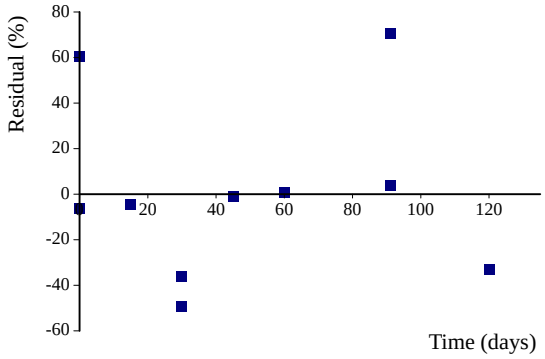
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k =0.001682	0.3471	-0.007489 — 0.011	32.5	5	0.01422	412	1370
FOMC	α = 0.02531; β = 3.07E-007	NA* NA*	Nd — nd* Nd — nd*	31.6	4	0.1693	>10,000	>10,000
DFOP	k_1 = 0.2017; k_2 = 2.01E-008; g = 0.386	0.4377; 0.5; NA	-2.625 — 3.028; -0.01556 — 0.016; -0.3789 — 1.151	34.6	3	0.1806	>10,000 (overall DT_{50}); 3.44 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.02703; k_2 = 6.07E-030; t_b = 18.44	0.1958; 0.5; NA	-0.04091 — 0.095; -0.01504 — 0.015; -30.56 — 67.45	34.4	3	0.1834	>10,000 (overall DT_{50}); 25.6 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.
One outlier was deleted at day 120 (but another replicate is available at day 120) as this concentration was a factor 10 times higher than the concentration observed at day 0.

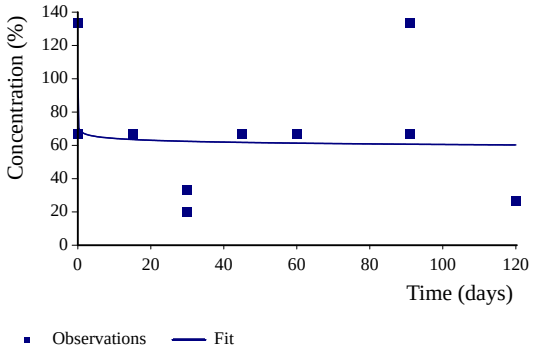
Improvement of χ^2 statistics for FOMC (31.6%) compared to the SFO model. However, it was not possible to assess the reliability of its individual rate parameter estimates (α and β) as no confidence interval and t-test are available. The covariance matrix used for describing parameter uncertainty can not be estimated by CAKE, due to the large correlation of parameters α and β in this fit. That is why the SFO model was the model selected for the prediction of the DT_{50} value for the $C_{14}Cl_3$ congener group, however, χ^2-test is >15%. For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_3$ congener group cannot be ruled out. A DT_{50} of 412 days is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_3$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

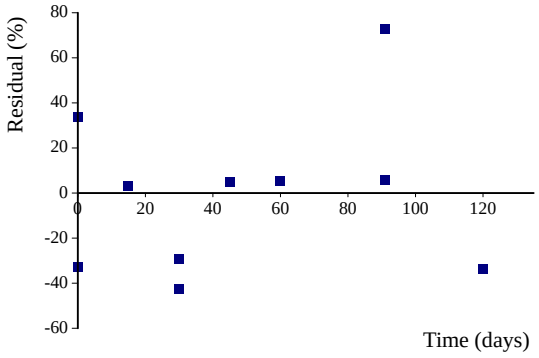
SFO model – $C_{14}Cl_3$



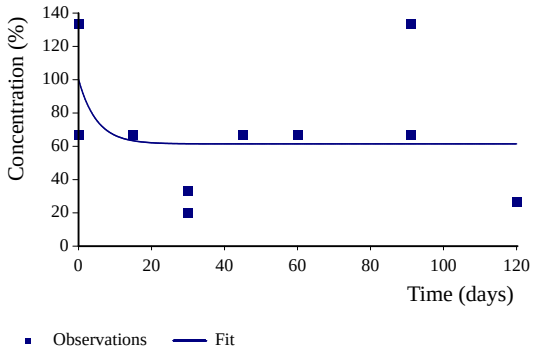


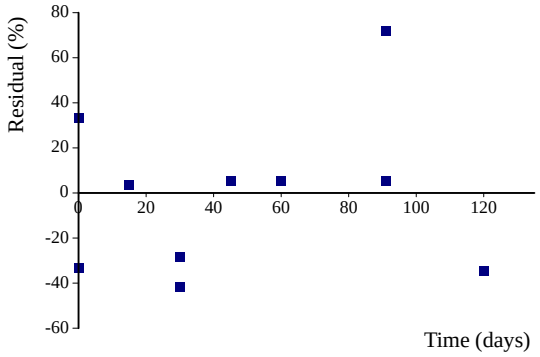
FOMC model – $C_{14}Cl_3$



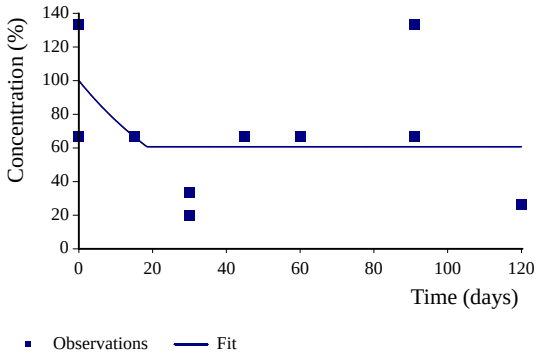


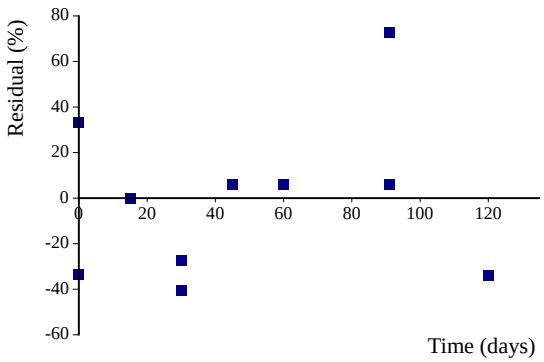
DFOP model– $C_{14}Cl_3$





HS model – $C_{14}Cl_3$





Results for the Water-Sediment system: Choptank River

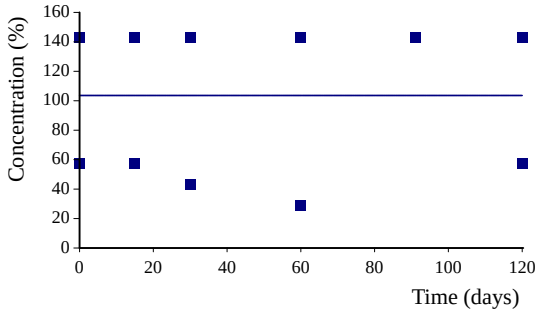
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 1.14E-014	0.5	-0.007562 — 0.008	14.1	4	0.02021	>10,000	>10,000
FOMC	α = 1.35E-009; β = 0.01766	NA* NA*	Nd— nd* Nd — nd*	15.5	3	0.006324	>10,000	>10,000
DFOP	k_1 = 0.1911; k_2 = 0; g = 0	Nd*; 0.5; NA*	Nd— nd* -0.008701 — 0.009; 0 — 0	17.7	2	nd	>10,000 (overall DT_{50}); 3.63 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0; k_2 = 0; t_b = 6.512	0.5; 0.5; NA*	-0.001065 — 0.001; -0.008964 — 0.009; nd — nd*	17.7	2	nd	>10,000 (overall DT_{50}); >10,000 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

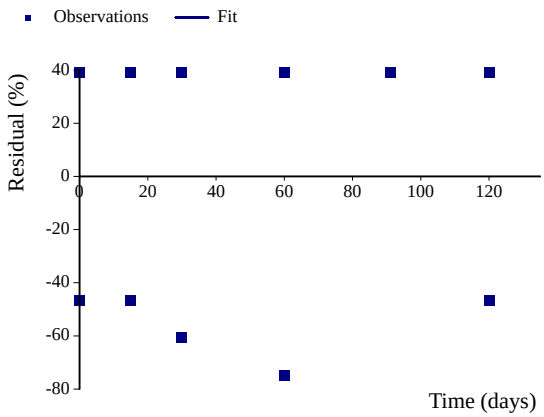
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

The SFO model is the best fit model (lowest χ^2-test value which is below 15%).

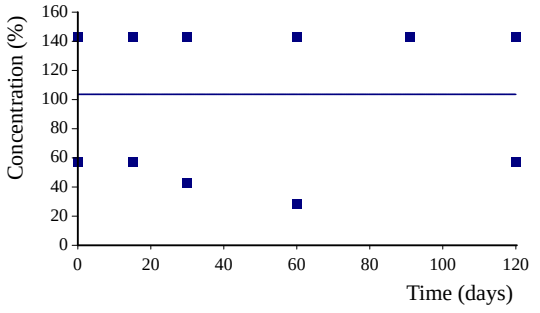
For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_3$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_3$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

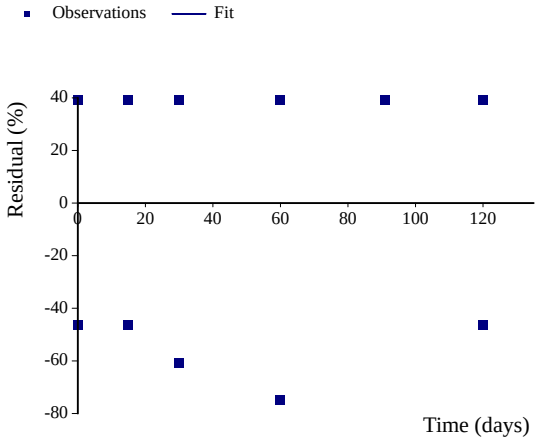
SFO model – $C_{14}Cl_3$



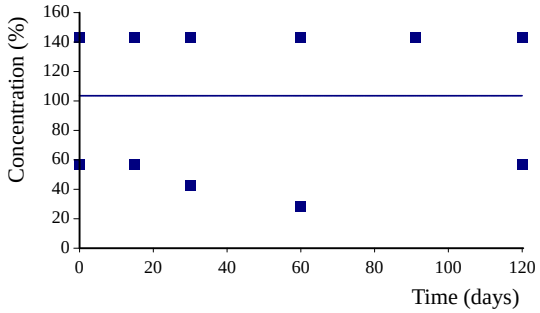


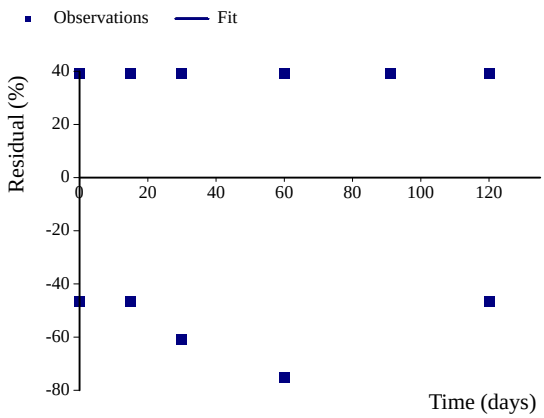
FOMC model – $C_{14}Cl_3$



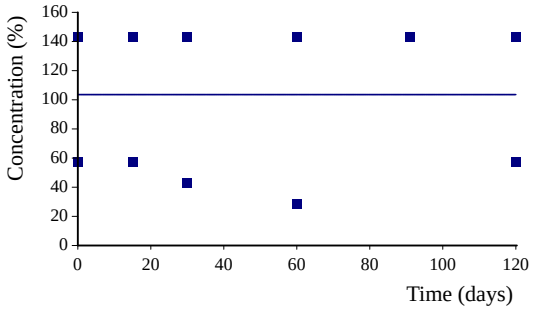


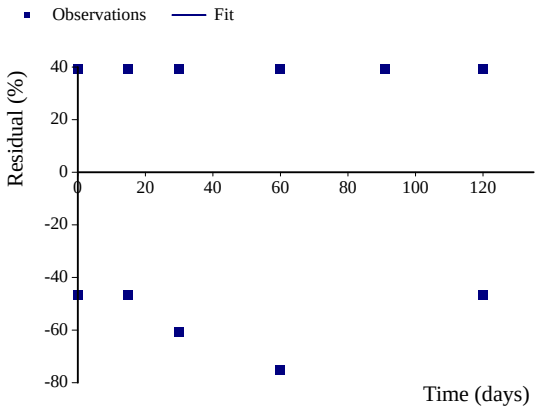
DFOP model– $C_{14}Cl_3$





HS model – $C_{14}Cl_3$





$C_{14}Cl_4$ congener group:

Results for the Water-Sediment system: Brandywine Creek

Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 3.95E-004	0.4704	-0.01102 — 0.012	36.1	5	0.000483	1760	5840
FOMC	α = 1.39E-008; β = 0.02103	NA*; NA*	Nd — nd* Nd — nd*	38.9	4	0.001094	>10,000	>10,000
DFOP	k_1 = 0.03892; k_2 = 4.88E-008; g = 0.1486	0.484; 0.5; NA	-2.098 — 2.176; -0.06633 — 0.066; -5.964 — 6.262	42.6	3	0.008152	>10,000 (overall DT_{50}); 17.8 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.005985; k_2 =7.25E-011; t_b =44.74	0.3123; 0.5; NA	-0.02074 — 0.033; -0.02332 — 0.023; 14.75 — 74.74	41.6	3	0.03265	>10,000 (overall DT_{50}); 116 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

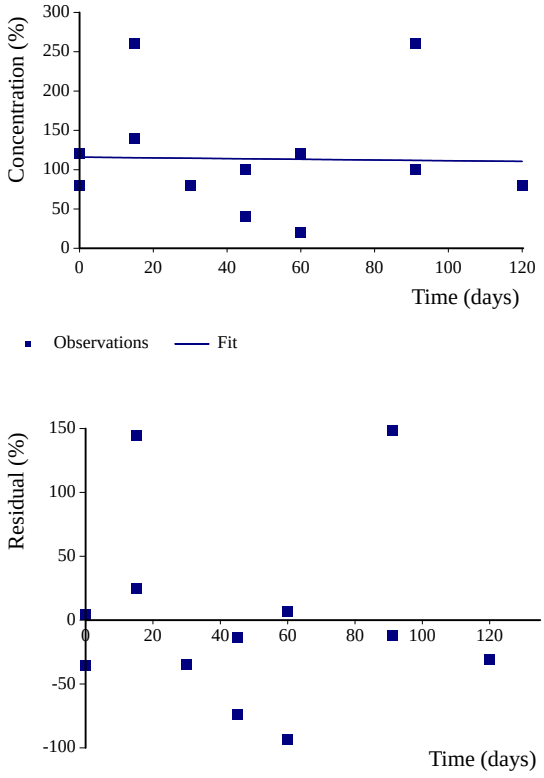
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

One outlier was deleted at day 120 (but another replicate is available at day 120) as this concentration was a factor ca. 5 times higher than the concentration observed at day 0.

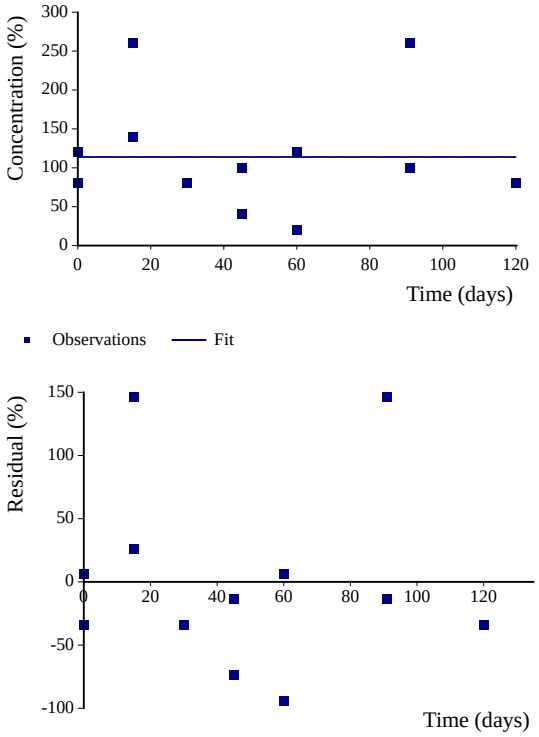
The SFO model is the best fit model, however, χ^2-test is >15%.

For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_4$ congener group cannot be ruled out. A DT_{50} of 1760 days is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_4$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

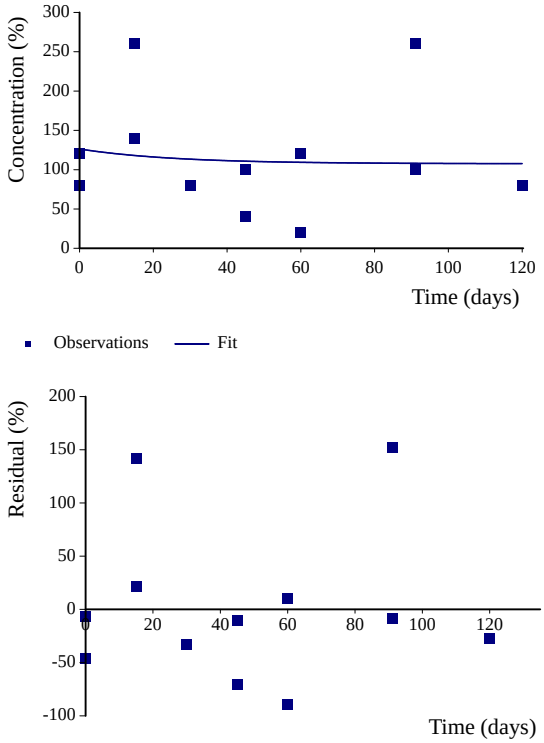
SFO model – $C_{14}Cl_4$



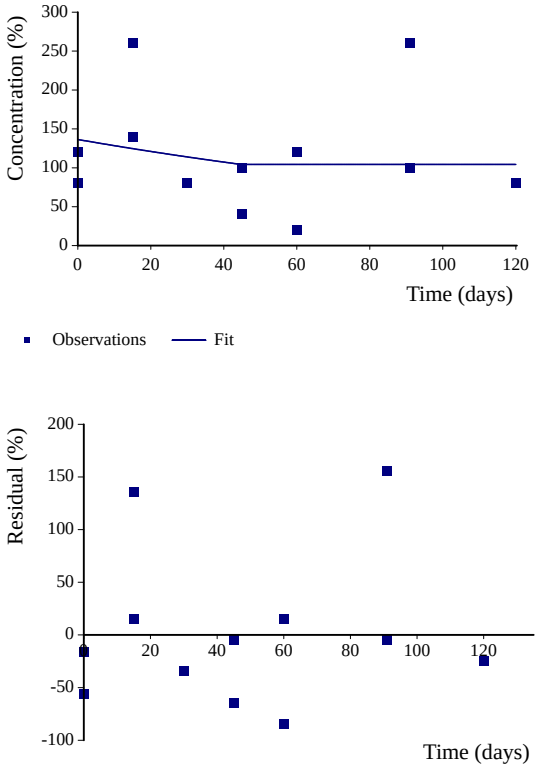
FOMC model – $C_{14}Cl_4$



DFOP model– $C_{14}Cl_4$



HS model – $C_{14}Cl_4$



Results for the Water-Sediment system: Choptank River

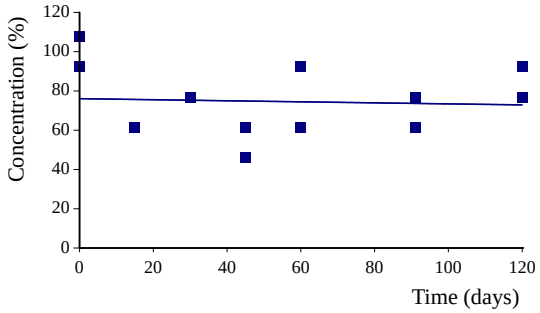
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 3.54E-004	0.4149	-0.003154 — 0.004	14.9	5	0.003585	1960	6510
FOMC	α = 0.01829; β = 2.88E-007	NA*; NA*	Nd — nd* Nd — nd*	11.5	4	0.3683	>10,000	>10,000
DFOP	k_1 = 0.74; k_2 = 0; g = 0.2951	0.4749; 0.5; NA	-24.78 — 26.26; -0.003855 — 0.004; -0.04759 — 0.543	12.1	3	0.401	>10,000 (overall DT_{50}); 0.937 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.02418; k_2 =1.24E-012; t_b =14.46	Nd*; 0.5; NA*	Nd — nd*; -0.00388 — 0.004; Nd — nd*	12.1	3	0.401	>10,000 (overall DT_{50}); 28.7 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

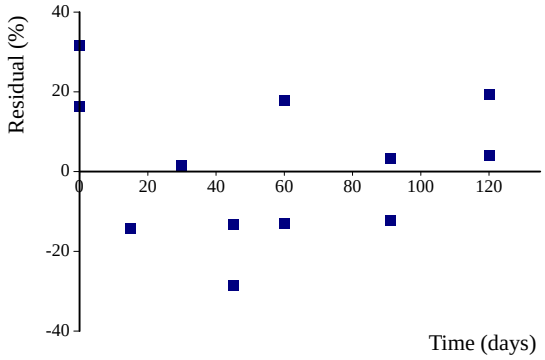
Improvement of χ^2 statistics for FOMC (11.5%), DFOP (12.1%) and HS (12.1%) compared to the SFO model. However, for the FOMC and HS models, it was not possible to assess the reliability of the individual rate parameter estimates (α and β; k_1 and t_b) as no confidence interval and t-test are available. That is why the DFOP model was the model selected for the prediction of the DT_{50} value for the $C_{14}Cl_4$ congener group (χ^2-test is <15%).

For this model, the parameters k_1 and k_2 do not differ significantly from zero as zero is included in the confidence interval, thus an absence of degradation for the $C_{14}Cl_4$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameters (k_1, k_2 and g) which are uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_4$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

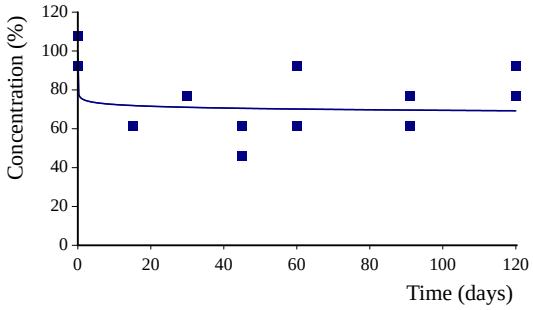
SFO model – $C_{14}Cl_4$



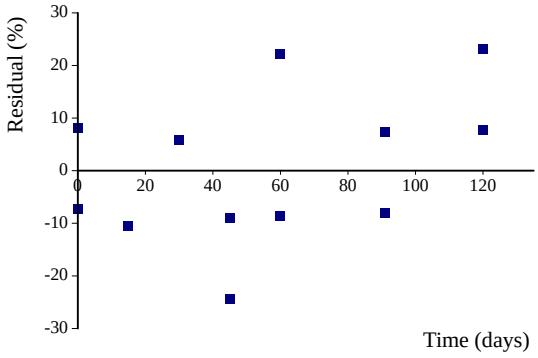
Observations Fit



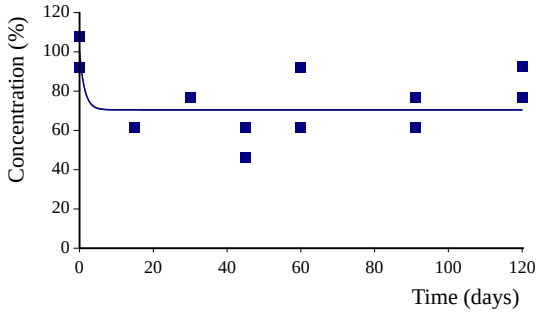
FOMC model – $C_{14}Cl_4$



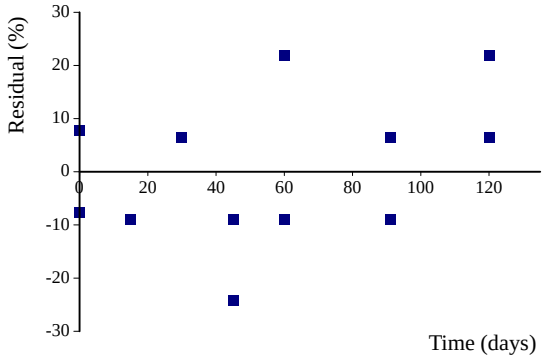
Observations Fit



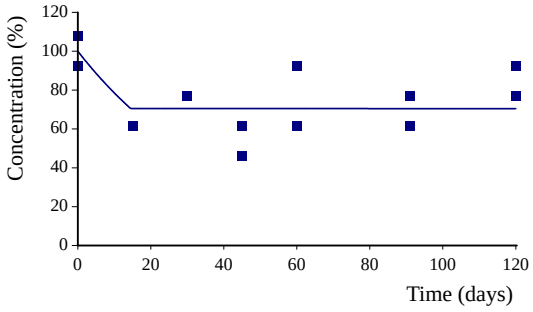
DFOP model– $C_{14}Cl_4$



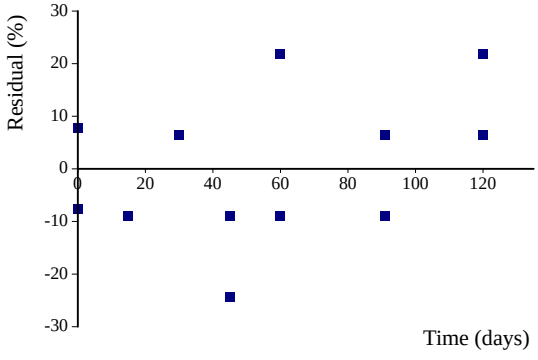
Observations Fit



HS model – $C_{14}Cl_4$



Observations Fit



$C_{14}Cl_5$ congener group:

Results for the Water-Sediment system: Brandywine Creek

Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 1.84E-004	0.4654	-0.004373 — 0.005	15.1	5	0.0007292	3760	>10,000
FOMC	α = 0; β = 0.01494	NA*; NA*	0 — 0 Nd — nd*	16.3	4	Nd	>10,000	>10,000
DFOP	k_1 = 0.0302; k_2 = 1.10E-004; g = 0.009199	0.4761; 0.492; NA	-1.078 — 1.138; -0.01196 — 0.012; -1.361 — 1.379	17.9	3	0.0007576	6220 (overall DT_{50}); 23 (k_1 DT_{50}); 6310 (k_2 DT_{50})	>10,000
HS	k_1 = 3.93E-008; k_2 =1.85E-004; t_b =0.07207	0.5; 0.4681; NA	-0.06167 — 0.062; -0.004895 — 0.005; -0.3324 — 0.477	17.8	3	0.0007354	3750 (overall DT_{50}); >10,000 (k_1 DT_{50}); 3750 (k_2 DT_{50})	>10,000

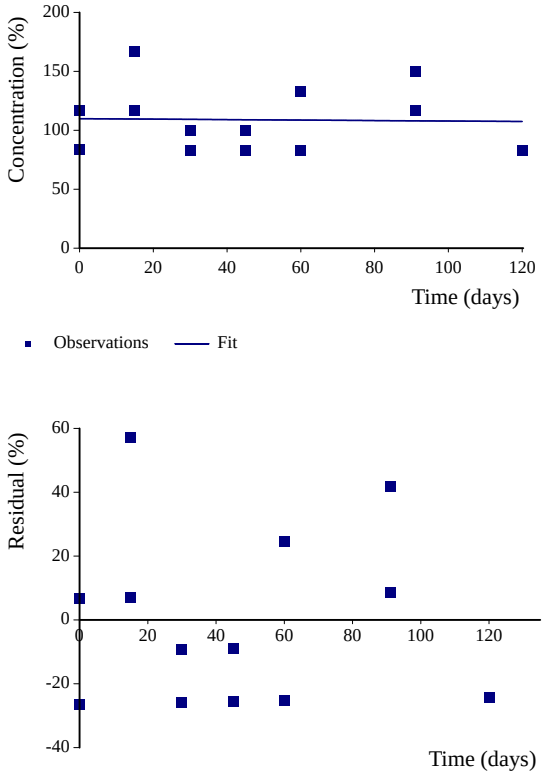
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

One outlier was deleted at day 120 (but another replicate is available at day 120) as this concentration was a factor ca. 2.5 times higher than the concentration observed at day 0.

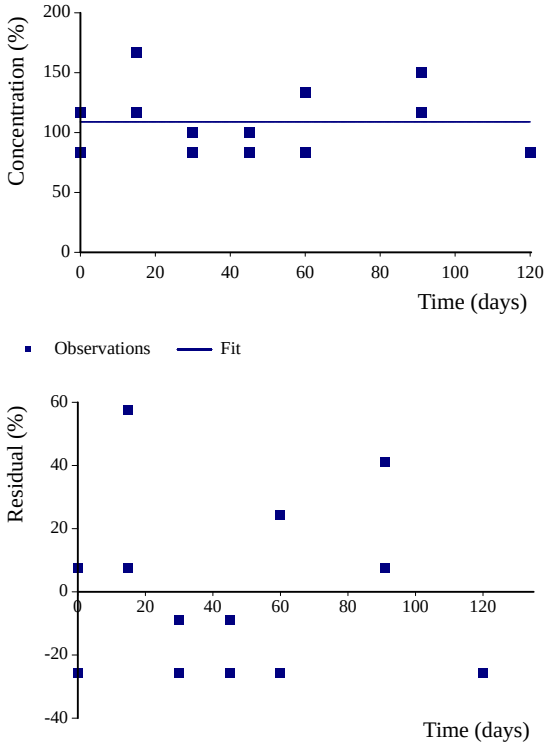
The SFO model is the best fit model, however, χ^2-test is slightly >15%.

For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_5$ congener group cannot be ruled out. A DT_{50} of 3760 days is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_5$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

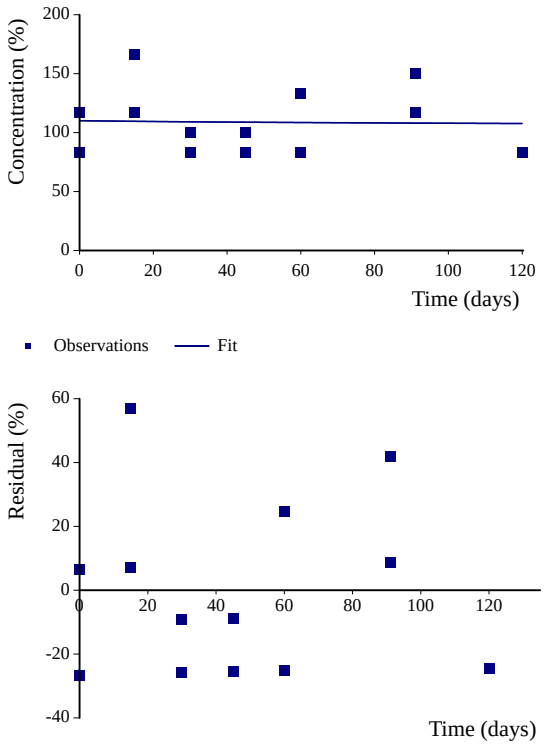
SFO model – $C_{14}Cl_5$



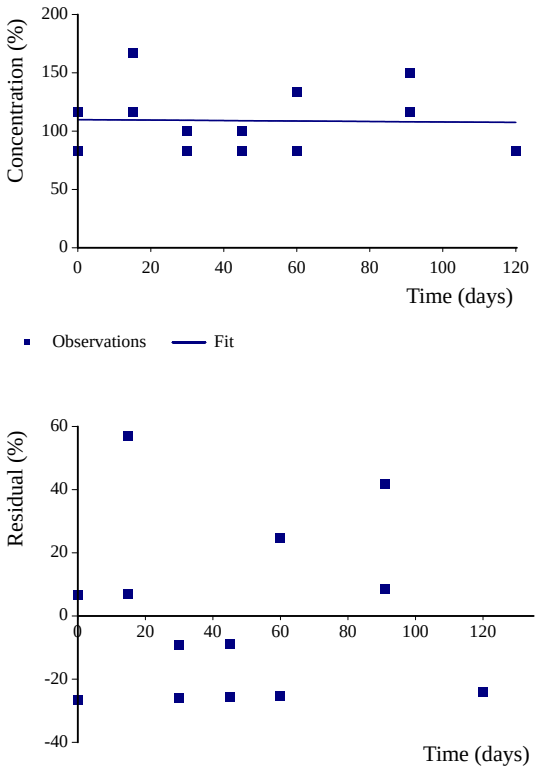
FOMC model – $C_{14}Cl_5$



DFOP model– $C_{14}Cl_5$



HS model – $C_{14}Cl_5$



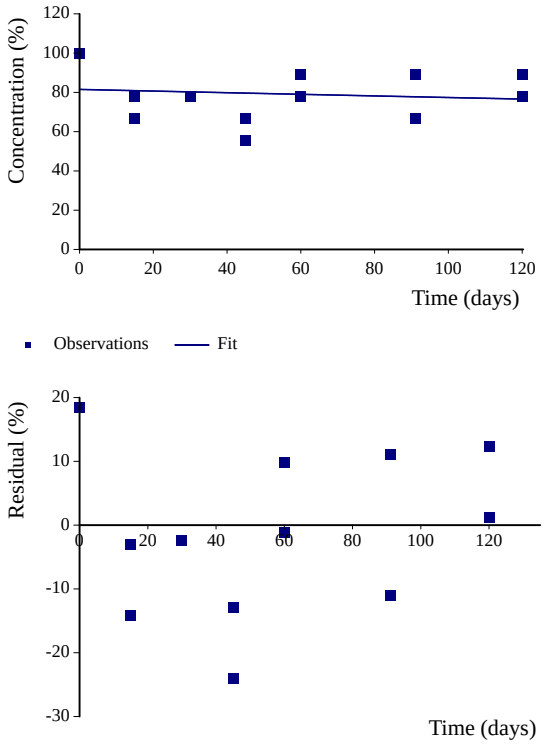
Results for the Water-Sediment system: Choptank River

Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 5.17E-004	0.3314	-0.002003 — 0.003	10.9	5	0.01527	1340	4450
FOMC	α = 0.01045; β = 1.52E-010	NA*; NA*	Nd — nd*; Nd — nd*	8.03	4	0.4329	>10,000	>10,000
DFOP	k_1 = 0.692; k_2 = 0; g = 0.2405	0.4727; 0.5; NA	-21.25 — 22.64; -0.002573 — 0.003; 0.05291 — 0.428	8.43	3	0.4544	>10,000 (overall DT_{50}); 1 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.0189; k_2 =1.38E-011; t_b =14.56	0.2365; 0.5; NA*	-0.03757 — 0.075; -0.002612 — 0.003; -29.1 — 58.21	8.43	3	0.4544	>10,000 (overall DT_{50}); 36.7 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

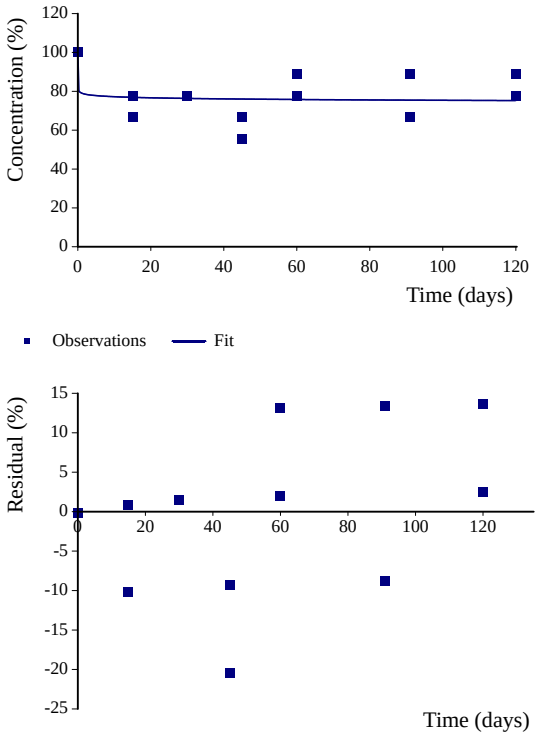
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

Improvement of χ^2 statistics for FOMC (8.03%), DFOP (8.43%) and HS (8.43%) compared to the SFO model. However, for the FOMC model, it was not possible to assess the reliability of its individual rate parameter estimates (α and β) as no confidence interval and t-test are available. That is why the DFOP and HS models were selected for the prediction of the DT_{50} value for the $C_{14}Cl_5$ congener group (χ^2-test is <15%).
For these models, the parameters k_1 and k_2 do not differ significantly from zero as zero is included in the confidence interval, thus an absence of degradation for the $C_{14}Cl_5$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group using these models. However, this prediction is derived from parameters (k_1 and k_2) which are uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_5$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

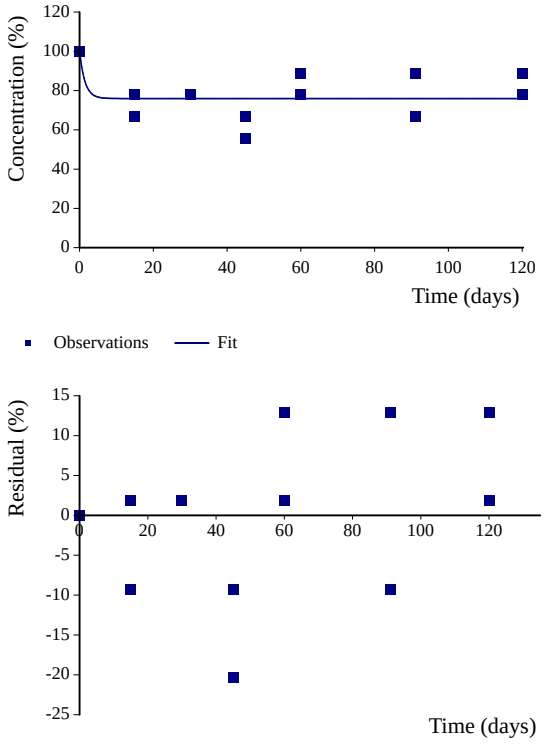
SFO model – $C_{14}Cl_5$



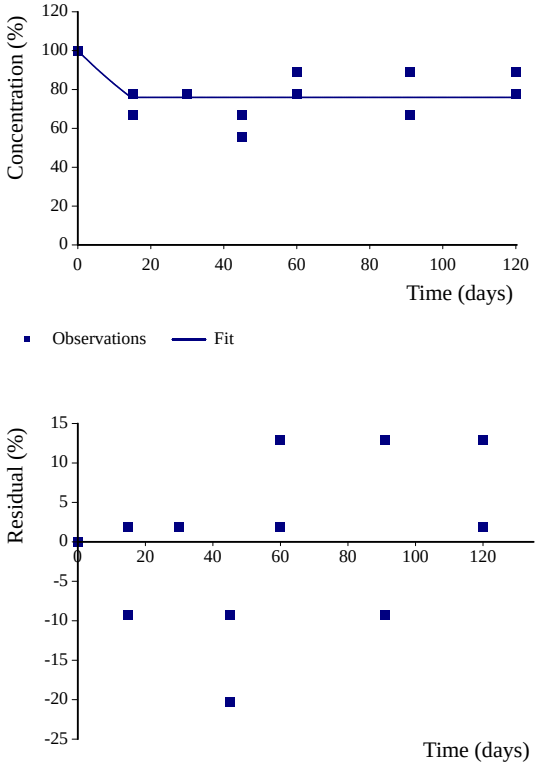
FOMC model – $C_{14}Cl_5$



DFOP model– $C_{14}Cl_5$



HS model – $C_{14}Cl_5$



$C_{14}Cl_6$ congener group:

Results for the Water-Sediment system: Brandywine Creek

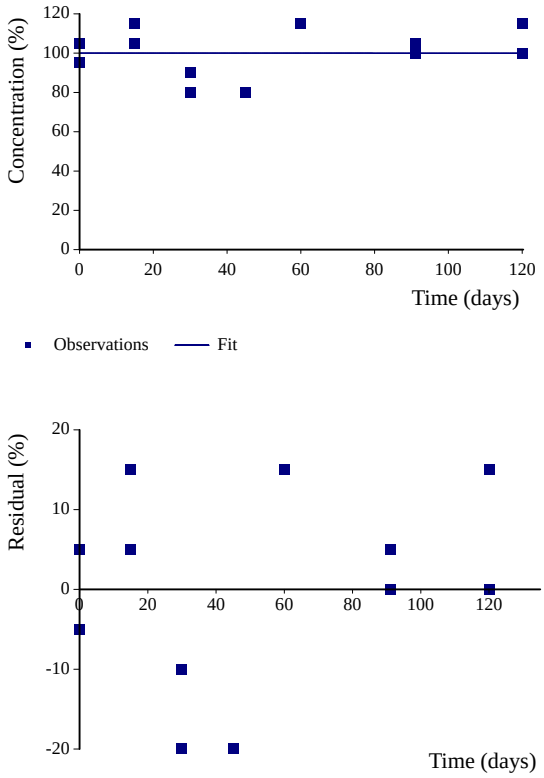
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 1.02E-018	0.5	-0.002051 — 0.002	9.56	5	nd	>10,000	>10,000
FOMC	α = 0; β = 0.009228	NA*; NA*	0 — 0; Nd — nd*	10.3	4	Nd*	>10,000	>10,000
DFOP	k_1 = 0.0936; k_2 = 9.40E-012; g = 0.0159	0.391; 0.5; NA	-0.64 — 0.827; -0.003066 — 0.003; -0.3259 — 0.358	11.4	3	0.001837	>10,000 (overall DT_{50}); 7.41 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0; k_2 =0.001446; t_b =133.3	0.5; 8.25E-014; NA	-0.00231 — 0.002; -0.001384 — 0.002; -106.3 — 372.8	11.4	3	0.05707	613 (overall DT_{50}); >10,000 (k_1 DT_{50}); 479 (k_2 DT_{50})	1730

* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

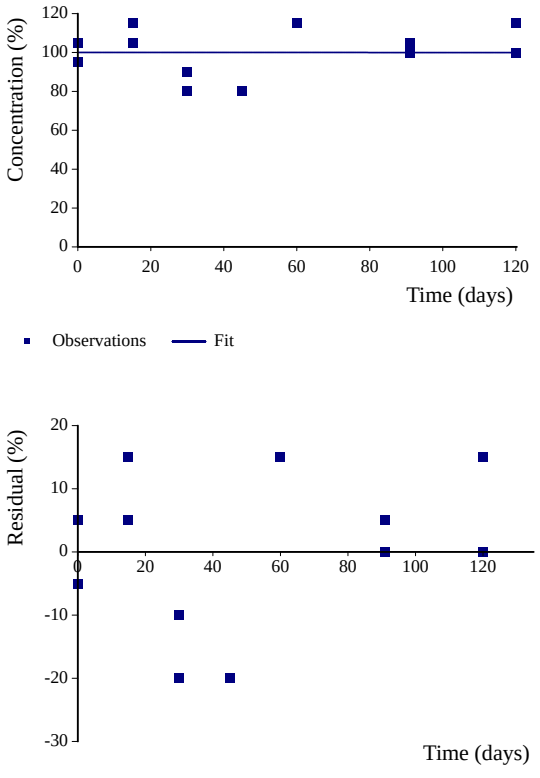
The SFO model is the best fit model (lowest χ^2-test value which is below 15%).

For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_6$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_6$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

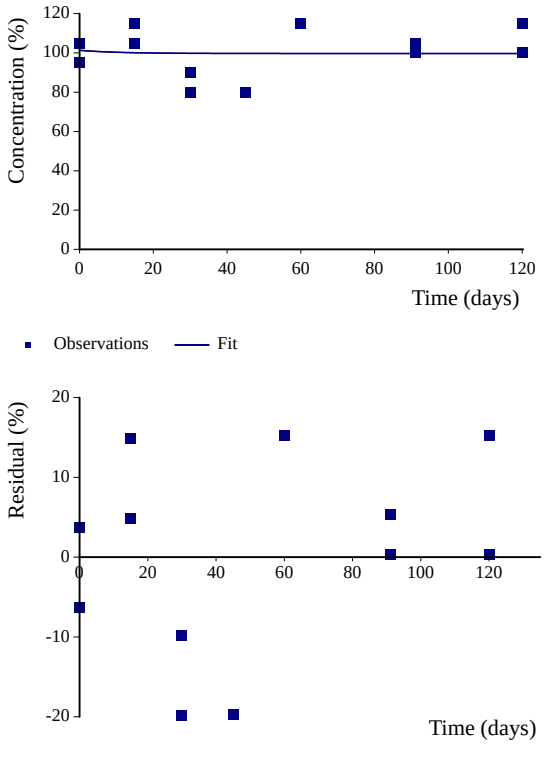
SFO model – $C_{14}Cl_6$



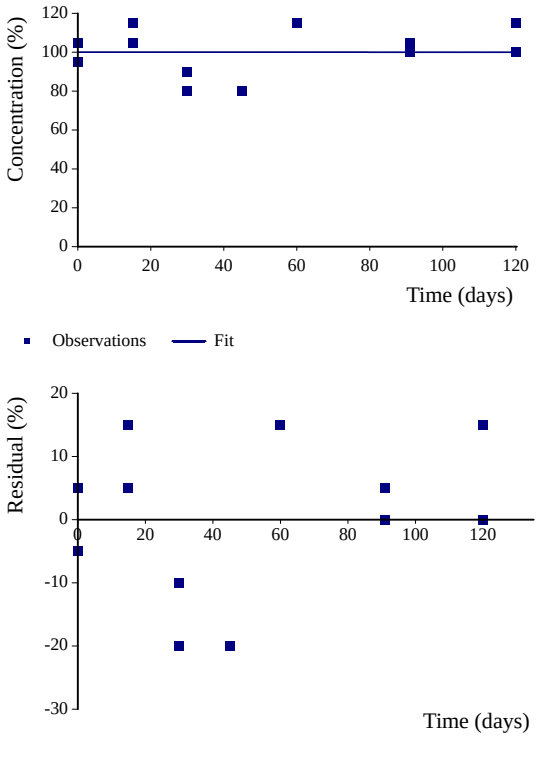
FOMC model – $C_{14}Cl_6$



DFOP model– $C_{14}Cl_6$



HS model – $C_{14}Cl_6$



Results for the Water-Sediment system: Choptank River

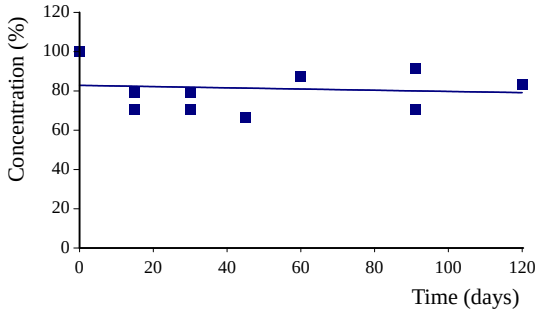
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 3.81E-004	0.353	-0.001765 — 0.003	9.62	5	0.01163	1820	6050
FOMC	α = 0.009365; β = 1.18E-010	NA*; NA*	Nd — nd*; Nd — nd*	6.91	4	0.4675	>10,000	>10,000
DFOP	k_1 = 0.8166; k_2 = 2.68E-013; g = 0.2187	0.4876; 0.5; NA	-56.24 — 57.88; -0.002082 — 0.002; 0.05939 — 0.378	7.31	3	0.4943	>10,000 (overall DT_{50}); 0.849 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 5.76E-004; k_2 =0; t_b =80.31	0.1546; Nd*; NA*	-0.0006216 — 0.002; Nd — nd*; Nd — nd*	11.5	3	0.03367	>10,000 (overall DT_{50}); 1210 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

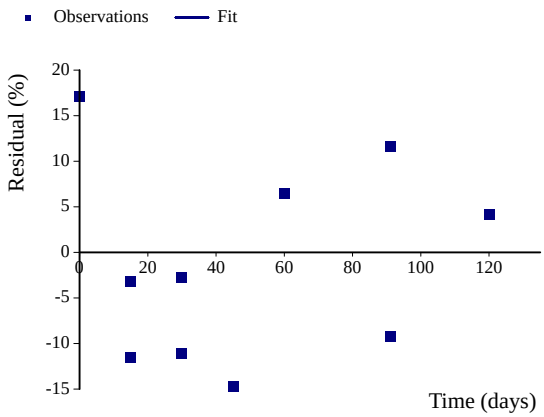
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

Improvement of χ^2 statistics for FOMC (6.91%) and DFOP (7.31%) compared to the SFO model. However, for the FOMC model, it was not possible to assess the reliability of its individual rate parameter estimates (α and β) as no confidence interval and t-test are available. The covariance matrix used for describing parameter uncertainty can not be estimated by CAKE, due to the large correlation of parameters α and β in this fit. That is why the DFOP model was selected for the prediction of the DT_{50} value for the $C_{14}Cl_6$ congener group (χ^2-test is <15%).

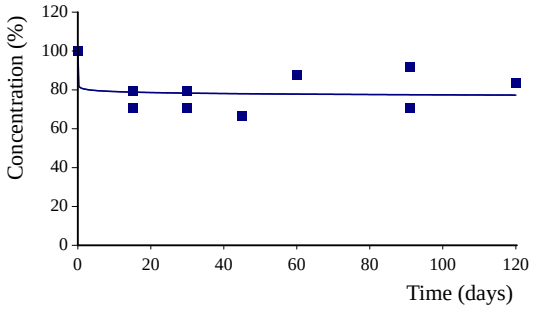
For this model, the parameters k_1 and k_2 do not differ significantly from zero as zero is included in the confidence interval, thus an absence of degradation for the $C_{14}Cl_6$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group using this model. However, this prediction is derived from parameters (k_1 and k_2) which are uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_6$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

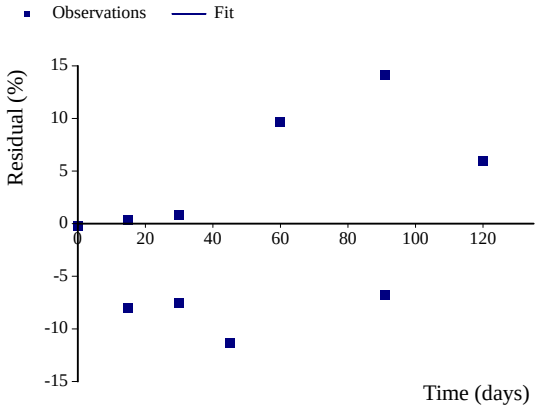
SFO model – $C_{14}Cl_6$



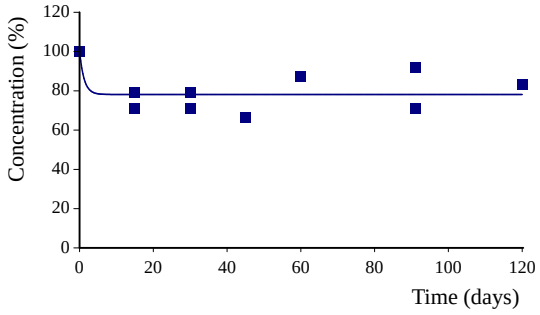


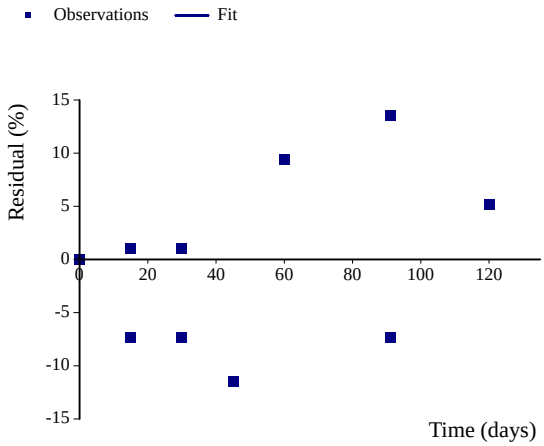
FOMC model – $C_{14}Cl_6$



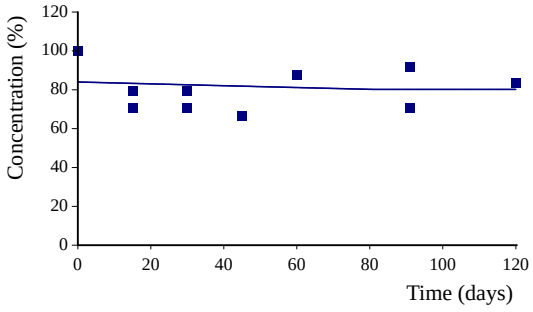


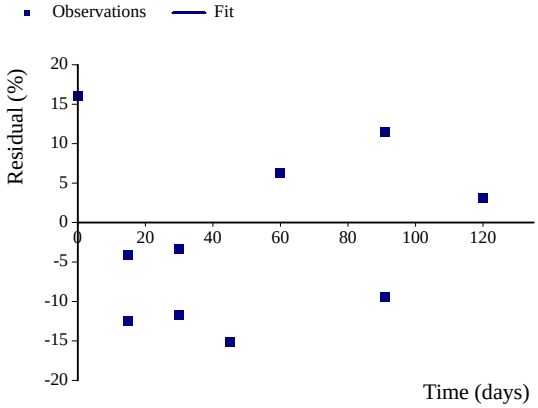
DFOP model– $C_{14}Cl_6$





HS model – $C_{14}Cl_6$





$C_{14}Cl_7$ congener group:

Results for the Water-Sediment system: Brandywine Creek

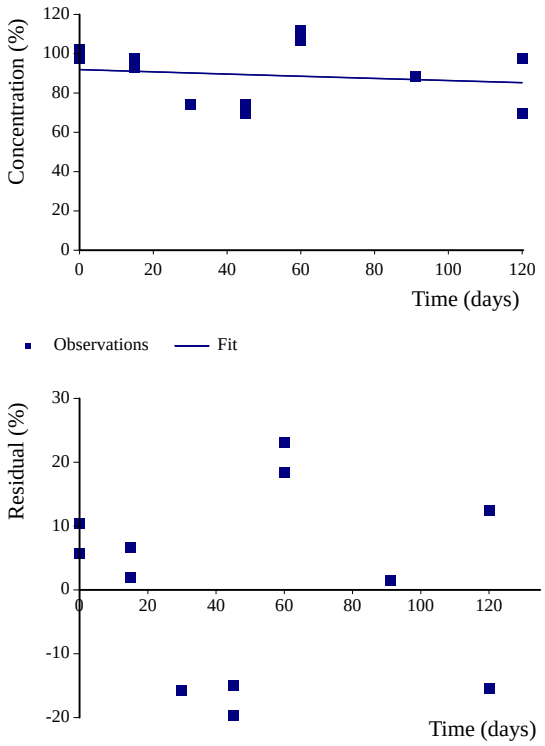
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 6.25E-004	0.2951	-0.001836 — 0.003	11	5	0.02476	1110	3680
FOMC	α = 0.007517; β = 6.30E-007	NA*; NA*	nd* nd*	11.3	4	0.1056	>10,000	>10,000
DFOP	k_1 = 0.1077; k_2 = 3.67E-007; g = 0.1401	0.393; 0.4999; NA	-0.7533 — 0.969; -0.004725 — 0.005; -0.2529 — 0.533	12.3	3	0.1235	>10,000 (overall DT_{50}); 6.43 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 3.60E-004; k_2 =0.001915; t_b =92.56	0.4258; 0.4429; NA	-0.003812 — 0.005; -0.02704 — 0.031; -434.2 — 619.3	13.1	3	0.02907	437 (overall DT_{50}); 1930 (k_1 DT_{50}); 362 (k_2 DT_{50})	1280

* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

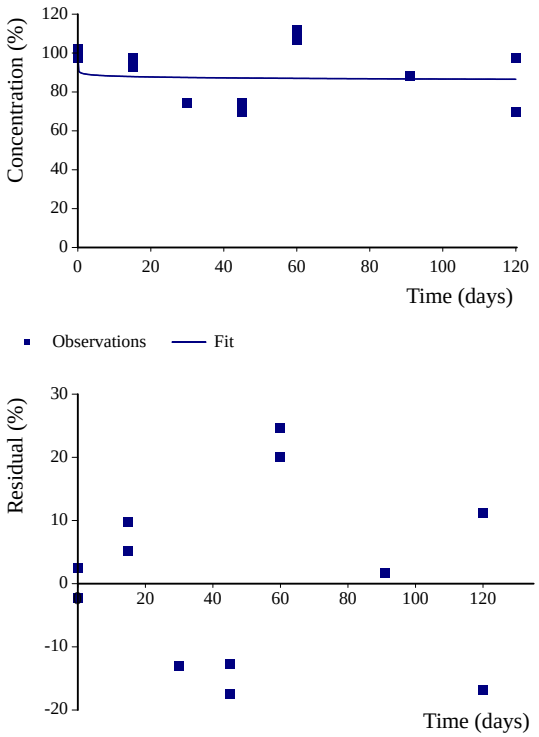
The SFO model is the best fit model (lowest χ^2-test value which is below 15%).

For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_7$ congener group cannot be ruled out. A DT_{50} of 1110 days is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_7$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

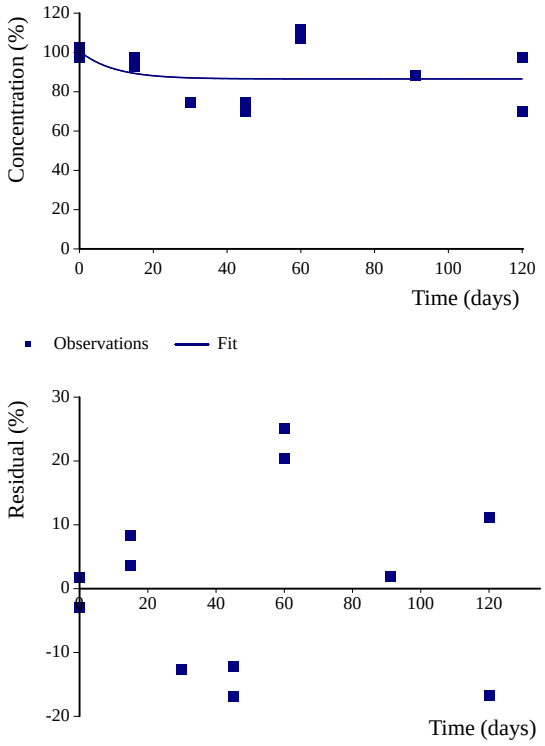
SFO model – $C_{14}Cl_7$



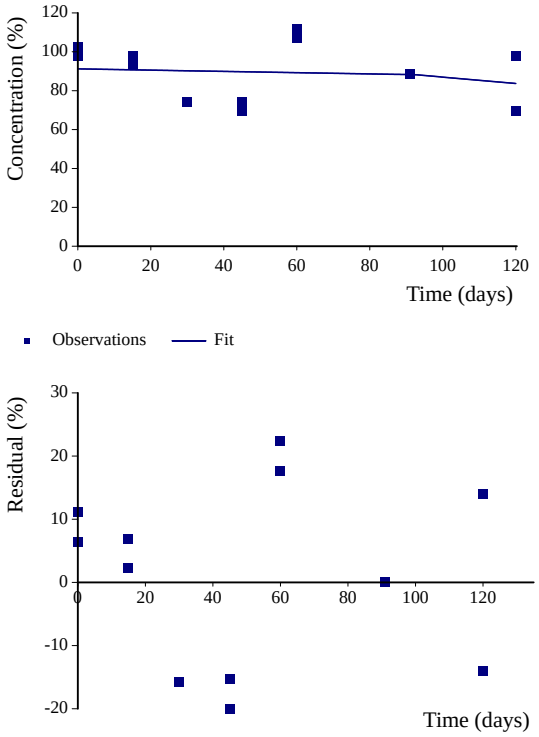
FOMC model – $C_{14}Cl_7$



DFOP model– $C_{14}Cl_7$



HS model – $C_{14}Cl_7$



Results for the Water-Sediment system: Choptank River

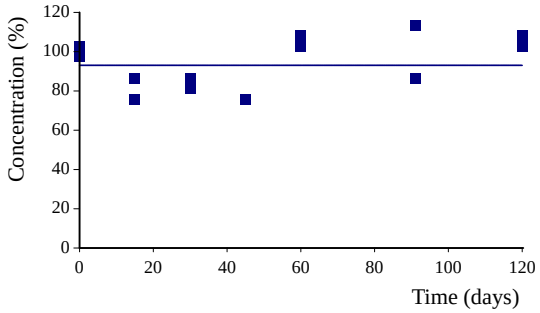
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 1.74E-021	0.5	-0.002225—0.002	9.7	5	nd	>10,000	>10,000
FOMC	α = 0.002653; β = 6.98E-012	NA*; NA*	Nd — nd* Nd — nd*	10.3	4	0.03232	>10,000	>10,000
DFOP	k_1 = 0.6461; k_2 = 0; g = 0.08098	0.4735; 0.5; NA	-20.48 — 21.77; -0.00292 — 0.003; -0.2009 — 0.363	11.2	3	0.04797	>10,000 (overall DT_{50}); 1.07 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0; k_2 =0.003874; t_b = 127	0.5; Nd*; NA*	-0.00254 — 0.003; nd — nd*; 110.4 — 143.6	11.5	3	0.1518	306 (overall DT_{50}); >10,000 (k_1 DT_{50}); 179 (k_2 DT_{50})	721

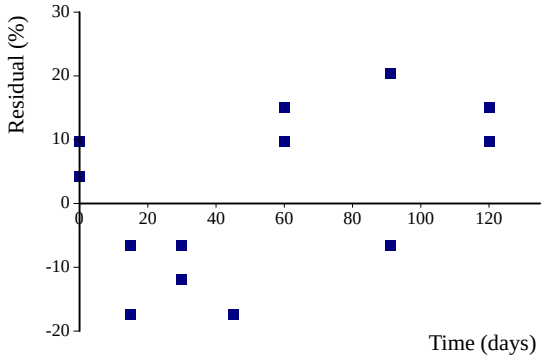
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

The SFO model is the best fit model (lowest χ^2-test value which is below 15%).

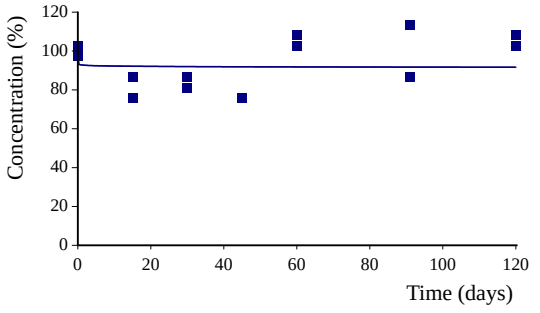
For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_7$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_7$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

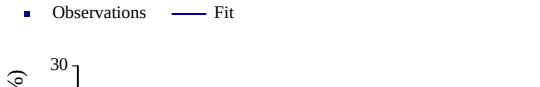
SFO model – $C_{14}Cl_7$

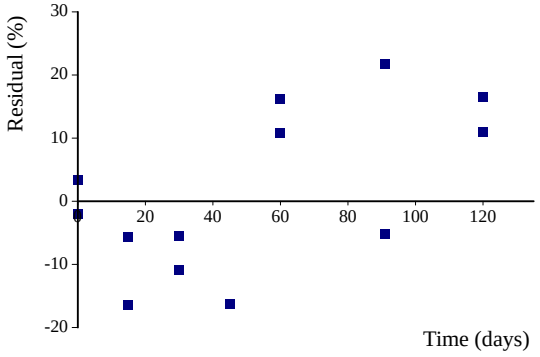




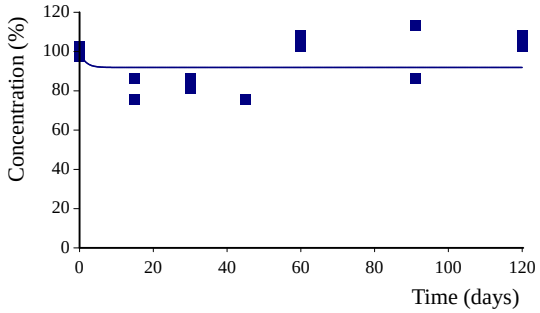
FOMC model – $C_{14}Cl_7$

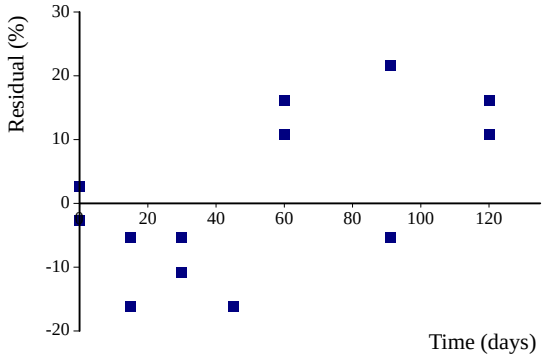




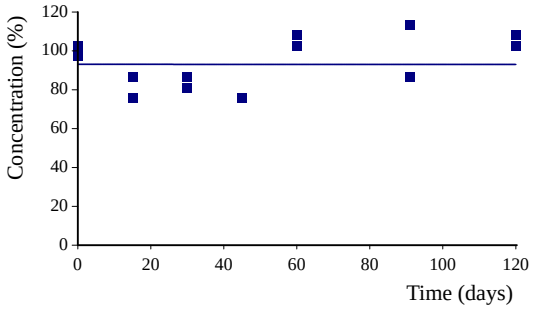


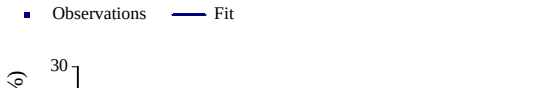
DFOP model– $C_{14}Cl_7$

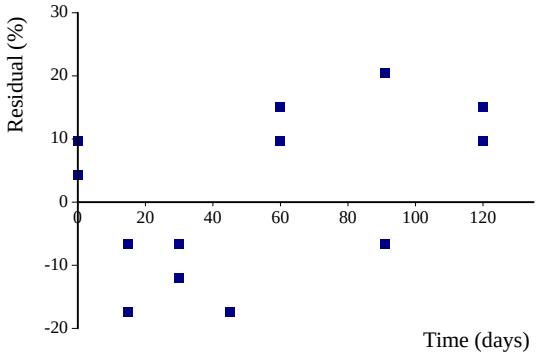




HS model – $C_{14}Cl_7$







$C_{14}Cl_8$ congener group:

Results for the Water-Sediment system: Brandywine Creek

Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 0.001174	0.2172	-0.001989 — 0.004	13.2	5	0.05069	590	1960
FOMC	α = 0.01272; β = 6.67E-007	NA; NA	nd* nd*	12.7	4	0.195	>10,000	>10,000
DFOP	k_1 = 0.107; k_2 = 1.13E-011; g = 0.2231	0.1986; 0.5; NA	-0.1626 — 0.377; -0.004468 — 0.004; -0.1279 — 0.574	13.6	3	0.2214	>10,000 (overall DT_{50}); 6.48 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.001174; k_2 =0.003079; t_b =126.5	0.242; 0.4998; NA	-0.002426 — 0.005; -17.34 — 17.35; - 34740— 35000	15.7	3	0.05069	303 (overall DT_{50}); 590 (k_1 DT_{50}); 225 (k_2 DT_{50})	826

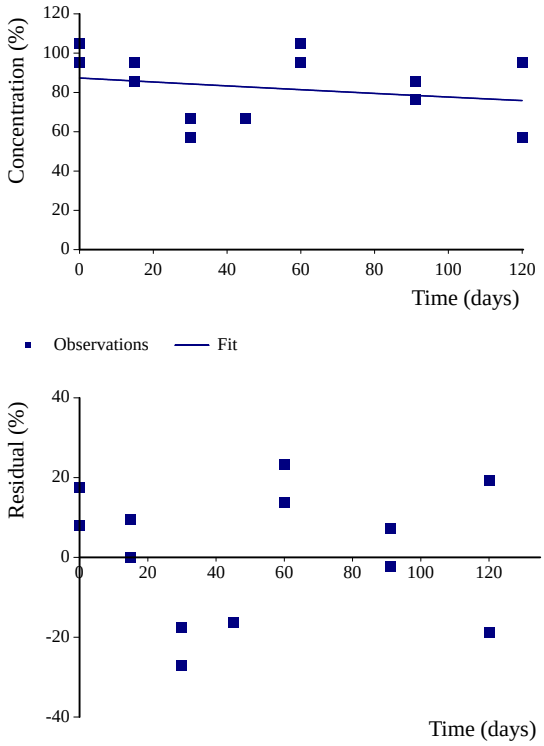
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

Improvement of χ^2 statistics for FOMC (12.7%) compared to the SFO model. However, it was not possible to assess the reliability of its individual rate parameter estimates (α and β) as no confidence interval and t-test are available. The covariance matrix used for describing parameter uncertainty can not be estimated by CAKE, due to the large correlation of parameters α and β in this fit. That is why the SFO model was the model selected for the prediction of the DT_{50} value for the $C_{14}Cl_8$ congener group (χ^2-test value is below 15%).

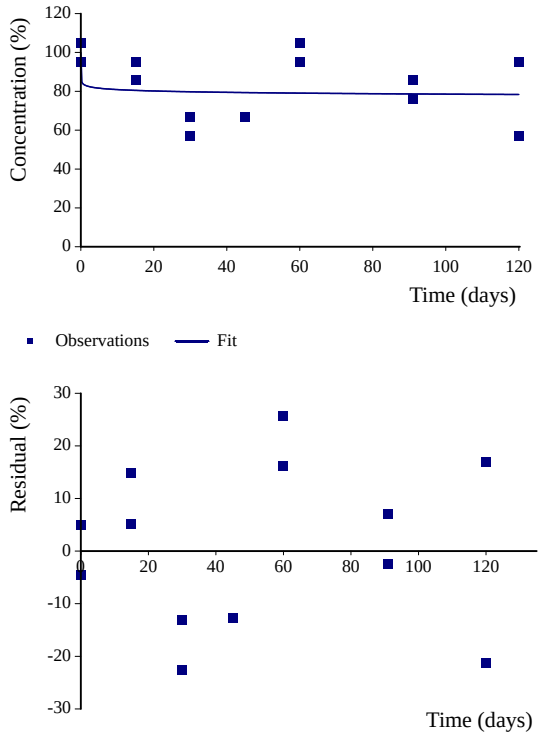
For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_8$ congener group cannot be ruled out. A DT_{50} of 590 days is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_8$ congener group of

MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

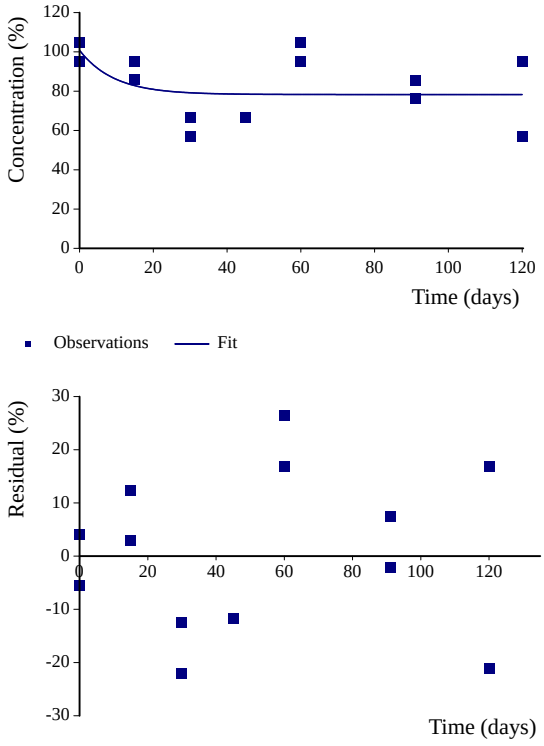
SFO model – $C_{14}Cl_8$



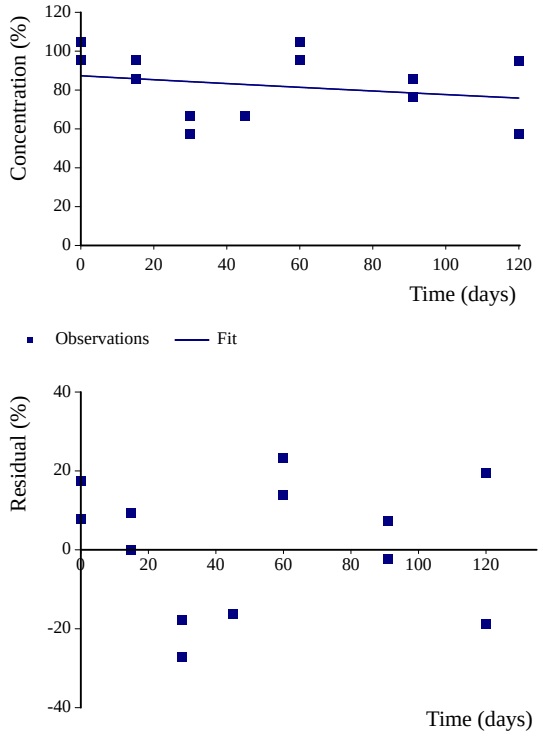
FOMC model – $C_{14}Cl_8$



DFOP model– $C_{14}Cl_8$



HS model – $C_{14}Cl_8$



Results for the Water-Sediment system: Choptank River

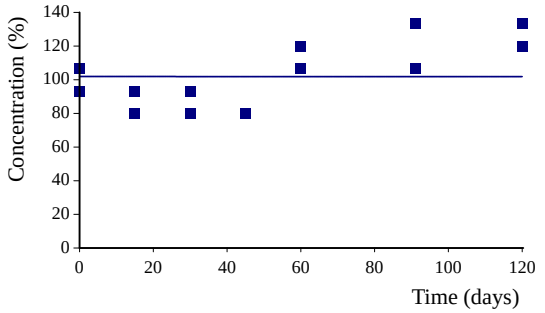
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 3.44E-016	0.5	-0.002919 — 0.003	13.2	5	0.5058	>10,000	>10,000
FOMC	α = 1.94-010; β = 0.01056	NA*; NA*	-4.717E-05— 0 nd — nd*	14.3	4	0.1042	>10,000	>10,000
DFOP	k_1 = 0.2421; k_2 = 0; g = 0	Nd*; 0.5; NA*	nd — nd*; -0.003416 — 0.003; 0 — 0	15.7	3	nd	>10,000 (overall DT_{50}); 2.86 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0; k_2 =0; t_b =4.024	0.5; 0.5; NA*	-0.0002605 — 0; -0.003493 — 0.003; nd — nd*	15.7	3	nd	>10,000 (overall DT_{50}); >10,000 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

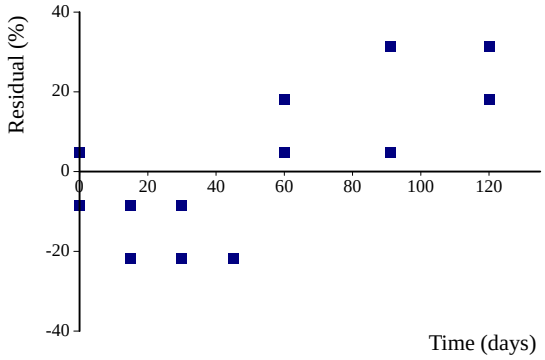
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

The SFO model is the best fit model (lowest χ^2-test value which is below 15%).

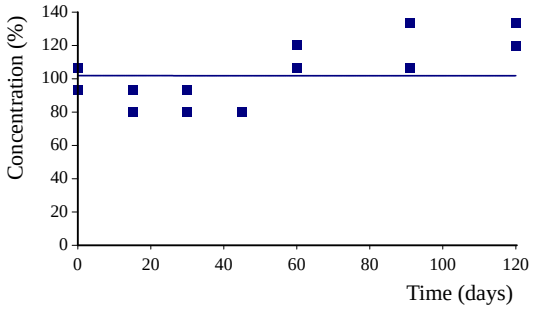
For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_8$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_8$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

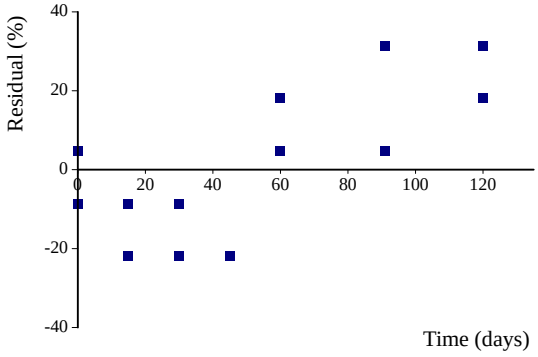
SFO model – $C_{14}Cl_8$



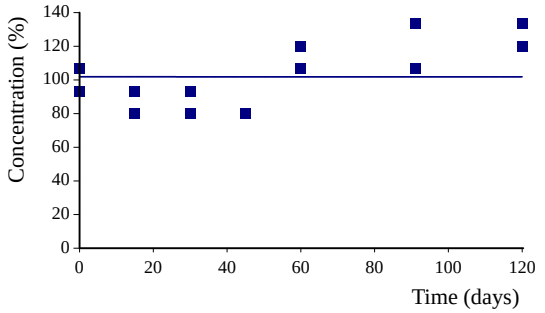


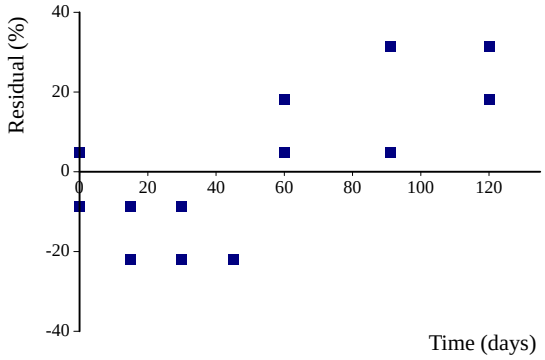
FOMC model – $C_{14}Cl_8$



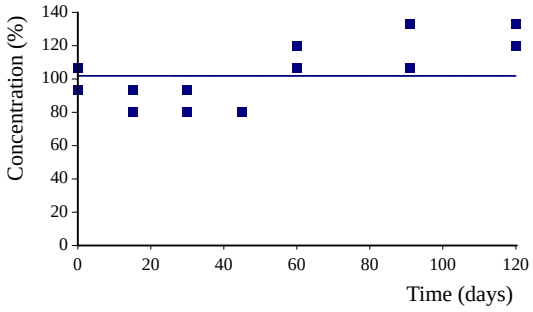


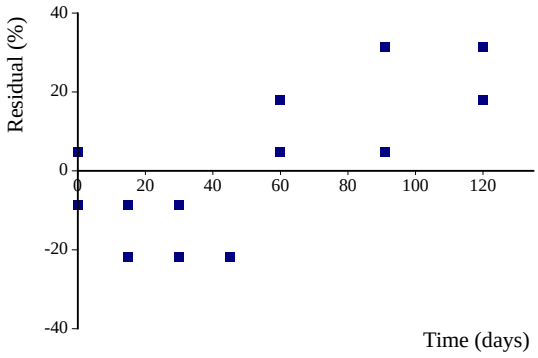
DFOP model– $C_{14}Cl_8$





HS model – $C_{14}Cl_8$





$C_{14}Cl_9$ congener group:

Results for the Water-Sediment system: Brandywine Creek

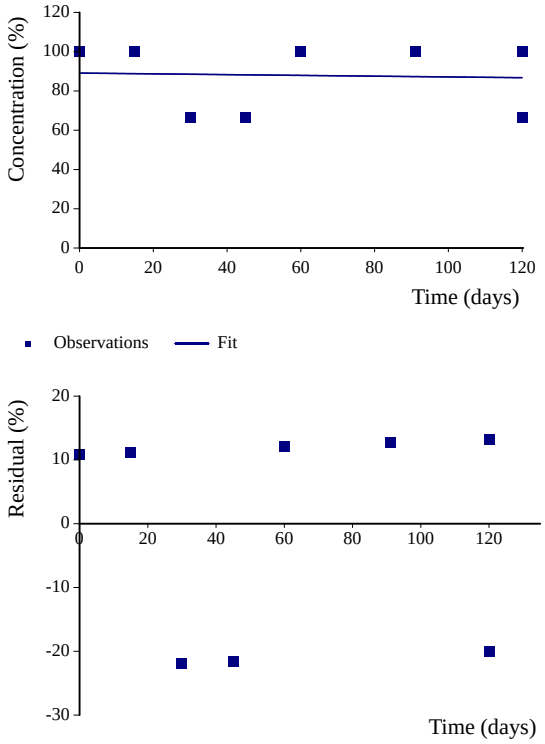
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 2.22E-004	0.4355	-0.002688 — 0.003	13.2	5	0.002209	3130	>10,000
FOMC	α = 0.007137; β = 6.38E-008	NA*; NA*	nd* nd*	13.5	4	0.08944	>10,000	>10,000
DFOP	k_1 = 0.09739; k_2 = 2.74E-011; g = 0.1608	0.2065; 0.5; NA	-0.1567 — 0.351; -0.004265 — 0.004; -0.2131 — 0.535	14.6	3	0.1212	>10,000 (overall DT_{50}); 7.12 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.006778; k_2 =9.43E-034; t_b =29.87	0.2765; 0.5; NA	-0.01782 — 0.031; -0.004803 — 0.005; - 73.86— 133.6	13.9	3	0.1881	>10,000 (overall DT_{50}); 102 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

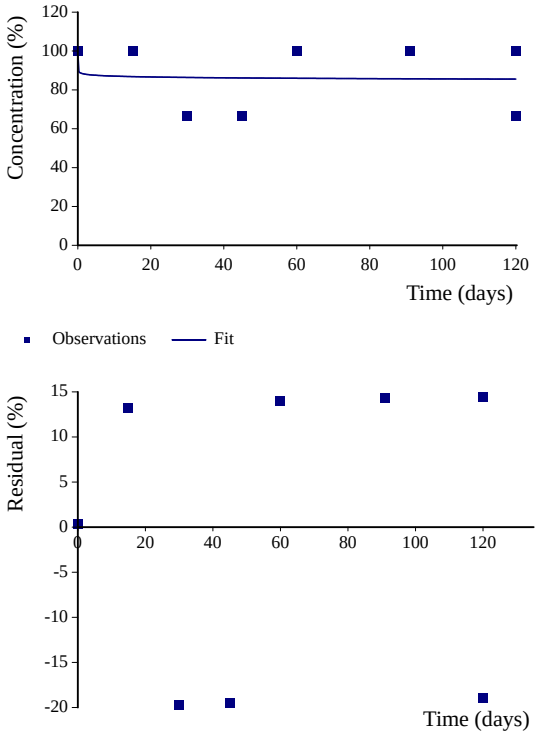
The SFO model is the best fit model (lowest χ^2-test value which is below 15%).

For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_9$ congener group cannot be ruled out. A DT_{50} of 3130 days is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_9$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

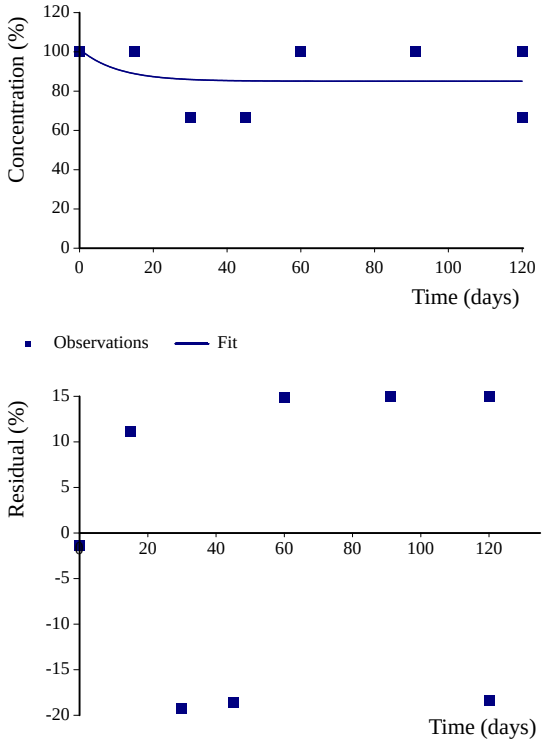
SFO model – $C_{14}Cl_9$



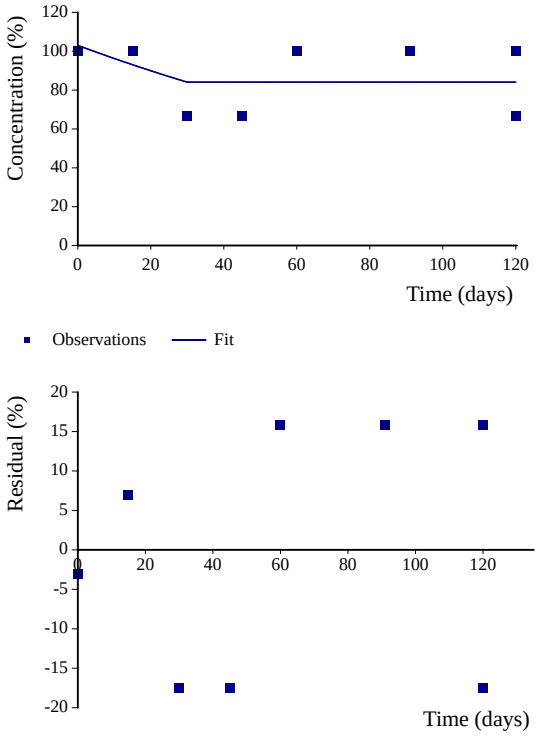
FOMC model – $C_{14}Cl_9$



DFOP model– $C_{14}Cl_9$

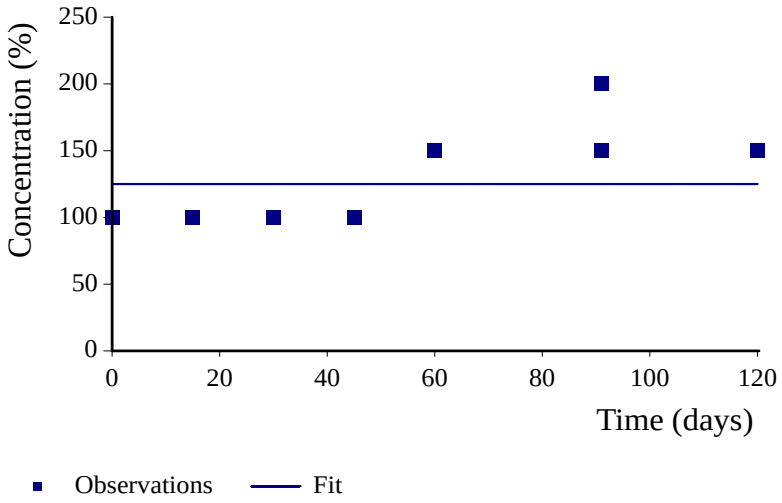


HS model – $C_{14}Cl_9$



Results for the Water-Sediment system: Choptank River

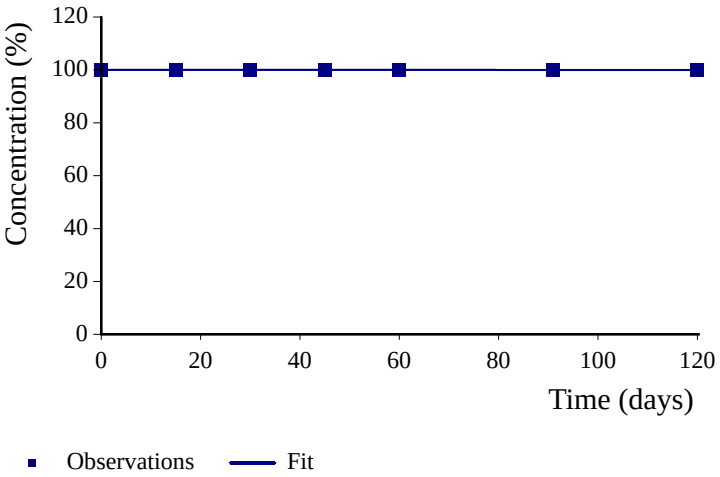
For the $C_{14}Cl_9$ congener group, no decrease in the concentration was observed during the test period (see below Figure). That is why it is concluded that the $C_{14}Cl_9$ congener group of MCCP does not degrade in the water-sediment system (DT_{50} >120 days).



$C_{14}Cl_{10}$ congener group:

Results for the Water-Sediment system: Brandywine Creek

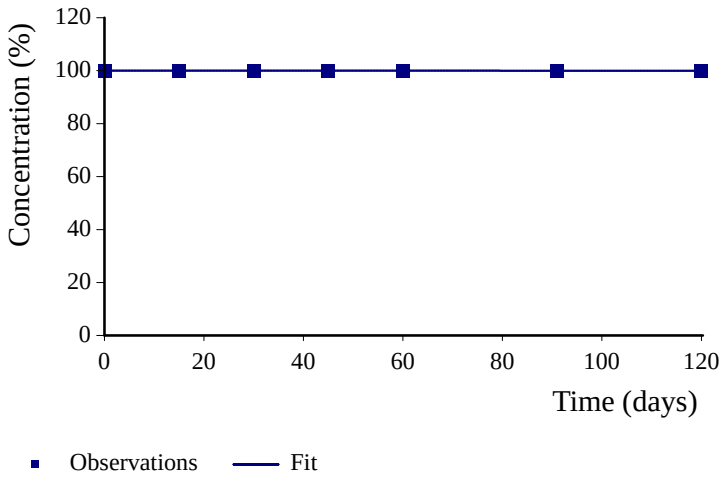
For the $C_{14}Cl_{10}$ congener group, no variation in the concentration was observed during the test period (see below Figure) and the results for the replicates were similar. That is why it is concluded that the $C_{14}Cl_{10}$ congener group of MCCP does not degrade in the water-sediment system (DT_{50} >120 days).



Results for the Water-Sediment system: Choptank River

For the $C_{14}Cl_{10}$ congener group, no variation in the concentration was observed during the test period (see below Figure) and the results for the replicates were similar. That is why

it is concluded that the $C_{14}Cl_{10}$ congener group of MCCP does not degrade in the water-sediment system (DT_{50} >120 days).



$C_{14}Cl_{11}$ congener group:

Results for the Water-Sediment system: Brandywine Creek

Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 1.41E-012	0.5	-0.003242 — 0.003	11.3	5	0.0002912	>10,000	>10,000
FOMC	α = 0.008054; β = 1.46E-010	NA; NA	nd* nd*	10.3	4	0.1465	>10,000	>10,000
DFOP	k_1 = 0.1376; k_2 = 3.57E-017; g = 0.197	0.3939; 0.5; NA	-0.9716 — 1.247; -0.005606 — 0.006; -0.232 — 0.626	11.1	3	0.1606	>10,000 (overall DT_{50}); 5.04 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.01028; k_2 =6.55E-012; t_b =21.72	0.2253; 0.5; NA	-0.01888 — 0.039; -0.005046 — 0.005; - 33.03— 76.47	10.9	3	0.1681	>10,000 (overall DT_{50}); 67.5 (k_1 DT_{50}); >10,000	>10,000

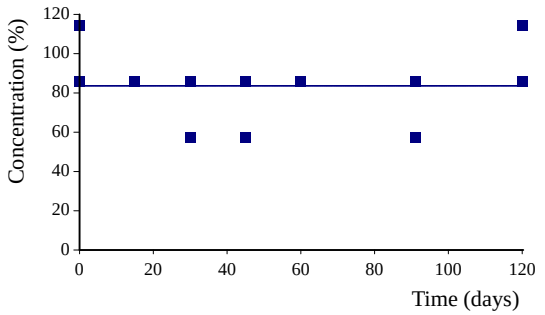
							(k_2 DT_{50})	

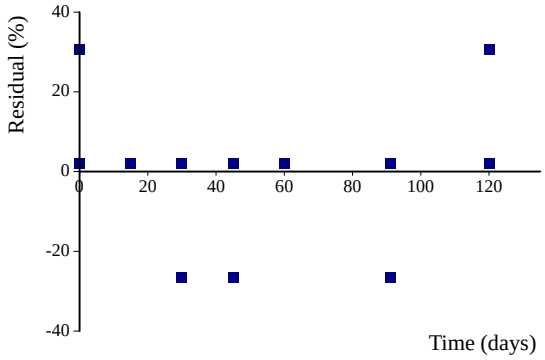
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

Improvement of χ^2 statistics for FOMC (10.3%) compared to other models. However, it was not possible to assess the reliability of its individual rate parameter estimates (α and β) as no confidence interval and t-test are available. The covariance matrix used for describing parameter uncertainty can not be estimated by CAKE, due to the large correlation of parameters α and β in this fit. That is why the HS model was the model selected for the prediction of the DT_{50} value for the $C_{14}Cl_{11}$ congener group (χ^2-test value is below 15%).

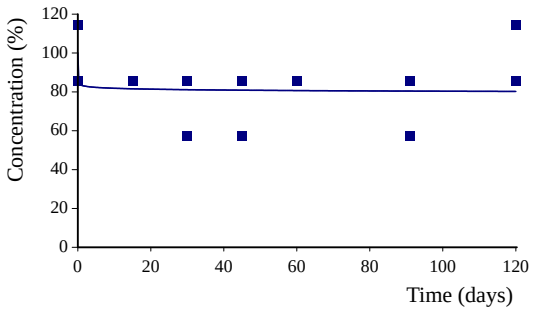
For this model, the parameters k_1 and k_2 do not differ significantly from zero as zero is included in the confidence interval, thus an absence of degradation for the $C_{14}Cl_{11}$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameters (k_1, k_2 and t_b) which are uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_{11}$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

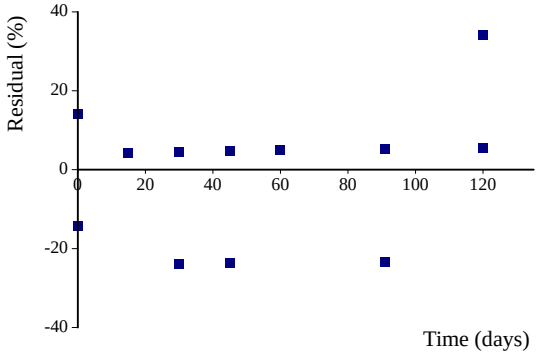
SFO model – $C_{14}Cl_{11}$



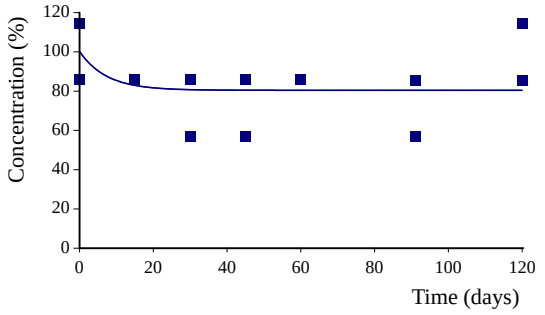


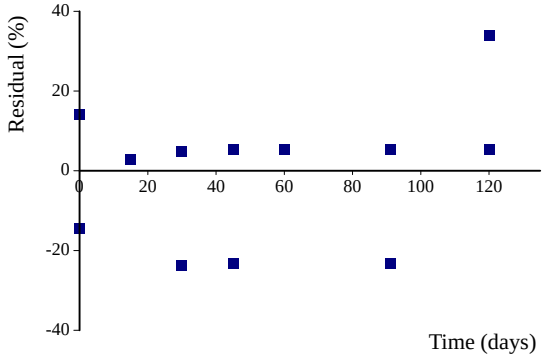
FOMC model – $C_{14}Cl_{11}$



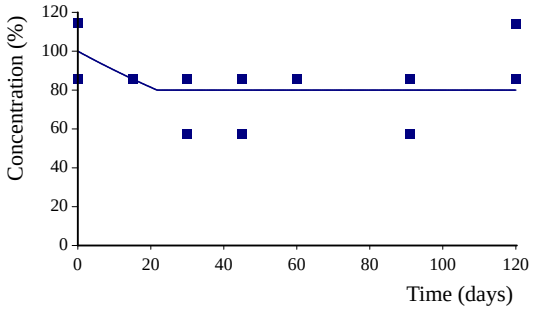


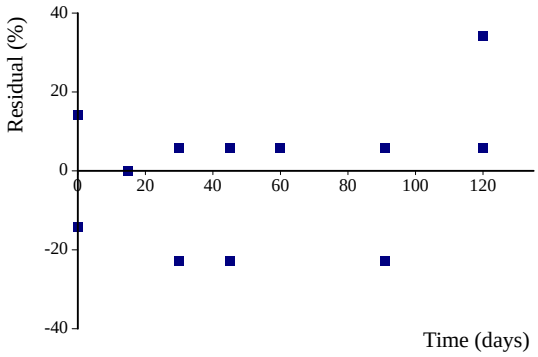
DFOP model– $C_{14}Cl_{11}$





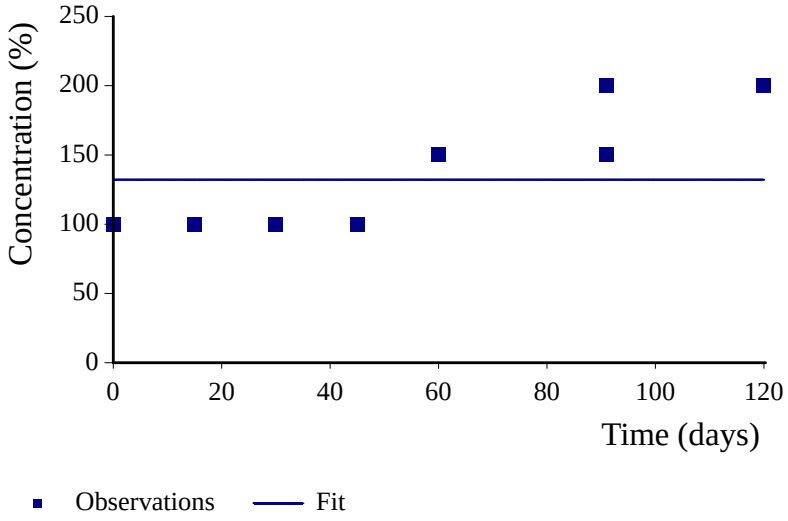
HS model – $C_{14}Cl_{11}$





Results for the Water-Sediment system: Choptank River

For the $C_{14}Cl_{11}$ congener group, no decrease in the concentration was observed during the test period (see below Figure). That is why it is concluded that the $C_{14}Cl_{11}$ congener group of MCCP does not degrade in the water-sediment system (DT_{50} >120 days).

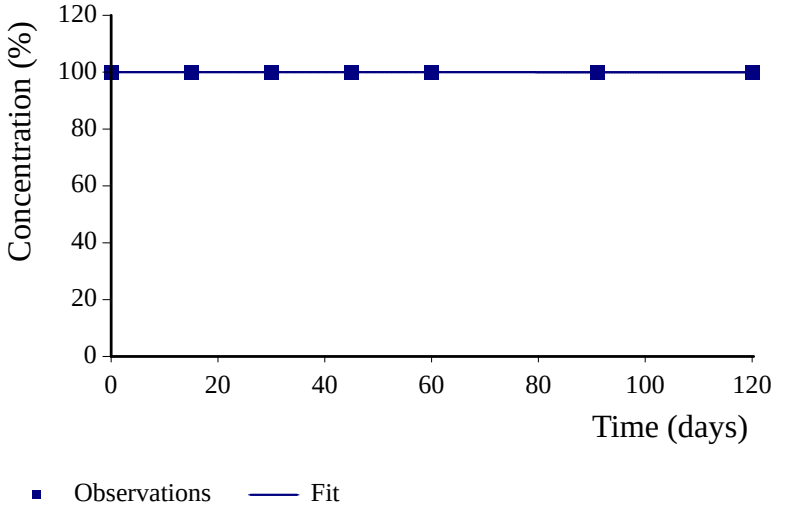


$C_{14}Cl_{12}$ congener group:

Results for the Water-Sediment system: Brandywine Creek

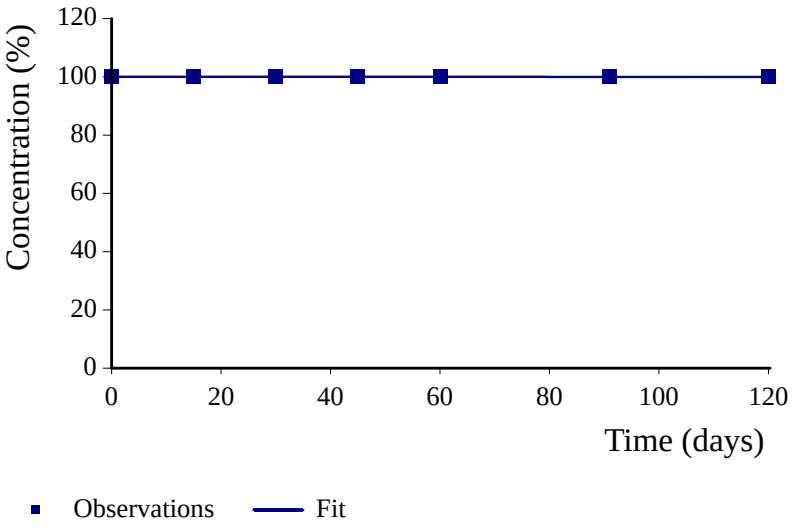
For the $C_{14}Cl_{12}$ congener group, no variation in the concentration was observed during the test period (see below Figure) and the results for the replicates were similar. That is why it is concluded that the $C_{14}Cl_{12}$ congener group of MCCP does not degrade in the water-sediment system (DT_{50} >120 days).

One outlier was deleted at day 45 (but another replicate is available at day 45) as this concentration is the only one which differs from the other data points.



Results for the Water-Sediment system: Choptank River

For the $C_{14}Cl_{12}$ congener group, no variation in the concentration was observed during the test period (see below Figure) and the results for the replicates were similar. That is why it is concluded that the $C_{14}Cl_{12}$ congener group of MCCP does not degrade in the water-sediment system (DT_{50} >120 days).



$C_{14}Cl_{13}$ congener group:

Results for the Water-Sediment system: Brandywine Creek

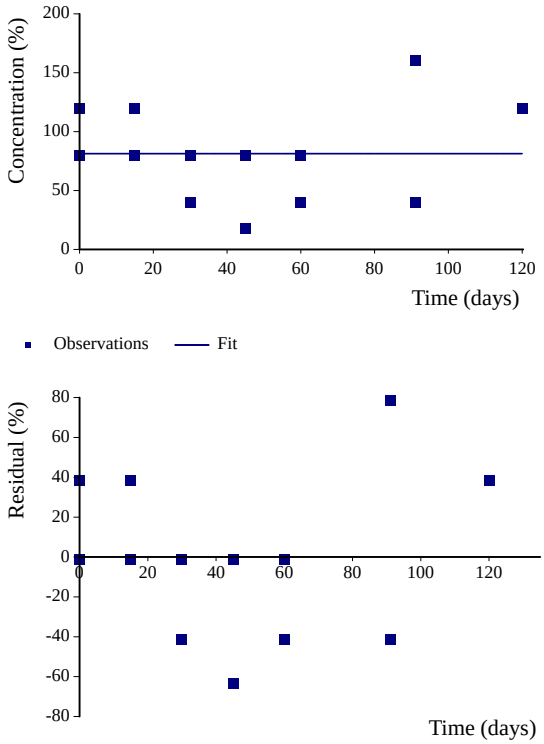
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 2.09E-013	0.5	-0.008914 — 0.009	23.8	5	0.01004	>10,000	>10,000
FOMC	α = 0.009442; β = 1.16E-010	NA*; NA*	nd* nd*	25	4	0.03921	>10,000	>10,000
DFOP	k_1 = 0.08625; k_2 = 7.33E-011; g = 0.263	0.2896; 0.5; NA	-0.2529 — 0.425; -0.01862 — 0.019; -0.8028 — 1.329	27.1	3	0.05812	>10,000 (overall DT_{50}); 8.04 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.01132; k_2 =2.41E-150; t_b =29.99	0.3348; 0.5; NA	-0.04674 — 0.069; -0.01863 — 0.019; - 138.4— 198.4	26.4	3	0.08401	>10,000 (overall DT_{50}); 61.2 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

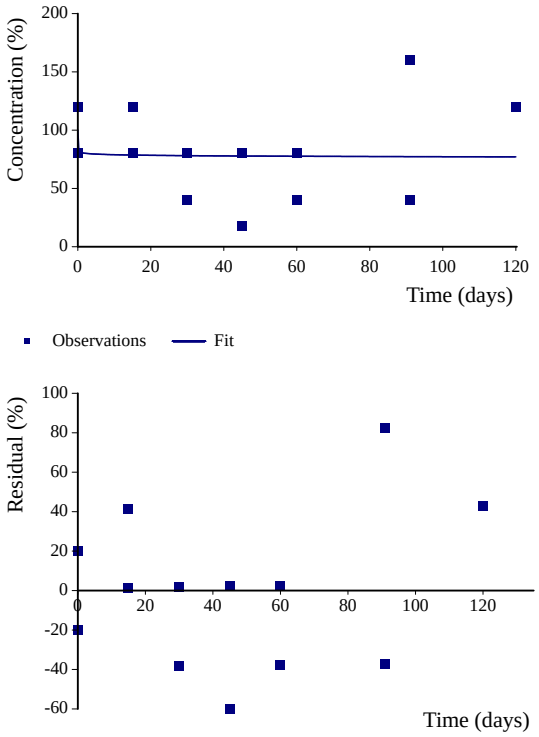
One outlier was deleted at day 120 (but another replicate is available at day 120) as this concentration was a factor ca. 3 times higher than the concentration observed at day 0.

The SFO model is the best fit model, however, χ^2-test is >15%. For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_{13}$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_{13}$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

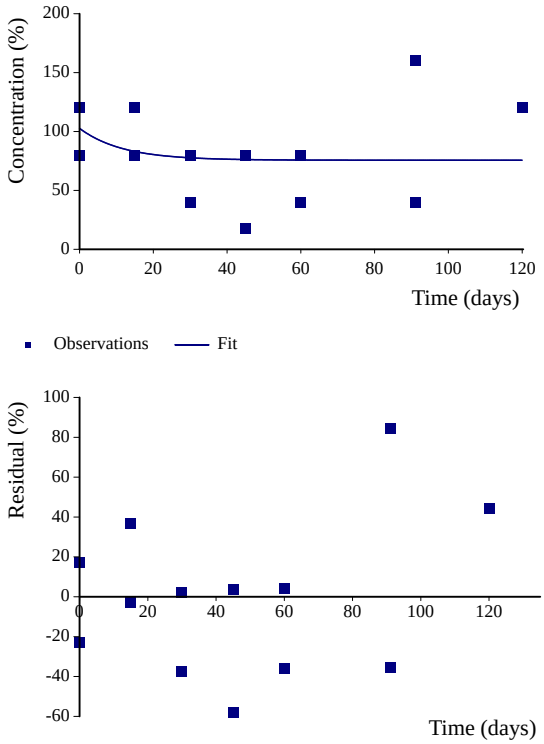
SFO model – $C_{14}Cl_{13}$



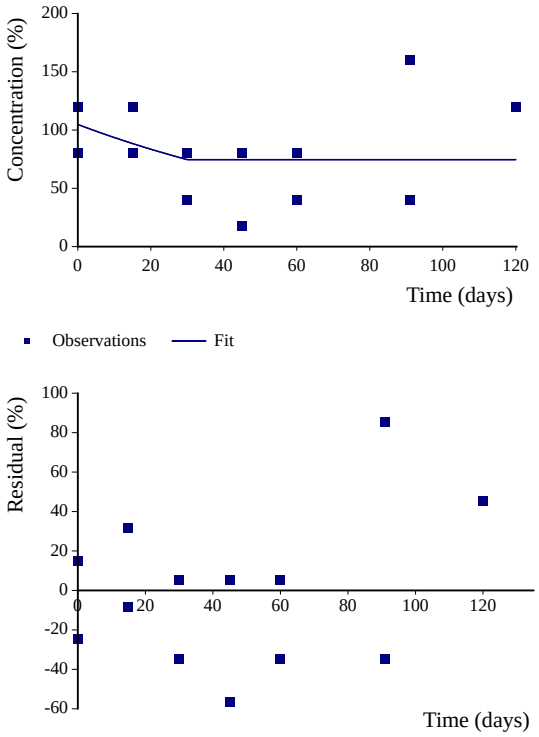
FOMC model – $C_{14}Cl_{13}$



DFOP model– $C_{14}Cl_{13}$



HS model – $C_{14}Cl_{13}$



Results for the Water-Sediment system: Choptank River

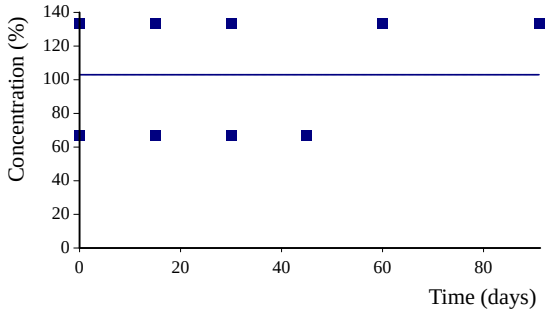
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 6.95E-019	0.5	-0.009067 — 0.009	17.1	4	nd	>10,000	>10,000
FOMC	α = 0; β = 0.009627	NA*; NA*	0 — 0* Nd — nd*	18.8	3	nd	>10,000	>10,000
DFOP	k_1 = 0.1654; k_2 = 0; g = 0	Nd*; 0.5; NA*	Nd — nd*; -0.01153 — 0.012; 0 — 0	21.5	2	nd	>10,000 (overall DT_{50}); 4.19 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0; k_2 =0; t_b =5.908	0.5; 0.5; NA*	-0.002927 — 0.003; -0.01207 — 0.012; Nd — nd*;	21.5	2	nd	>10,000 (overall DT_{50}); >10,000 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

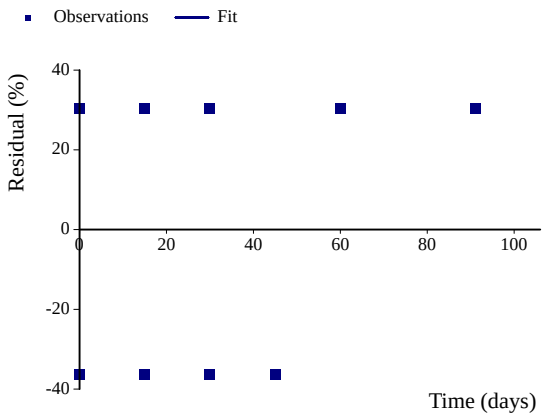
* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

One outlier was deleted at day 91 (but another replicate is available at day 91) and two outliers were deleted at day 120. These three outliers were deleted as their concentrations were a factor ca. 2 to 3 times higher than the concentration observed at day 0.

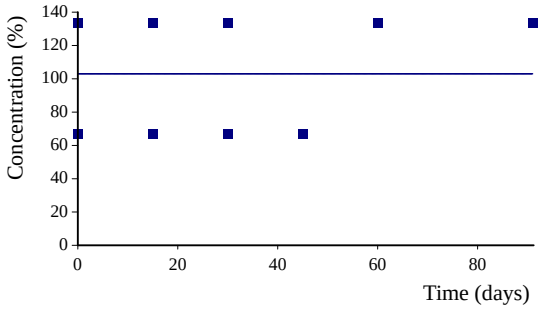
The SFO model is the best fit model, however, χ^2-test is >15%. For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_{13}$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_{13}$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

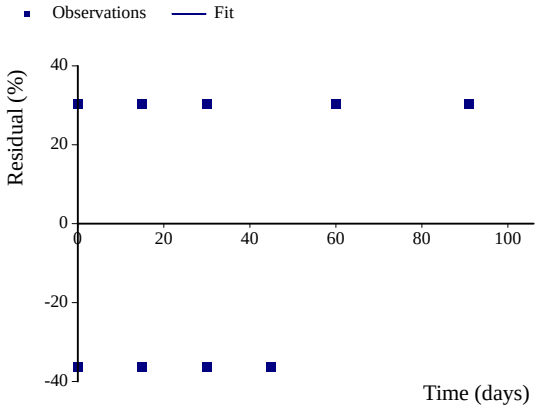
SFO model – $C_{14}Cl_{13}$



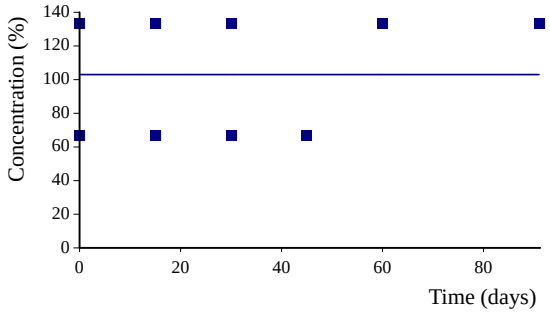


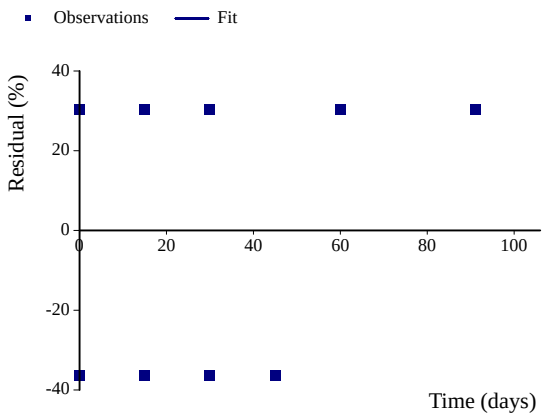
FOMC model – $C_{14}Cl_{13}$



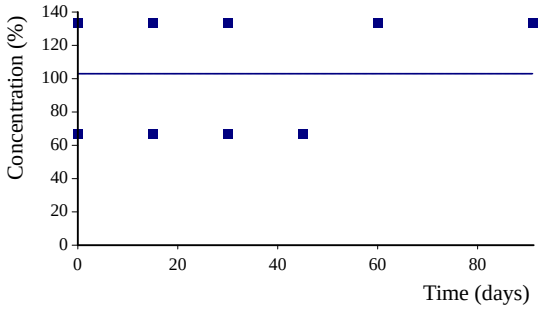


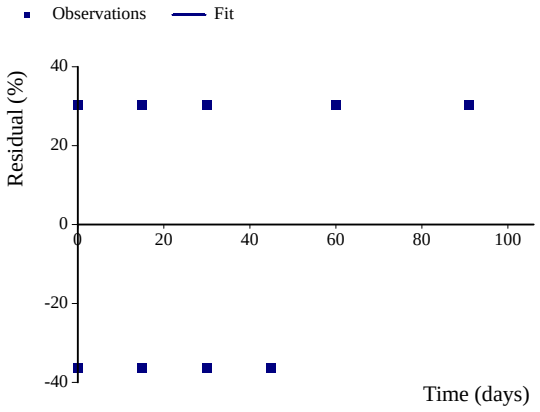
DFOP model– $C_{14}Cl_{13}$





HS model – $C_{14}Cl_{13}$





$C_{14}Cl_{14}$ congener group:

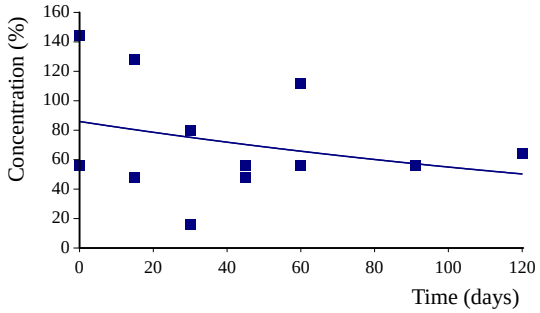
Results for the Water-Sediment system: Brandywine Creek

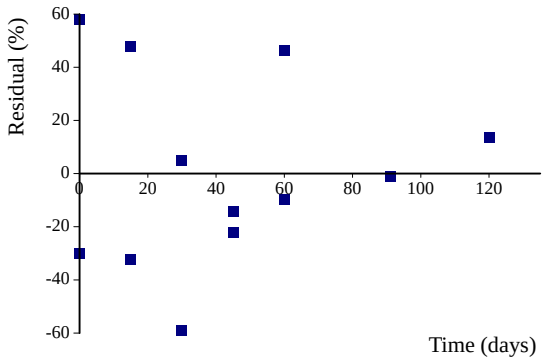
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 0.004461	0.194	-0.006549 — 0.015	18.3	5	0.07382	155	516
FOMC	α = 0.1177; β = 1.267	NA; NA	-0.6271 — 0.862; -28.91 — 31.45	16.5	4	0.1393	457	>10,000
DFOP	k_1 = 0.07458; k_2 = 1.52E-008; g = 0.391	0.3885; 0.5; NA	-0.5126— 0.662; -0.0274— 0.027; -1.035— 1.817	17.2	3	0.1564	>10,000 (overall DT_{50}); 9.29 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0.01683; k_2 = 3.77E-011; t_b =29.94	0.1265; 0.5; NA	-0.01467 — 0.048; -0.01651 — 0.017; 19.19 — 40.69	15.2	3	0.188	>10,000 (overall DT_{50}); 41.2 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000

Two outliers were deleted: one at day 91 and one at day 120 (but replicates are available at day 91 and at day 120) as these concentrations were a factor ca. 2 and 5 times higher than the concentration observed at day 0.

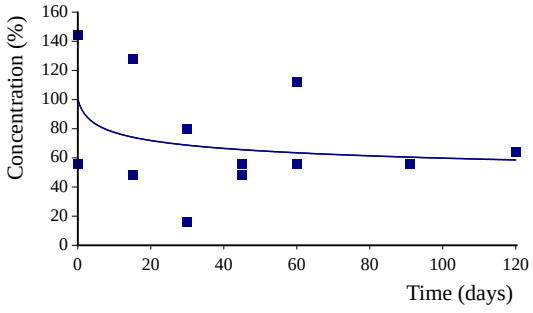
Improvement of χ^2 statistics and of deviation of residuals for HS (15.2%) compared to the SFO model. That is why the HS model is the best fit model, however, χ^2-test is slightly >15%.
For this model, the parameters k_1 and k_2 do not differ significantly from zero as zero is included in the confidence interval, thus an absence of degradation for the $C_{14}Cl_{14}$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameters (k_1 and k_2) which are uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_{14}$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

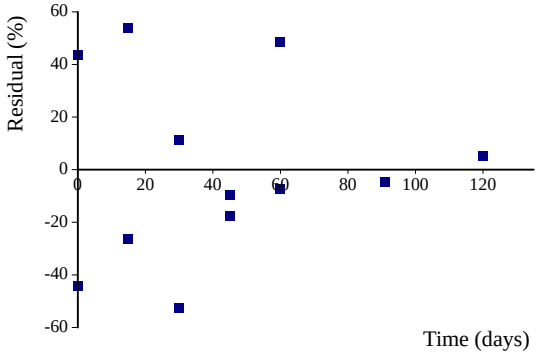
SFO model – $C_{14}Cl_{14}$



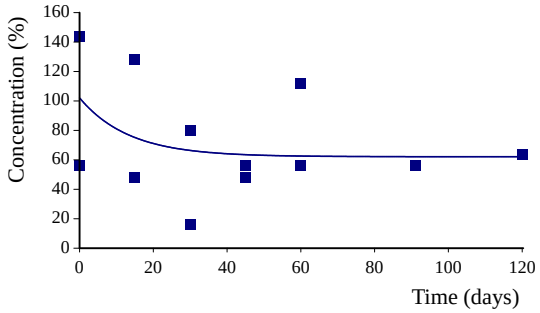


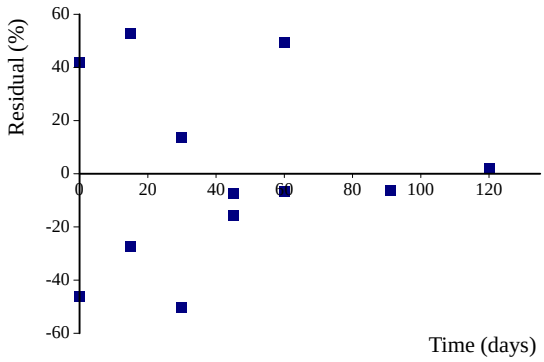
FOMC model – $C_{14}Cl_{14}$



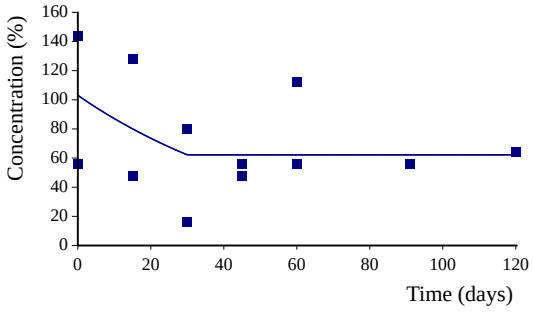


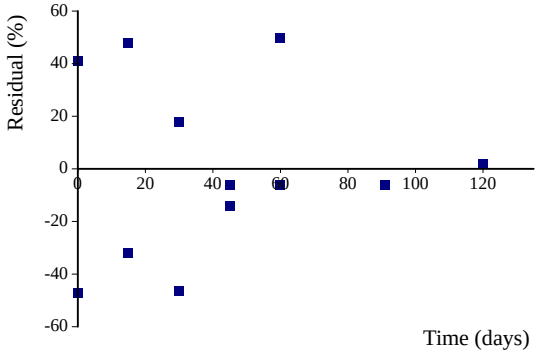
DFOP model– $C_{14}Cl_{14}$





HS model – $C_{14}Cl_{14}$





Results for the Water-Sediment system: Choptank River

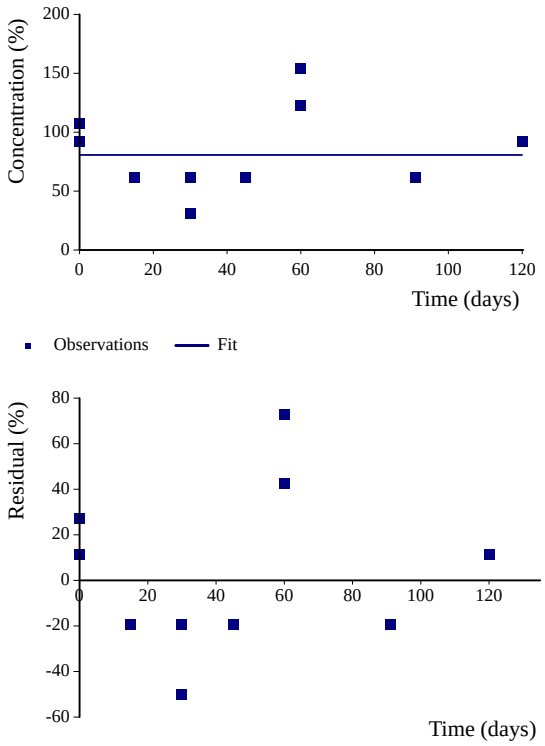
Model	Parameter estimated value	t-test (Prob. > t)	Confidence interval 95%	χ^2-test (error %)	Degrees of freedom	r^2 (Obs v Pred)	DT_{50} (days)	DT_{90} (days)
SFO	k = 7.08E-013	0.5	-0.008233 — 0.008	29.1	5	0.02554	>10,000	>10,000
FOMC	α = 0.01007 ; β = 9.03E-010	NA*; NA*	Nd — nd* Nd — nd*	30.4	4	0.0569	>10,000	>10,000
DFOP	k_1 = 0.9074; k_2 = 7.24E-012; g = 0.231	0.4963 ; 0.5; NA	-215.2 — 217; -0.01142 — 0.011; -0.4605 — 0.922	33.3	3	0.06924	>10,000 (overall DT_{50}); 0.764 (k_1 DT_{50}); >10,000 (k_2 DT_{50})	>10,000
HS	k_1 = 0; k_2 = 0.004; t_b =142.2	Nd*; Nd*; NA*	Nd — nd*; Nd — nd*; Nd — nd*	34.6	3	nd	307 (overall DT_{50}); >10,000 (k_1 DT_{50}); 165 (k_2 DT_{50})	689

* Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

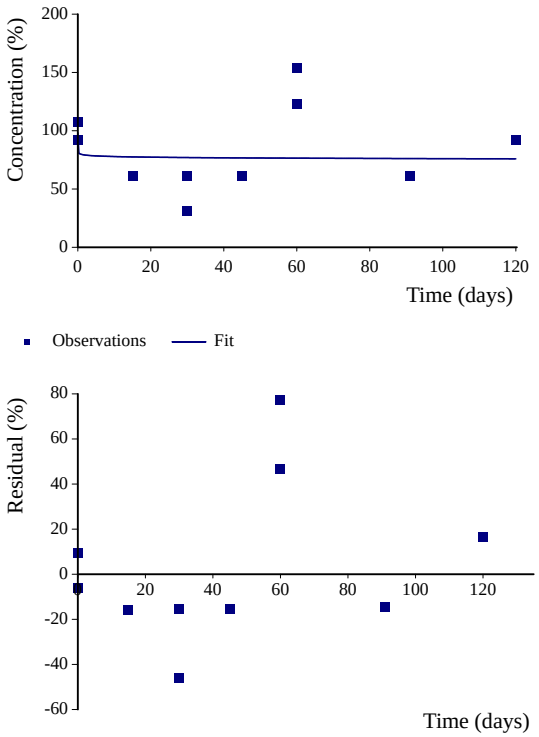
Two outliers were deleted: one at day 91 and one at day 120 (but replicates are available at day 91 and at day 120) as these concentrations were a factor ca. 3 times higher than the concentration observed at day 0.

The SFO model is the best fit model, however, χ^2-test is >15%. For this model, parameter k does not differ significantly from zero (p>0.1), thus an absence of degradation for the $C_{14}Cl_{14}$ congener group cannot be ruled out. A DT_{50} >10,000 days (default value) is predicted for this congener group. However, this prediction is derived from parameter k which is uncertain. Therefore, this DT_{50} value should be interpreted with caution. However, this very high DT_{50} value indicates that the $C_{14}Cl_{14}$ congener group of MCCP does not degrade significantly in the water-sediment system (DT_{50} >180 days).

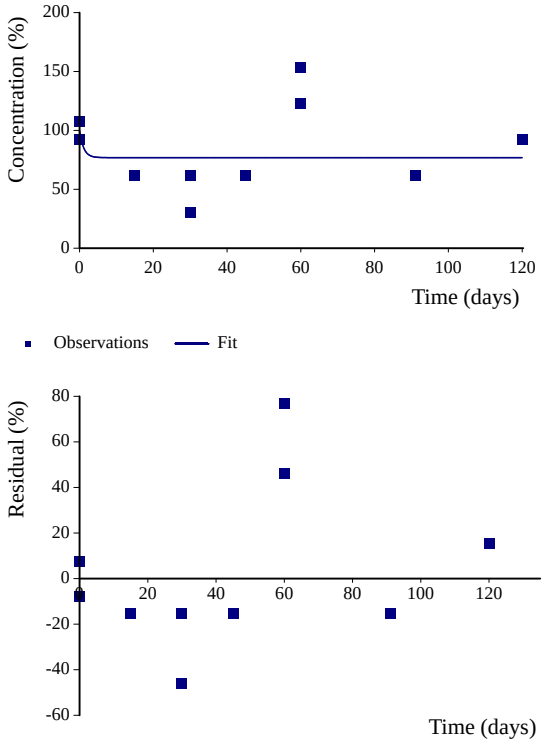
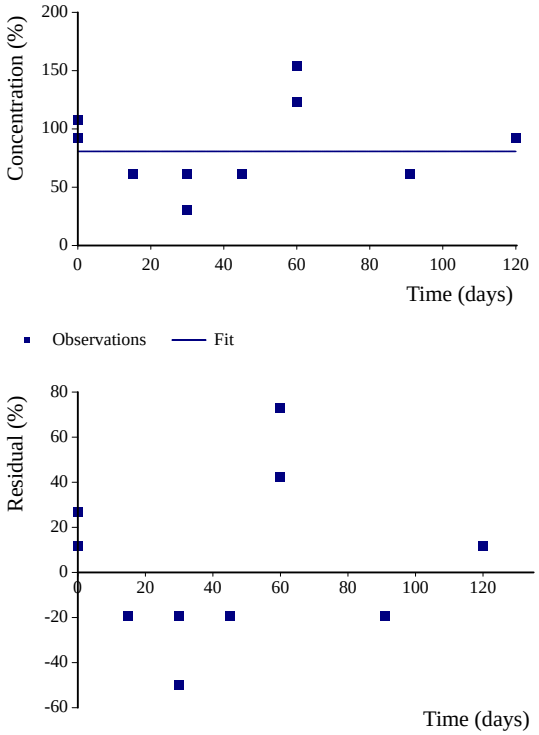
SFO model – $C_{14}Cl_{14}$



FOMC model – $C_{14}Cl_{14}$



DFOP model– $C_{14}Cl_{14}$



HS model – $C_{14}Cl_{14}$