Persistent, Bioaccumulative and Toxic (PBT) properties of Long Chain Chlorinated Paraffins (LCCPs)

Chief Scientist's Group report

July 2022

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Published by:

Environment Agency
Horizon House, Deanery Road,
Bristol BS1 5AH

www.gov.uk/environment-agency

Further copies of this report are available from our publications catalogue: www.gov.uk/government/publications or our National Customer Contact Centre: 03708 506 506

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Keywords:
Chlorinated paraffins, Halogenated n-alkanes, chlorinated alkanes, PBT, Persistent, Bioaccumulative, Toxic

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Citation:
Environment Agency (2022). Persistent, Bioaccumulative and Toxic (PBT) Properties of Long Chain Chlorinated Paraffins (LCCPs), Environment Agency, Bristol.

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Dr Jo Nettleton
Chief Scientist

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Acknowledgements

The Environment Agency has liaised extensively with representatives of the LCCPs REACH Consortium, in particular INOVYN ChlorVinyls Limited. We wish to formally acknowledge their helpful assistance, along with input kindly provided by the following experts.

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Dr Helen McGarry (Health and Safety Executive, UK)

Dr Andreas Buser (Federal Office for the Environment, Switzerland)

Mr John Pasternak (Environment and Climate Change Canada)

Mr Danny Lee (Environment and Climate Change Canada)

Members of the Hazardous Substances Advisory Committee (DEFRA, 2021) also provided comments on specific issues identified during the preparation of this report.

Executive summary

There is growing international regulatory concern about the presence of chlorinated paraffins in the environment. This report addresses one product type, known as long-chain chlorinated paraffins (LCCPs), and focusses on its persistent, bioaccumulative and toxic (PBT) properties. Chemicals with such properties are of significant concern because they can remain in the environment for a long time and accumulate in food chains with unpredictable consequences. The report updates a previous Environment Agency evaluation published in 2009, using data from the European Chemicals Agency's (ECHA) public registration dissemination site, an updated academic literature search, and more recent national and international industry and regulatory outputs.

LCCPs is a very complex substance and can be either liquid or solid depending on the range of congener carbon chain lengths and degree of chlorination. Due to the number of constituents involved, a wide range of values are encountered for various properties (e.g., water solubility), which affects their environmental behaviour. Chemical analysis is also complicated and limited by the absence of completely characterised test substances and reference materials. Comparison between studies is therefore challenging. To address this issue, we examined trends observed for other types of chlorinated paraffin for additional context.

A large amount of information is available for LCCPs, although much of the data is of doubtful or unknown reliability. This applies particularly to the evaluation of persistence and bioaccumulation endpoints, as there are no studies available that meet current regulatory standards.

We conclude that a significant proportion of LCCP constituents will have long half-lives in freshwater sediments, most likely exceeding 180 days at 12 °C. This is based on read across of information from medium-chain chlorinated paraffins (MCCPs), which are theoretically more bioavailable and so rates of degradation are likely to be higher than those for LCCPs. This view is supported indirectly by the detection of LCCPs in sediment cores. The Environment Agency therefore concludes that LCCPs meets the persistent (P) and very persistent (vP) criteria in Annex 13 of the UK REACH Regulation, based on likely sediment half-life. Based on similarity to MCCPs, it is possible that low chlorine content congeners (e.g., < 30% Cl wt.) might not be persistent, but there are no definitive data available to confirm this. Evaluation of potential for bioaccumulation is made difficult by the age of the available studies and lack of guidance for the interpretation of monitoring data in single tissues like bird muscle:

- Shorter chain length congeners of LCCPs meet the screening criteria in Annex 13 of the UK REACH Regulation for both a bioaccumulative (B) and very bioaccumulative (vB) substance. They also screen for a high bioaccumulation potential in air-breathing organisms. Only highly chlorinated congeners (> 60% Cl wt.) with greater than 22 carbon atoms are considered too large to pass biological membranes.

- The available laboratory bioaccumulation data for fish and molluscs using aqueous exposure are not reliable. A recent study of bioaccumulation in the water flea *Daphnia magna* indicates that uptake of LCCP congeners by passive diffusion can occur over 48 hours. The study reported very high bioaccumulation factors, but major uncertainties in the numerical values make them unreliable for regulatory decision making. Information from MCCPs cannot be readily extrapolated either.

- We estimated depuration rate constants and half-lives from 2 non-standard fish studies of unknown reliability that used dietary exposure. These estimates are consistent with information from other substances that are known to have fish bioconcentration factors (BCF) above 5 000 L/kg.

- LCCP congeners have been detected in a wide range of aquatic and terrestrial wildlife, including sensitive life stages (e.g., frog eggs), species at the top of the food chain, and in human breast milk. Terrestrial species are more likely to accumulate longer, larger molecular weight CPs than aquatic species (although the amounts are often small).

We conclude that whilst there is no unequivocal evidence that LCCPs meet the definitive criteria in REACH Annex 13 for being bioaccumulative (B) or very bioaccumulative (vB), there is sufficient information to be concerned, particularly for LCCPs with chain lengths between C_{18} and C_{25} and chlorination levels of 42 to 49%. In terms of ecotoxicity, aquatic invertebrates appear to be the most sensitive trophic group, with a 21-day NOEC for *Daphnia* reproduction of 29 to 32 µg/L (and ≥2 µg/L) for a $C_{18–20}$, 52% Cl wt. product and ≥55 µg/L for a $C_{>20}$, 43% Cl wt. CP substance. These are higher than the toxicity (T) criterion 10 µg/L in Annex 13 of REACH. There is insufficient evidence to indicate that LCCPs meet the T criterion based on effects in mammals and birds. However, the available studies do not cover all LCCP product types.

We consider that further work is needed to address the uncertainties in the available data, using modern analytical methods to provide information about variation with chain length and the degree of chlorination. This could include:

- More representative measurements of water solubility and partition coefficient values.
- Investigation of the level of bioaccumulation of $C_{18\text{-}20}$ congener groups using modern methods. Additional biomonitoring of terrestrial predatory organisms and their food items – and measurement of a half-life in humans – could be useful.
- Additional toxicity testing with daphnids.
- Monitoring in remote areas.
- Assessing the relevance of transformation products.
- The development of better analytical standards.

Introduction

Chlorinated paraffins (CPs) are treated as three distinct product types for regulatory purposes within Europe, North America and Australia, related to carbon chain length:

- Short-chain chlorinated paraffins (SCCPs, $C_{10\text{-}13}$);
- Medium-chain chlorinated paraffins (MCCPs, $C_{14\text{-}17}$); and
- Long-chain chlorinated paraffins (LCCPs, C_{18+}).

SCCPs and MCCPs meet the persistent, bioaccumulative and toxic (PBT) and very persistent, very bioaccumulative (vPvB) criteria specified in Annex XIII of the Registration, Evaluation, Authorisation and restriction of CHemicals (REACH) Regulation (ECHA, 2008 & 2019). This conclusion is assumed to apply to product types with varying degrees of chlorination because they will all contain shared constituents with PBT/vPvB properties above 0.1% w/w. Chemicals that have PBT or vPvB properties are of significant concern because they can remain in the environment for a long time and accumulate in food chains with unpredictable consequences.

This report assesses whether the recent conclusion for MCCPs affects the PBT/vPvB status of LCCPs. It describes substance identity, structural analogues, analytical chemistry, various properties connected to its environmental fate and behaviour, and ecotoxicity (including a brief summary of the relevant mammalian toxicology data that are available). This is followed by an assessment against the PBT/vPvB criteria. The final section summarises the findings of this review. This is not a formal UK REACH evaluation.

The starting point is a previous Environment Agency evaluation (Environment Agency, 2009a). This has been supplemented with data presented in the European Chemicals Agency's (ECHA) public dissemination site (ECHA, 2021a, b and c), the findings for MCCPs (ECHA, 2019), an updated academic literature search focussing on publications from 2009 to 2021 (see Appendix A: Literature search), as well as other industry and regulatory outputs (both national and international). Where suitable, the Environment Agency has used predictive software and curated databases such as Comptox™ (US EPA, 2021) and VEGA Hub (IRSCC, 2021) as a screening tool to fill data gaps.

Environment Agency (2009a) was based on the assessment methods outlined in Parts II and III of the pre-REACH Technical Guidance Documents (ECB, 2003 a and b). The methodology used in this assessment follows ECHA Guidance Document R.11 (ECHA, 2017a). The basic PBT criteria have not changed, but several additional factors are now considered compared with the earlier guidance, including biomagnification and trophic magnification. Updates to OECD test guideline studies

and their interpretation have also occurred (in particular the fish bioaccumulation test guideline).

LCCPs have a very complex composition. This affects their physical state, with some products liquid and others solid due to differing ranges of congener carbon chain lengths and degree of chlorination. This means that a range of values is to be expected for various properties (e.g. water solubility), even though a single numerical value is often reported in laboratory studies. There is also often a lack of clarity about the exact composition of test substances, especially in older studies, which can make comparisons between studies difficult. We aim to provide a sufficient level of detail to characterise the various products in terms of their environmental fate, behaviour, and effects, without overcomplicating the assessment. To help provide further context, we have also considered data and trends observed for the homologues SCCPs and MCCPs, where appropriate.

Original study reports reviewed for Environment Agency (2009a) were not re-reviewed although data were re-interpreted where relevant. Reliability scores provided by the European Union (EU) REACH Registrant on the ECHA public registration dissemination site (2021b) will have been produced using ECHA Guidance Document R.4 (ECHA, 2011). We have provided our own view of data reliability for key endpoints.

1 Substance identity

1.1 Name and other identifiers

LCCPs are composed primarily of straight chain n-alkanes (paraffins) that have chlorine atoms situated at various positions along the chains. Two substances were identified as being covered by the term “LCCPs” in Environment Agency (2009a), as summarised in Table 1.

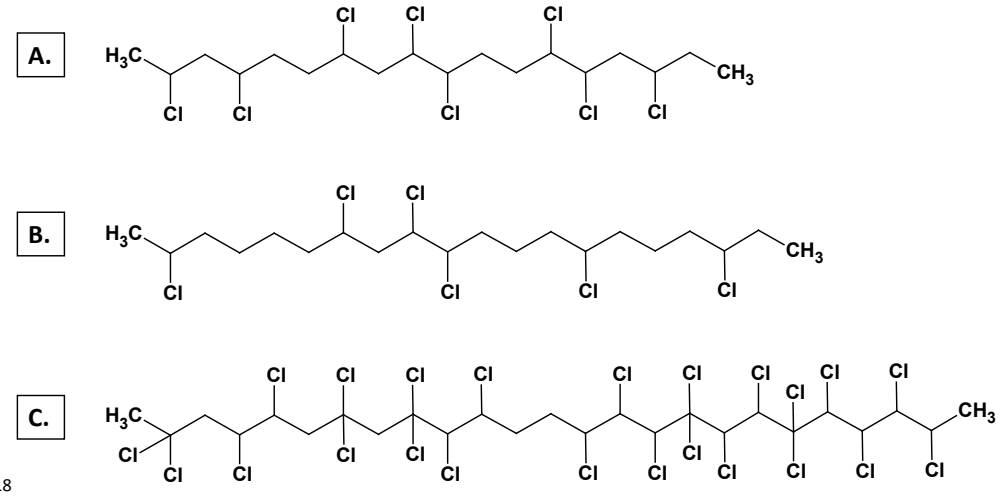
Table 1 Substance identities for LCCPs (Environment Agency, 2009)

EC name	**Paraffin oils, chloro**	**Paraffin waxes and hydrocarbon waxes, chloro**
EC number	287-196-3	264-150-0
CAS number	85422-92-0	63449-39-8
Molecular formula	$C_xH_{2x+2-y}Cl_y$, where x ≥18	$C_xH_{2x+2-y}Cl_y$, where x = 18 to 30 and y = 1 to 30[1]
Molecular weight range	320 to 500 g/mole (approximately)	420 to 1 355 g/mole (approximately)
Synonyms	Long-chain chlorinated paraffins (LCCPs); alkanes, C_{18-30}, chloro; chlorinated paraffins, C_{18-30}; chlorinated paraffin wax; chloroparaffin; chlorinated paraffin waxes and hydrocarbon waxes; hydrocarbon waxes, chlorinated; chlorparaffin; paraffin oils and hydrocarbon oils, chloro	Long-chain chlorinated paraffins (LCCPs); alkanes, C_{18-30}, chloro; chlorinated paraffins, C_{18-30}; chlorinated paraffin wax; chloroparaffin; chlorinated paraffin waxes and hydrocarbon waxes; hydrocarbon waxes, chlorinated; chlorparaffin; paraffin oils and hydrocarbon oils, chloro
Composition	UVCB: consists primarily of straight chain carbon aliphatic compounds $C_{<20}$ (US EPA, 2021)	UVCB (section 1.2 below)

[1] The Environment Agency notes that longer chained LCCPs have been detected.

Note: UVCB- unknown or variable composition, complex reaction products or biological materials.

Figure 1 Example structures of LCCPs



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A. $C_{18}H_{30}Cl_8$ LCCP 54% chlorine content by weight (Cl wt.)
B. $C_{20}H_{36}Cl_6$ LCCP 44% Cl wt.
C. $C_{25}H_{29}Cl_{23}$ LCCP 71% Cl wt.

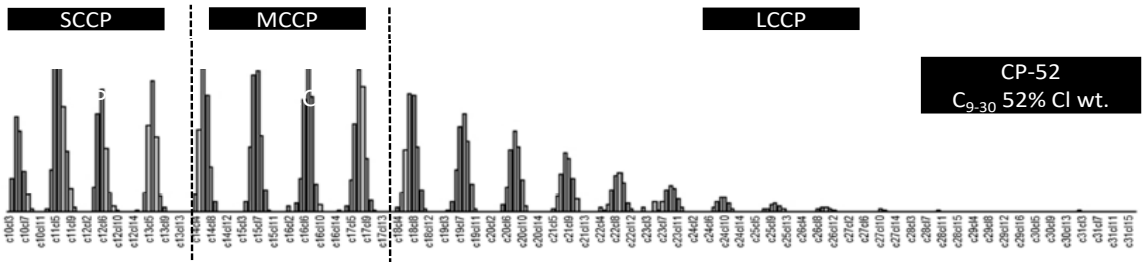
The ECHA public dissemination site (accessed December 2021; ECHA 2021c) lists 7 active and 2 inactive EU Registrants for CAS no. 63449-39-8. Of the 7 active Registrants, 1 submitted a dossier update in 2020, 2 submitted dossier updates in 2019 and 1 submitted a dossier update in 2016. The remaining Registrants have not submitted dossier updates since initial registrations in 2010 and 2015. Fifteen legal entity compositions are presented in the EU REACH registrations. These demonstrate the complexity of the registered substance. No information was presented on percentage distribution of constituents for each declared composition. Paraffin oils, chloro (CAS no. 85422-92-0) has not been registered as a discrete substance under EU REACH (ECHA, 2021c). Many alternative CAS numbers apply to LCCPs in different parts of the world, and a global inventory is presented in Appendix C: Global LCCP inventory.

Representatives of the LCCP REACH Consortium asked ECHA about the implications of using different feedstocks for LCCP products and were informed that they were appropriately covered under the existing registration (see also Section 1.2) (Personal Communication with LCCP REACH Consortium Representatives, 2019).

In Europe, North America and Australia, CPs are described as three distinct product types – SCCPs, MCCPs and LCCPs. However, Asian manufacturers use different feedstocks, producing CPs with a very wide range of chain lengths characterised by the chlorination level. These can include SCCP, MCCP and LCCP congeners in a single product. For example, Wei *et al*. (2016) discussed three commercial substances that are manufactured in large quantities in China: CP-42, CP-52 and CP-70, of which CP-52 accounts for 80-90% of the total commercial production. Castro *et al*. (2018) performed semi-quantitative mass fraction analysis of the

congeners contained within a CP-52 sample obtained from the author's colleagues at Tongji University (China) (Personal communication, M. Castro, University of Stockholm, September 2020). Using a negative ion atmospheric pressure chemical ionisation-quadrupole time-of-flight-high resolution mass spectrometry (APCI-qTOF-HRMS) method in conjunction with mathematical deconvolution, individual congener groups were resolved from the mass spectrum to produce a congener group fingerprint. A total of 224 congener groups from C_9Cl_3 to $C_{31}Cl_{16}$ were measured. The CP-52 product had a carbon chain length distribution in the range $C_{9\text{-}30}$ and 52% Cl wt., around a third of the constituents were congeners normally associated with SCCPs (Figure 2). This product has not been registered under EU REACH (as of December 2021) but may be present in imported articles.

Figure 2 Congener profiles of a current commercial Chinese CP product



Adapted and reprinted from Castro *et al*. (2018) supporting information. Copyright © 2018. Published by the American Chemical Society.

It is possible that similar materials are made in other countries such as India. However, industry has indicated that most CPs produced in India are used domestically (Personal Communication with LCCP REACH Consortium Representatives, 2019).

1.2 Composition

Environment Agency (2009a) contained a summary of substance composition compiled from several historical sources. As more modern analytical methods are available this older information is not repeated here.

In August 2019, the EU REACH Registrants updated the boundary composition description in their registrations. According to the LCCP REACH consortium representatives, they were advised that they should not be exclusive in their definition of LCCPs since there is no prescribed carbon number definition based on the EINECS/CAS numbers (Personal Communication with LCCP REACH Consortium Representatives, 2019). They subsequently provided a non-confidential summary statement to the Environment Agency, as follows:

"LCCPs are primarily comprised of chloroalkanes, predominantly in the carbon number range of C_{18} to C_{36}, with 20 to 75% Cl wt. LCCP is estimated to have 10^5 to

10^6 isomers based on the calculation referenced to Tomy *et al*. (1997). It is a UVCB substance. There are currently no analytical techniques capable of identifying individual constituents. For the boundary composition, as a UVCB substance, LCCP is effectively 100% "pure". Provided that the substance is a predominantly C_{18}+ polychlorinated alkane (20-75% chlorine by weight) it is within this boundary composition for the joint registration."

1.3 Chain length distribution

Representatives of the LCCP REACH Consortium (Personal Communication, 2019) noted that the LCCPs have a very broad composition range in comparison to MCCPs. As the paraffin feed stocks used in the synthesis of LCCPs increase in chain length, the cut-off between products become less precise. Therefore, quoted carbon numbers are typically an average and not the absolute carbon chain length. The UK-based EU REACH Registrant (at the time) noted that their paraffin feed stocks are sourced from plant-based materials and their general approach is to have a sharp cut-off in alkane chain length (C_{20-30}). This is different from the C_{14-17} feedstock for MCCP production, which is sourced from the petroleum industry. In the USA it is also common to use alpha-olefin (1-alkene) feedstocks. Alpha-olefins are oligomers of ethylene, and these feedstocks produce CPs which are almost exclusively even numbered.

Environment Agency (2009a) presented information on other chain lengths that might be present in LCCPs (Table 2).

Table 2 Minor chlorinated paraffin constituents in LCCPs (Environment Agency, 2009)

Feedstock	Constituent and typical concentration by weight
C_{18-20}	C_{16} <1% C_{17} 17% (range: 10 to 20%)
$C_{>20}$	C_{19} 0% C_{20} <0.2%

Liquid $C_{18–20}$ LCCP products may therefore contain a significant proportion of $C_{16–17}$ CPs, which are also constituents of MCCPs. Representatives of the EU REACH LCCP Consortium have confirmed that this composition is still relevant for current $C_{18–20}$ LCCP products (Personal Communication, 2019).

Environment Agency (2009a) stated that the $C_{>20}$ chlorinated paraffin products are virtually free from other related CP components. The LCCP REACH Consortium has

stated that “full-range” LCCP starting materials (both paraffin and alpha-olefin feedstocks) have <0.1% $C_{<18}$ constituents and generally only small amounts of $C_{<20}$ constituents (0 to 3%).

Chloroalkanes with carbon numbers greater than C_{36} have been detected (Brandsma *et al*., 2021 and Brits *et al*., 2020) in European monitoring samples, although their origin cannot be confirmed.

1.4 Chlorination

The MCCP REACH Consortium previously stated via personal communication (2019) that carbon atoms are randomly chlorinated, multiple chlorination of individual carbon atoms is unlikely and that terminal chlorination is not typical for these substances.

Academic studies over the last 10 years have explored the chlorination pattern of CPs. Although they considered MCCPs, the Environment Agency considers that the principles will be applicable to LCCPs.

Sprengel *et al*. (2019) characterised CPs using combinations of ^{1}H-nuclear magnetic resonance spectroscopy (NMR), ^{13}C-NMR, 2D-heteronuclear single quantum coherence (HSQC) spectroscopy and elemental analysis-isotope ratio mass spectrometry (EA-IRMS). Twenty-one single chain mixture CPs were synthesised and analysed alongside 29 CP technical mixtures ($C_{10\text{-}17}$). Chlorination levels were between 41.8% and 62.6% Cl wt. CP synthesis followed the method of Sprengel and Vetter (2019). In brief, the respective n-alkane ($C_{10\text{-}17}$) was irradiated in dichloromethane and sulfuryl chloride with a UV-lamp. The irradiation time was adjusted to control the chlorination degree. Commercially, CPs are synthesized on an industrial scale through the reaction of chlorine gas with liquid n-paraffin or paraffin wax at temperatures between 80 and 100 °C. From the data generated a calculation model was developed that could estimate the chlorination degree of single carbon chain length CPs (monochlorinated carbons [-CHCl-]). In addition, the data verified the presence of [$CHCl_2$-] and [-CCl_2-] groups in highly chlorinated (41.8 - 62.2% Cl wt.) single chain length mixtures and indicated the presence of non-chlorinated n-alkanes. As this work was performed using laboratory synthesised single carbon chain length CPs the Environment Agency cannot gauge how comparable these data would be to commercial products without further work being performed.

Building on the work of Sprengel *et al*. (2019), Yuan *et al*. (2020) demonstrated that chlorine atoms are not evenly distributed in CPs using a predictive NMR pattern matching framework to discriminate isomers in complex mixtures. The CPs used in

this study were supplied by the Chlorinated Paraffin Industry Association (Washington, DC, USA). The CPs had carbon chain lengths of C_{14} and C_{15} and chlorination levels between 39.75% and 60.14% Cl wt. (totalling nine different congener groups). The molar composition of each congener group was characterised using the non-linear algorithm described in Yuan *et al*. (2017a) and references therein. Fragments were identified using ^{13}C-NMR (^{1}H NMR spectra provided less detail). ^{13}C-NMR analysis identified that with increasing chlorination the number of $–CH_2-$ and methyl groups in the CP mixtures decreased and confirmed that dichloro-substituted carbons were present (trichlorinated carbons were also observed in small quantities). In brief the results showed that: 1) chlorine substitution at each carbon atom is not statistically evenly distributed in any CP mixture; and 2) the third carbon from the end of an n-alkane chain is the most reactive to chlorine in mixtures with low and intermediate chlorination levels (40 to 56 % Cl wt.). Yuan *et al*. (2020) calculated that the number of possible isomers for $C_{14}Cl_{1\text{-}10}$ and $C_{15}Cl_{1\text{-}7}$ CPs exceeds 41 000 (assuming $-CCl_2-$ groups are present). This number is approximately 25 times greater than previously calculated, which assumed that no more than one chlorine atom will be bound per carbon atom in a CP product. For LCCPs the potential number of isomers will exceed this value of 41 000 by more than an order of magnitude.

Endo *et al*. (2020) presented modelled synthesis data, which indicated that there is a lower probability for the terminal carbons to chlorinate, but noted an increased probability in chlorination at carbons near the terminal ends.

Environment Agency (2009a) presented the theoretical percent by weight chlorine contents (% Cl wt.) of several theoretical constituents of LCCPs. This has been updated and is presented in Appendix D.

1.5 Impurities

Commercial chlorinated paraffins may also contain several impurities, although these are not typically mentioned in the EU REACH registrations. For example, Environment Agency (2009a) states that isoparaffins may comprise about 1% of the paraffin feedstock (in the case of petroleum sources), so these could also be present in the final mixture; aromatic compounds are present at levels usually less than 100 parts per million (ppm). Chlorinated alkenes (i.e. olefins) might also be present as transformation products from dehydrohalogenation reactions.

In particular, some products of Asian origin have been shown to contain significant proportions of other impurities such as chlorinated fatty acid methyl esters (CFAMES), which may have endocrine disrupting effects (Sun *et al*., 2020).

1.6 Additives

Environment Agency (2009a) noted that long-chain epoxidised soya oil or glycidyl ether is added at concentrations <0.05% by weight to some CPs to inhibit the release of hydrogen chloride at elevated temperatures. For some high thermal stability formulations other additives, such as organophosphorus compounds, have been reported to be used in conjunction with these at <1% by weight. The Environment Agency was unable to verify whether these intentionally added components would be present in test materials used in regulatory studies or most academic tests and therefore cannot examine how they would influence the results. However, given the low concentrations, it is unlikely to be a major confounder in study interpretation.

1.7 Structurally related substances

Table 3 Substance identifiers for close analogues of LCCPs

	SCCPs	MCCPs
EC name	Alkanes, C_{10-13}, chloro	Alkanes, C_{14-17}, chloro
EC number	287-476-5	287-477-0
CAS number	85535-84-8	85535-85-9
Index number in Annex VI of the CLP Regulation	602-080-00-8	602-095-00-X
Molecular formula	$C_xH_{(2x - y+2)}Cl_y$, where x = 10 to 13 and y = 1 to 13	$C_xH_{(2x - y+2)}Cl_y$, where x = 14 to 17 and y = 1 to 17
Molecular weight range	176 to 632 g/mol (approximately)	232 to 826 g/mol (approximately)
Synonyms	Short-chain chlorinated paraffins (SCCPs); alkanes, C_{10-13}, chloro; chlorinated paraffins, C_{10-13} (used in Annex VI of the CLP Regulation)	Medium-chain chlorinated paraffins (MCCPs); Chlorinated paraffins, C_{14-17} (used in Annex VI of the CLP Regulation)

Environment Agency (2009a) noted that it was possible that $C_{\geq 18}$ chain lengths may be present in MCCP products. For example, a typical 52% Cl wt. MCCP product was reported to contain 0.16% C_{18} and <0.1% C_{19}. This might have some implications for the interpretation of monitoring data in terms of potential sources given the very high tonnage of MCCP's but is not a major issue for this assessment.

Environment Agency (2009a) mentioned two other CAS numbers that may be relevant related substances to LCCPs:

- Alkenes, polymerised, chlorinated (also known as chlorinated polyolefins) CAS no. 68410-99-1 (EC no. 614-454-8)
- Alkenes, C_{12-24}, chloro CAS no. 68527-02-6 (EC no. 271-247-1)

A search of the ECHA's public dissemination site (https://echa.europa.eu, last accessed April 2022) indicates that both substances were pre-registered under EU REACH but are not currently registered. There are entries for them on ECHA's Classification and Labelling Inventory, so they might be supplied at quantities below 1 tonne/year by individual companies, or alternatively they may no longer be used. Products formed from the chlorination of alkenes are expected to have the same environmental properties as the equivalent CP.

Environment Agency (2009a) also noted that Dover Chemical Corporation in the USA supplied mixtures of various compounds that may include mixed chlorinated and brominated paraffins (for example DOVERGUARD 9122 was described as a bromo-chlorinated paraffin/phosphorous blend; this product is no longer listed on the company's website https://www.doverchem.com/ last accessed November 2020). A search of ECHA's public dissemination site identified the following substances:

- Alkanes, C_{10-18}, bromo chloro CAS no. 68955-41-9 (EC no. 273-276-5)
- Alkenes, C_{12-30} α-, bromo chloro CAS no. 68527-01-5 (EC no. 271-246-6)

Both substances were pre-registered under EU REACH but have not been registered. There are no entries for them on ECHA's Classification and Labelling Inventory. Such products are likely to be equally or more hazardous than their chlorinated analogues, but as they appear to no longer be commercially relevant, they are not discussed further in this report.

2 Analytical chemistry

2.1 Analytical methods

The LCCP REACH Registrants do not recommend any analytical methods in their registrations (ECHA, 2021b). Environment Agency (2009a) contains a summary of analytical methods (pre-2009) for LCCPs in environmental matrices. Academic and regulatory interest in more accurate, precise, robust, and reliable methodology for CPs has gained traction in recent years as analytical capabilities have improved (van Mourik *et al*., 2015 and 2018; Yuan *et al*., 2018a and 2019a).

Chemical analysis of CPs is very difficult due to their compositional complexity (Yuan *et al*., 2020). The analysis of CPs is highly demanding in their pure form, where strong mass interferences can be evident i.e. where high molecular weight MCCPs and low molecular weight LCCPs cannot be differentiated due to low mass resolution of the detection method (Schinkel *et al*., 2018). In environmental samples, many common organic contaminants interfere with analysis alongside extraction challenges, i.e. other anthropogenic organo-halogen substances are co-extracted (see Section 4.2.5). Instrumental methods and reference standard selection can also impact the quality of the data produced.

Following the regulation of SCCPs under the Stockholm Convention, internationally validated monitoring methods are available for SCCPs – and to some extent MCCPs – in textiles, leather, and plastics (for example ISO/DIS 18219-1 and ISO/DIS 18219-2). EFSA (2020) recommended the need for a validated analytical method for the determination of CPs in food and feed as well as suitable reference standards (see Section 2.2). van Mourik *et al*. (2018) conducted a comparative study using 33 laboratories to assess the consistency of measured SCCP concentrations. This work is discussed in detail in the REACH Substance Evaluation report for MCCPs (ECHA, 2019) and is not repeated here.

A literature search conducted by the Environment Agency for analytical methods for the detection of LCCPs and their related structural analogues (SCCPs and MCCPs) in environmental matrices (fresh and marine water, sediment, sludge, soil, air and biota) generated > 80 results for the period 2009 to 2022. The thesis of van Mourik (2015) contains a full summary of methods used in the sample preparation and detection of CPs in a variety of media. Further comprehensive discussion is provided in the critical review paper of Yuan *et al*. (2019a) which also provides practical guidance to analytical chemists for the interpretation of generated data (e.g. deconvolution of C_nCl_m congener groups in a spectrum, following the methodology of

Bogdal *et al*. (2015)). Appendix G and Appendix H notes the current studies that contain the following desired details:

- Instruments and variables, including chromatographic column, temperature, mobile phase composition, flow rates, gradient or isocratic separation and the detector optimisation and configuration.
- Certified reference standards, calibration range and sensitivity, limit of detection, limit of quantification, column recoveries, stability and reproducibility.
- Sample preparation including clean-up consumables, concentration techniques and use of internal standards (plus justification for choice) for validation and recoveries, etc.
- Identification and discussion of technical limitations.

Even though the reliability and robustness of the methods have improved, Brandsma *et al*. (2017), Yuan *et al*. (2019a), and Krätschmer and Schächtele (2019) all highlight the caution that must be applied when comparing homologue and congener level characterisation of CPs.

The most common methods for quantifying "MCCPs" at a homologue and congener level are LC-API-HRMS[1], GC-ECNI-HRMS[2] (including direct injection APCI-HRMS[3]) and GC-ECNI-LRMS[4], respectively. Each of these analytical methods corresponds to the following form of evaluation pattern deconvolution, homologue specific, and linear regression, detailed in Bogdal *et al*. (2015), Yuan *et al*. (2017a) and Chen *et al*. (2011), respectively. These three methods are respectively capable of discerning different CP congeners (same carbon chain length with a given number of chlorine atoms e.g. C_nCl_m), congener groups (a selected range of carbon chain lengths, usually with an averaged degree of chlorination), and homologues (same chain length but varying number of chlorine atoms). Advantages and disadvantages that exist for these 3 approaches are discussed in detail in Krätschmer and Schächtele (2019). Cross comparison of results obtained with these methods should be approached with caution, particularly when applying a generalisation in terms of the degree of chlorination. For example, lower resolution methods – i.e. Gas

[1] LC-API-HRMS – Liquid chromatography – atmospheric pressure ionisation – high resolution mass spectrometry
[2] GC-ECNI-HRMS – Gas Chromatography – electron capture negative ionisation – high resolution mass spectrometry
[3] APCI-HRMS – Atmospheric pressure chemical ionisation- high resolution mass spectrometry
[4] GC-ECNI-LRMS – Gas Chromatography – electron capture negative ionisation – low resolution mass spectrometry

Chromatography - Electron Capture Negative Ionisation/ Low Resolution Mass Spectrometry (GC-ECNI/LRMS) and Gas Chromatography-Electron Capture Detection (GC-ECD) (a common method up to 2011, and still in use) – have insufficient sensitivity to identify and quantify congeners with fewer than 5 chlorine atoms and only allow for an approximate homologue/congener level identification. Furthermore, for LCCPs specifically, and especially very long CPs, elution in the GC column becomes the limiting factor. Low resolution GC does not allow the user to separate interferences like other halogenated compounds from the CPs either. Therefore, values may be overestimated (Personal communication, S Brandsma, Vrije Universiteit Amsterdam, December 2021).

Even using high resolution methods – i.e. high-resolution mass spectrometry (HRMS) like those employed by Krätschmer *et al*. (2018) and Bogdal *et al*. (2015) – CPs with lower chlorination degrees (<5 chlorine atoms) appear to be particularly difficult to accurately quantify (van Mourik *et al*. 2015). For methods that quantify the total concentrations of SCCPs, MCCPs or LCCPs based on the detectable ≥5 chlorine atom homologues. As a result, even though <5 chlorine atom homologues are “invisible”, the quantification methods may compensate the “missing concentration” by using a steeper calibration curve – the concentrations could be the real values, but of very high uncertainty (Personal Communication, B Yuan, University of Stockholm, 2021).

Measured values reported in academic literature pre-2011 should be considered indicative but not quantitative. After 2011, detections of “MCCPs” in biota and the environment are considered to be semi-quantitative in the following discussion. This is due to the number of different methods, instruments and laboratories involved. The most recent HRMS methods (2015 onwards) where mathematical corrections have been applied to account for variance between ‘standards’ and samples are considered accurate but cannot be described as fully quantitative due the absence of certified reference standards (See Section 2.2).

No chromatographic method is currently available that allows for the separation of congeners into their different isomers. NMR analysis is required for this level of detail (Sprengel *et al*., 2019). A recent study highlighted that GCxGC can separate some lower chlorinated CP isomers, furthermore it illustrated that NMR spectra are too complex in CP isomer mixtures to interpret the structures. NMR can only identify general substructures and can confirm the structure of single isomers (van Mourik *et al*. 2021).

Furthermore, an inherent difficulty in CP analysis lies in the highly variable constituents of commercial products, relating to the wide range of chlorination and chain lengths.

The use of commercial products as standards also introduces a potential bias towards the commercial product used in the synthesis of external calibration curves, as evidenced in several academic publications (Bogdal *et al*., 2015) (see Section 4.2.5). Commercial products have been acquired from different manufacturers for many studies, which therefore introduces further variation. This, however, reflects the range of substances that may be detected in the environment and enables reconstruction of the congener/ homologue patterns with confidence.

2.2 Analytical reference standards

Data presented throughout this report should be considered semi-quantitative, unless certified reference standards were available, or synthesis of a standard (with full characterisation) was performed.

Many academic papers published since 2015, beginning with that of Bogdal *et al*. (2015), present work that used technical product mixtures obtained from CP manufacturers to create a 'standard'. By characterising these products using high resolution mass spectrometry in conjunction with pattern matching and deconvolution, the accuracy and precision of congener pattern interpretation has improved. The deconvolution model is presented in Bogdal *et al*. (2015). These advances enabled authors such as Du *et al*. (2018, 2019 and 2020), Yuan *et al*. (2017a, 2018a, 2019, 2020, and 2021), and Zhou *et al*. (2019) to tentatively identify specific CP products detected within biota, by comparing deconvoluted congener patterns in product and tissue. Other academic groups such as Hilger *et al*. (2011) and Sprengel *et al*. (2019) have synthesised their own CP substances in the laboratory prior to analysis. Overall, it has been recognised by both the academic community and regulators that there is an urgent need for specific CP analytical standards, of varying chain length and chlorination level, to be available to improve comparability of data (Schinkel *et al*., 2018).

2.3 Statistical analysis

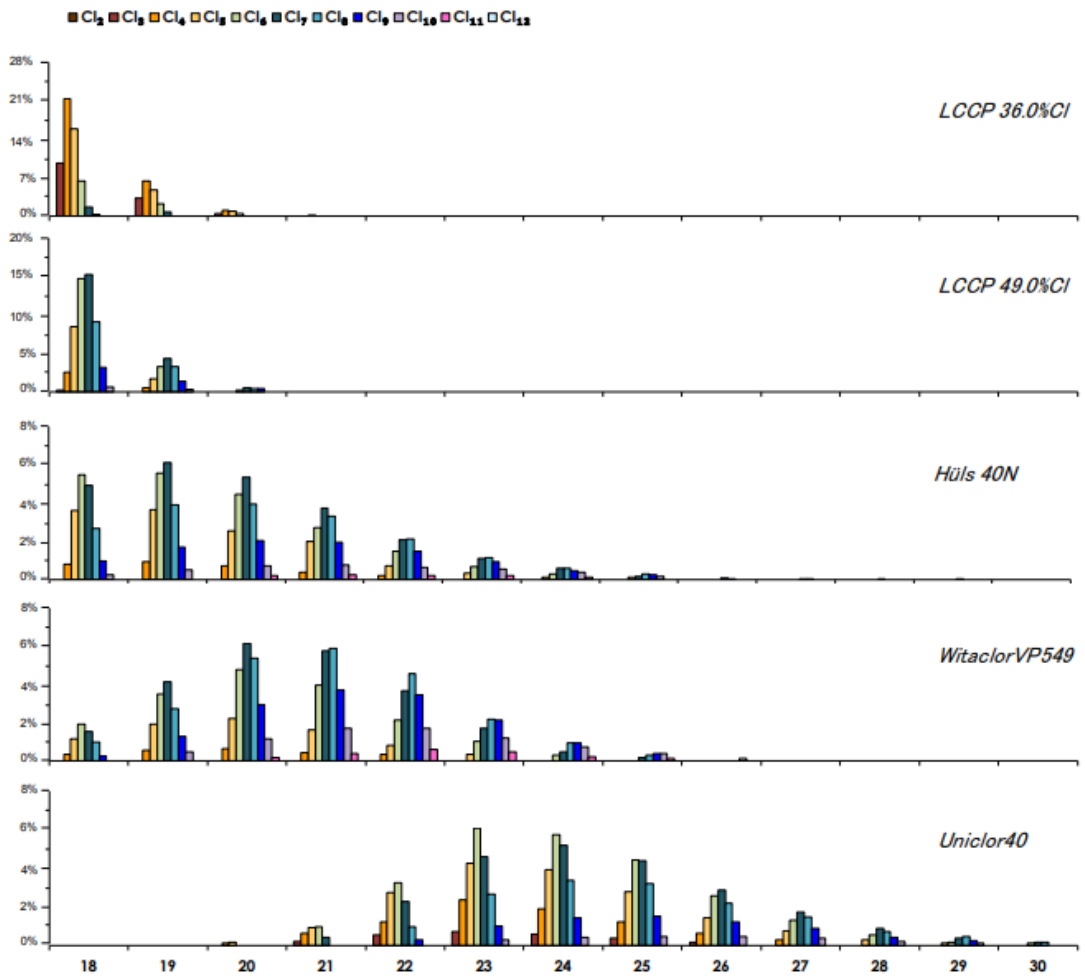
The Environment Agency considers that statistical uncertainty and outlier indicators, which would normally make reported concentration data unreliable, should not be applied for CPs. Concentration data for LCCPs can generate metrics such as standard deviations that are likely to exceed mean reported values. Standard deviations indicate precision for a normally distributed data set. For normally distributed data the standard deviation exceeding the mean indicates poor precision in measurements, the presence of outliers and occurrence of random errors, which should indicate that re-analysis is required. However, LCCPs are UVCBs, comprising congeners with chain lengths primarily from 18 to 37 carbons and varying

chlorination degrees. The relative contribution of each congener to the final product does not generate a single Gaussian peak in the detection and a skewed congener profile or fingerprint is frequently observed that will contain multiple peaks (see Figure 3). These fingerprints are unique to each commercial product.

Quantification is performed using commercial technical products that are selected to reflect the CPs expected to be detected in an environmental sample. It is important that they match as closely as possible, since otherwise confidence-of-fit in the reconstruction algorithm for the congeners decreases. This is discussed in the papers of Bogdal *et al*. (2015) and Brandsma *et al*. (2017). Figure 3 shows that technical products do not contain a normal symmetrical distribution of congeners (although a congener group with a single chain length and varying degrees of chlorination is assumed to be normally distributed) and can be dominated by specific chain lengths and chlorination degrees. Therefore, quantification of non-normally distributed components (covering a wide range of chain lengths) is performed against a technical product that also contains non-normally distributed components. The standard deviation is consequently not the best measure of accuracy or central tendency. The median or modal average and range could better reflect the breadth and variance of the data sets. Many of the field monitoring studies (Sections 4.3.1.4 and 4.3.2.4) have presented data this way.

Figure 3 **Congener profiles of LCCP technical commercial products using APCI-QTOF-MS (Du *et al.*, 2019 supporting information)**

.



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3 Physico-chemical properties

This evaluation focusses on vapour pressure, water solubility and n-octanol-water partition coefficient, because they are the key physico-chemical endpoints for the PBT assessment.

Commercial LCCP products can be free-flowing mobile liquids, highly viscous glassy liquids, or waxy solids and powders, depending on their carbon chain length distribution and chlorine content (Environment Agency, 2009). The substance can therefore be divided into sub-groups based on physical state, as outlined in Table 4.

Table 4 Sub-groups of commercial LCCPs (Environment Agency, 2009)

Carbon chain length	Chlorine content % wt.	Physical state
$C_{18\text{-}20}$	~ 30 – 35	Liquid
$C_{18\text{-}20}$	~ 44	Liquid
$C_{18\text{-}20}$	~ 48 - 52	Liquid
$C_{>20}$	~ 40 – 43	Liquid
$C_{>20}$	~ 48 - 54	Liquid
$C_{>20}$	~ 70 - 72	Solid

Note: The Environment Agency recognises that there is significant overlap in constituent congeners between the three subgroups.

The majority of data (including software predictions) presented in the EU REACH registrations (ECHA, 2021a) were also presented in Environment Agency (2009a). Environment Agency (2009a) did not assign reliability scores to these data and the software has since been updated. For the purposes of this evaluation, the Environment Agency has performed additional predictions using EPI Suite™ version 4.1 (US EPA, 2012) and the VEGA platform (IRSCC, 2021) where appropriate. A search of the US EPA curated COMPTOX database of in silico derived data was performed in December 2021, using the CAS numbers (USE EPA, 2021). This did not identify any data that were relevant for this assessment.

3.1 Vapour pressure

3.1.1 Measured data

Environment Agency (2009a) and the EU REACH registrations (ECHA, 2021a) cite the same studies for the vapour pressure endpoint:

- Howard *et al*. (1975) reported that the vapour pressures of C_{23} CPs containing 42%, 48% or 54% Cl wt. were all in the region of 2×10^{-5} mmHg (2.67×10^{-3} Pa) at 65 °C. Few details of how these were measured appear to be available.
- A value of 2.67×10^{-6} kPa (2.67×10^{-4} Pa) at 80 °C for a $C_{>20}$, 42% Cl wt. CP product was calculated from measurements generated using an effusiometric technique, as reported by Ineos Chlor (2005). No details of methodology were presented.

It is likely that the measured vapour pressures represented those of the most volatile components of the CPs. Lower vapour pressures would be expected at ambient temperature and pressure; the Clausius-Clapeyron equation could have been used to perform corrections, but this would require information on specific latent heat and the pressures at which the original measurements were made. These data are not available. The Environment Agency consider these data to be Klimisch 4 (unknown reliability), due to the lack of detailed information in their derivation.

Volatility and evaporation rates of LCCPs were considered in Environment Agency (2009a) and are not repeated in this report.

3.1.2 Predicted data

The Environment Agency predicted vapour pressures from SMILES codes for a series of hypothetical CP structures (terminally and evenly chlorinated) with carbon chain lengths in the range C_{18} to C_{30} and chlorine contents between 42 and 71% Cl wt. using the MPBPVP v1.43 model contained within the EPISuite™ v4.11 platform (US EPA, 2012; Appendix E). The Environment Agency was able to modify inputs to the software by using experimentally derived melting points which allowed for trends to be identified against chain length and chlorination levels. Values range from $< 10^{-7}$ to 2.5×10^{-4} Pa at 25 °C, with only lower molecular weight constituents (e.g. $C_{18}H_{33}Cl_5$) having vapour pressures exceeding 10^{-4} Pa. The guidance provided with the model indicates that the relationship between the experimental and predicted vapour pressure values, for a test set of 1 642 compounds, was good with an R^2 of 0.949, standard deviation of 0.59 and an average deviation of 0.32. However, no structural analogues of CPs or homologues of LCCPs were in the training set.

Therefore, these predictions should be treated with caution. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

In addition, the Environment Agency acquired predicted vapour pressure values for several of the above hypothetical LCCPs derived using the COSMOtherm software (Personal Communication, J Glüge, ETH Zurich, 2021). The data are presented in Appendix E. COSMOtherm software calculates the free energy of compounds in solution using quantum chemistry macroscopic thermodynamics to predict the chemical potential and thereby related properties (Dassault Systèmes, 2021). This model has previously been shown to have greater predictive accuracy for CPs compared to other commonly used models (Glüge *et al*., 2013). Much lower vapour pressures were indicated for the modelled LCCPs with the highest vapour pressure of 2.2 x 10^{-8} Pa predicted for $C_{18}H_{33}Cl_5$ at 25 °C. Vapour pressure decreased with increasing chain length and with increasing degree of chlorination, with degree of chlorination having a larger impact on the decrease in vapour pressure than chain length. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

Endo (2021) used COSMO-RS to generate training and validation data for fragment contribution models (FCM) for CPs. A set of CP congener structures (SMILES codes) built using a Monte-Carlo Model was passed to the trained FCMs to predict property distributions for CP mixtures. $C_{18\text{-}20}$ LCCP fragments were present in both the training and the validation sets. The full training and validation set consisted of SCCP, MCCP and LCCP chain lengths at two chlorination levels (53% Cl wt. and 75% Cl wt.). 1 070 CP congeners were included in the training set and 420 congeners were included in the validation set. The median log vapour pressure (at 25 °C) for $C_{18}Cl_1$ was -2.69 (2.04 × 10^{-3} Pa), decreasing to -13.06 (8.71 × 10^{-14} Pa) for $C_{18}Cl_{19}$. The log vapour pressure for a non-chlorinated C_{18} alkane was -1.65 (0.02 Pa). The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

3.1.3 Data from structural analogues

There is no experimental information available on the variation of vapour pressure with carbon chain length or chlorine content for LCCPs. Based on evidence for SCCPs (see ECHA, 2019), vapour pressure is expected to decrease with both increasing carbon chain length and chlorine content.

ECHA (2019) reports a measured vapour pressure of 1.3 to 2.7×10^{-4} Pa at 20 °C for a $C_{14\text{-}17}$ CP, 52% Cl wt. product. Based on molecular weight considerations, LCCPs would be expected to have a lower vapour pressure.

Glüge *et al*. (2013) calculated subcooled-liquid vapour pressure for 29 constituents of MCCPs using COSMOtherm, SPARC and EPI Suite™ (this study did not consider LCCPs). For C_{17} CPs with 1 chlorine atom, the vapour pressure was predicted to be around 0.004 Pa at room temperature. Vapour pressure was predicted to decrease with increasing chlorine content: The vapour pressure was consistently predicted to be ≤ 6.2×10^{-6} Pa for C_{17} CPs with 7 or more chlorine atoms. This provides a further indication of an upper limit of vapour pressures for LCCPs.

Hammer *et al*. (2021) determined the vapour pressures of CPs using a gas saturation method. A generator column was used to measure the partial vapour pressure (P) and saturated vapour pressure (P*) of each congener group between 20 °C and 50 °C. Quantification was performed using electrospray ionisation-tandem mass spectrometry (ESI-MS/MS). Limits of Quantification (LOQs) for SCCPs and MCCPs were 1.7 to 65.0 ng/mL and 0.49 to 3.0 ng/mL, respectively. Three technical mixtures with differing congener contributions were selected for investigation (Paroil 179-HV, Chlorowax 500C and SYCT-wax). Characterisation of the technical mixtures showed that Paroil 179-HV consisted of C_{10} to C_{13} chain lengths with 7 to 14 chlorine atoms per molecule, Chlorowax 500C consisted of C_{10} to C_{13} chain lengths with 4 to 10 chlorine atoms per molecule and SYCT-wax consisted of C_{10} to C_{17} chain lengths with 4 to 10 chlorine atoms per molecule. It is necessary to note that this method does not detect CPs with fewer than 4 chlorinated atoms per molecule, and these ranges reflect this. The measured P* decreased with increasing carbon chain length and chlorine content. Fewer data points were achieved at 20 °C than the higher temperatures for each of the commercial mixtures. The higher the temperature the greater the number of congeners identified at all chain lengths. Mean values of log P^* at 20 °C ranged from -2.08 ($C_{10}Cl_4$) to -4.73 ($C_{13}Cl_7$) for SYCT-wax. This was not measured for the other products at this temperature. The authors noted that data generated as part of this study were used to validate and calibrate a new model that could be applied to a broad range of CP congeners. However, for congeners with more than 10 chlorine atoms data were limited due to low volatility at ambient temperatures. Additionally, in the absence of certified calibration standards for highly chlorinated congeners, absolute values of P could not be measured even at the highest temperatures. The extrapolation of linear regression models to highly chlorinated congeners may cause further error due to a non-linear relationship between P* and the number of chlorine atoms. The Environment Agency considers these data to be Klimisch 2 (reliable with restrictions).

3.1.4 Summary

Available measured vapour pressure data for LCCPs are of unknown reliability and limited in their coverage of the products available (and are not extrapolated to room temperature). However, they suggest that the vapour pressure will generally be

below 10^{-4} Pa at 20 °C. Predicted data and evidence from MCCPs support this assumption, with many constituents likely to have much lower vapour pressures. Congeners with chain lengths at the lower end of the distribution range and a small number of chlorine atoms (e.g. 1 to 5) are likely to be the most volatile.

Averaged vapour pressure values estimated by the Environment Agency using EPI Suite™ may provide a rough indication of vapour pressure for different physical forms: 1.6×10^{-4}, 2.2×10^{-5} and $< 2.2\times10^{-5}$ Pa at room temperature for $C_{18\text{-}20}$ liquids, $C_{>20}$ liquids and $C_{>20}$ solids, respectively. Similarly, the COSMOtherm software indicated very low vapour pressures with a decrease in vapour pressure with increasing chain length and degree of chlorination.

Given the enormous complexity of LCCP compositions, further analysis is not considered appropriate.

3.2 Water solubility

3.2.1 Measured data

Environment Agency (2009a) and the EU REACH registrations (ECHA, 2021a) cite the same study for the water solubility endpoint. This is an unpublished pre-GLP study by Madeley and Gillings (1983), which investigated two radiolabelled LCCP products: 13-[^{14}C] n-pentacosane (C_{25} average chain length) 43% Cl wt. (liquid) and 70% Cl. wt. (solid). The study was performed using the guidance set out in EPA OPPTS 830.7840 (Water Solubility). The Environment Agency could not locate the 1983 version of the guideline, so potential differences from currently accepted guidelines could not be identified.

The test substances were prepared using radiolabelled n-paraffin, which was diluted with a non-radiolabelled n-paraffin feedstock (CWX40) prior to chlorination. The radiochemical purity of the 13-[^{14}C] n-pentacosane (C_{25}) substance was 98% and the chemical purity was approximately 90 % (the major impurity was n-tetracosane; C_{24} average chain length). The tests were carried out by weighing 50 mg of the test substance onto a glass slide and placing the glass slide substance-side up into the test vessel containing five litres of water. The vessel was stirred gently (100 rpm) in the dark for 91 days at 19±0.7 °C. After this period, the test system was maintained for a further 87 days with no stirring. Samples were taken at approximately 7-day intervals for analysis. Both ^{14}C and non-radiolabelled analyses were carried out using a thin layer chromatography (TLC) method. Measured concentrations were inconsistent during the stirring phase of the experiment, possibly owing to the presence of suspended droplets of test substance in the aqueous phase. The non-stirring phase of the experiment allowed for settlement of any suspended droplets of

test substance and for equilibrium to become established. By the end of this phase, the ^{14}C measurements indicated that the concentration had reached steady state, where measurements remained constant between 7 and 24 days. Mean concentrations determined at steady state were 6.4 µg/L in the experiments with the $^{14}C_{25}$, 43% Cl wt. substance and 5.9 µg/L with the $^{14}C_{25}$, 70% Cl wt. substance. The mean concentration calculated from non-radiolabelled analyses was <5 µg/L. This was below the detection limit of the method used. No further information about methodology was presented in Environment Agency (2009a) or ECHA (2021a).

LCCPs fall into the “difficult to test” category described in OECD Guidance Document 23 (OECD, 2019), as a UVCB substance. The method described is similar to that for achieving a water accommodated fraction as an exposure concentration for ecotoxicity assessment and does not correspond to the column elution or flask methods set out in OECD Test Guideline (TG) 105 (OECD, 1995). ECHA Guidance Document R.7a (ECHA, 2017b) states that both methods are suitable for substances with low solubility, but the slow stirring flask method in conjunction with an extended equilibrium time is also acceptable.

The Environment Agency notes the following:

- The test substance was dosed via a glass slide, which is inconsistent with the usual recommendation to dissolve the test substance at an elevated temperature and then cool to the desired test temperature prior to the initiation of stirring.
- No characterisation data were presented for the composition of the n-paraffin feedstock (CWX40) which was combined with the radiolabel (13-$^{14}C_{25}$ n-alkane) prior to chlorination.
- The lack of data detailing any characterisation of the substance that was dosed to the test systems does not allow assessment of any degradation to the radiolabel during the chlorination process.
- It is unclear how the analysis of the ‘parent’ substance was performed using TLC and whether this was also combined with radio-detection via phosphor-imaging.
- Environment Agency (2009a) noted that the TLC method was at the limit of its detection capabilities and therefore the results should be treated with caution.
- Radioactivity measurements are absolute and assuming the absence of transformation, the Environment Agency considers that the study is reliable with restrictions (Klimisch 2). The water solubility of both the C_{25} 43% Cl wt. and 70% Cl wt. CP products was around 6 µg/L at 20 °C.
- The reported water solubilities (3 - 9.4 µg/L) are similar to those of the shorter chained MCCPs, which is higher than expected. The methods used may not be appropriate for difficult to test substances.

Two supporting studies are also available:

- Tomy *et al*. (1998) presented a water solubility range of 8.6 to 9.4 µg/L for C_{18} 36-54% Cl wt. CP product (liquid). The Environment Agency has not been able to access the full text and therefore cannot evaluate the origin of the value.
- A seawater solubility of 3 µg/L at a temperature of 16 to 20 °C was reported for a C_{25}, 42% Cl wt. CP product based on radioactive tracer measurements (Campbell and McConnell, 1980). The Environment Agency has not been able to access the full text and therefore cannot establish the validity of this value.

3.2.2 Predicted data

The Environment Agency predicted water solubility from SMILES codes for a series of hypothetical chlorinated paraffin structures (preferentially terminally and evenly chlorinated) with carbon chain lengths of C_{18} to C_{30} and chlorine contents between 42 and 71% Cl wt. using the WSKOWWIN v1.41 and WATERNT v1.01 models contained within the EPI Suite™ v4.11 platform (US EPA, 2012; Appendix E). The Environment Agency was able to modify inputs to the software by using experimentally derived melting points which allowed for trends to be identified against chain length and chlorination levels. The highest value was 1.4×10^{-5} mg/L (0.014 µg/L) at 25 °C, with most congeners predicted to have a much lower water solubility. The WATERNT v1.01 model uses a "fragment constant" method like that used to estimate log K_{OW} values. Fragment-based methods may not estimate actual log K_{OW} values of CPs very well (see Section 3.2.3), which therefore casts uncertainty about the relevance of these predictions. In addition, there is no universally accepted definition of applicability domain for either model. The maximum molecular weight for substances in the training set for both models is 627.6 g/mol. Only one of the theoretical structures used to make the predictions had a molecular weight greater than this. However, the lowest predicted solubility was less than the minimum solubility of the lowest solubility substance in the test set (4×10^{-7} mg/L for both models). No structural analogues of CPs or homologues of LCCPs were in the training set. Therefore, these predictions should be treated with caution. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

In addition, the Environment Agency acquired predicted water solubility values for several of the above hypothetical LCCPs derived using the COSMOtherm QSAR modelling software (Personal Communication, J Glüge, ETH Zurich, 2021). The data are presented in Appendix E. This model has previously been shown to have greater predictive accuracy for CPs compared to other commonly used models (Glüge *et al*., 2013). Predicted data derived from the software indicate very low water solubility

with the highest water solubility of 1.67×10^{-3} mg/L (1.67 µg/L) at 25 °C determined for randomly chlorinated $C_{18}H_{33}Cl_5$. Interestingly, the water solubility of a CP with the same molecular formula, but with slight preference for terminal chlorination was an order of magnitude lower than when chlorination was assumed to be entirely random. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

Endo (2021) used COSMO-RS to generate training and validation data for fragment contribution models (FCM) for CPs. A set of CP congener structures (SMILES codes) built using a Monte-Carlo Model was passed to the trained FCMs to predict property distributions for CP mixtures. $C_{18\text{-}20}$ LCCP fragments were present in both the training and the validation sets. The full training and validations set consisted of SCCP, MCCP and LCCP chain lengths at two chlorination levels (53% Cl wt. and 75% Cl wt.). 1 070 CP congeners were included in the training set and 420 congeners were included in the validation set. The median log water solubility (mol/L, 25 °C, log solubility) for $C_{18}Cl_1$ was -10.30 M (1.4×10^{-8} g/L), increasing to -8.88 M (6.5×10^{-7} g/L) for $C_{18}Cl_7$, and decreasing to -11.84 M (1.3×10^{-9} g/L) for $C_{18}Cl_{19}$. The log water solubility for a non-chlorinated C_{18} alkane was -10.77 M (4.3×10^{-9} g/L). The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

3.2.3 Data from structural analogues

A modern non-GLP OECD TG 105 (column elution method) study for a C_{14} CP, 50 % Cl wt. test substance is described in ECHA (2019). The water solubility of C_{14} congeners with different chlorine numbers varied from 0.011 to 2.3 µg/L at 19 °C. Total water solubility values ranged from 3.56 to 11.11 µg/L, with an average of 6.1 µg/L (0.0061 mg/L). It would be expected that LCCP constituents would have lower water solubility values due to their longer chain lengths.

Glüge *et al*. (2013) calculated subcooled-liquid solubility in water for 29 constituents of MCCPs using COSMOtherm, SPARC and EPI Suite™ (this study did not consider LCCPs but may provide a further indication of an upper limit). In general, good, or very good agreement between calculated and measured data were obtained for COSMOtherm whilst EPI Suite™ showed the largest discrepancies. For C_{17} CPs with 1 chlorine atom, the water solubility was predicted to be around 0.09 µg/L at room temperature. Water solubility was predicted to increase with the number of chlorine atoms – up to around 12.7 µg/L for 9 chlorine atoms – before declining once more. The data also suggested that the water solubility is likely to decrease with increasing carbon chain length. However, the predictions for C_{14} congeners were up to an order of magnitude higher than the values measured in a modern OECD TG

105 study (see ECHA, 2019 for further details), so these conclusions should be treated with caution.

3.2.4 Summary

The available experimental data suggest a water solubility of between 3 and 10 µg/L at ambient temperature for LCCPs of differing chain lengths and chlorine contents. However, these are old studies, using non-standard methods with limited experimental detail. According to predicted data, water solubility is likely to decrease with increasing carbon chain length. These measured values are therefore much higher than would be expected based on the results of a modern OECD TG 105 study for a C_{14} CP, 50 % Cl wt. test substance (which had an average solubility of 6.1 µg/L).

The Environment Agency considers it would be valuable to measure the water solubility of different LCCP product types using a modern method. Without this information, it is not appropriate to speculate on the actual water solubility of different products or congener groups. However, it can be concluded that LCCPs is a relatively insoluble substance and solid products are likely to have a lower solubility than liquid ones.

The Environment Agency notes that much higher concentrations (up to around 4 mg/L) have been reported for some LCCP substances in aquatic tests (e.g. see Section 4.3.1.1). These may not be truly dissolved concentrations, based on the water solubility data.

3.3 n-Octanol-water partition coefficient (log K_{ow})

3.3.1 Measured data

The key study in the EU REACH registrations (ECHA, 2021a) is for a structural homologue (see Section 3.3.3).

Renberg *et al*. (1980) is also cited in the EU REACH registrations as supporting information. The study determined K_{OW} using a high-performance thin layer chromatography (HPTLC) method. Chromatographic separation was performed using pre-coated plates from EG Merck with an octadecyl (C_{18}) stationary phase. TLC spots were visualised using a silver nitrate reagent followed by UV-irradiation. Retention factors (Rm) were calculated using the equation: $Rm = \log(1/Rf - 1)$, where Rf is defined as the distance travelled by the compound divided by the distance travelled by the solvent front. For each HPTLC separation, two sets of

substances (analytical samples or high purity products) were used as internal standards (no further details such as the type of solvent used as the mobile phase were given). A linear standard curve was calculated, and the resulting equation was used to calculate log K_{OW} values for the target compounds. The reported values are provided in Table 5. The range of measured values for a given commercial product reflects the different HPTLC retention times of the constituents. It is apparent that log K_{OW} increases with the chain length.

Table 5 Log K_{ow} values for selected LCCP products (Renberg *et al.*, 1980)

Commercial product	Carbon chain length	% Cl wt.	Log K_{ow} range	Log K_{ow} average
Hüls 40N	$C_{21.5}$	42	7.63 to 12.83	10.23
Witaclor 44	C_{18-26}	44	7.46 to 11.48	9.47
Cereclor 42	C_{22-26}	42	9.29 to 12.83	11.06
Cereclor 48	C_{22-26}	49	8.69 to 12.83	10.76

This is a non-standard method that could be considered equivalent to OECD TG 117 (OECD, 2004a), which is usually applicable to substances with log K_{OW} values in the range of 0 to 6, but can be expanded to cover the log K_{OW} range between 6 and 10 in exceptional cases. Some of the measurements exceeded this range. Log K_{OW} values generated using HPLC methods should be treated with caution as this is not a direct measurement but a comparative assessment relying on external reference substances, with known log K_{OW} values. The same is true of TLC methods. The EU REACH Registrants have assigned a Klimisch score of 2 (reliable with restrictions) stating that it is an acceptable, well documented publication. However, the lack of information about the reference standards and mobile phase and failure to use substance-specific analytical methods, means the Environment Agency considers this study to be of unknown reliability (Klimisch 4).

ECHA (2019) summarises a non-GLP study by Hilger *et al*. (2011), which is not included in the current EU REACH registrations (ECHA, 2021a). This study used reversed-phase high performance liquid chromatography (RP-HPLC) for the analysis of synthesised polychlorinated n-alkanes with varying chlorination degrees and chain lengths (C_{10} to C_{28}), an SCCP technical mixture (Cereclor 63L), and 15 in-house synthesized C_{10}, C_{11} and C_{12} chloroalkanes with known chlorine positions. The method used was identical to that of OECD TG 117 (OECD, 2004a), including the handling of homologue substances. Interlaboratory comparison tests of the OECD 117 and the Shake-flask method (OECD TG 107, 1995) obtained log P_{OW} values within ± 0.5 log units.

Separation of the substances was performed using an ODS Hypersil column (40 °C) in conjunction with an isocratic mobile phase of methanol/water (90:10 v/v) and flow rate of 0.5 mL min^{-1}. Detection was performed using a diode array detector at a wavelength of 200 nm. Ten reference substances of known log K_{OW} (ranging from 2.37 to 7.86) were analysed to generate the capacity factor curves from which the log K_{OW} of the test substances would be derived. The estimated log K_{OW} values of the test substances most relevant to LCCPs are presented in Table 6.

Table 6 Estimated log K_{ow} values (and standard deviations) of LCCP constituents (adapted from Hilger *et al.*, 2011)

Carbon chain length	% Cl wt.	Log K_{ow} peak top[a]	Log K_{ow} peak range[b]
18	57.7	7.33 ± 0.05	6.58 to 8.60
22	52.2	8.57 ± 0.04	7.55 to 9.52
24	56.2	8.90 ± 0.04	8.26 to 10.42
28	54.8	10.1 ± 0.09	9.08 to 11.34

Note: a - Values correspond to the retention time of the chromatographic peak at its maximum.
b - Values correspond to the retention time of the start and end of the eluting chromatographic peak.

The authors note that when the entire data set was considered (including SCCP and MCCP congeners), it was apparent that the log K_{OW} value was relatively independent of the chlorine content for a given carbon chain length, for chlorine contents between approximately 45 and 55% Cl wt. For higher chlorine contents (up to 70% Cl wt.), the log K_{OW} increased with increasing chlorine content in a non-linear fashion. The correlation between chlorination degree and log K_{OW} was found to follow a second-order polynomial relationship.

The effect of carbon chain length on the log K_{OW} was investigated by grouping the substances by similar chlorine contents [< 60% Cl wt. (45% Cl wt. - 55% Cl wt.), ca. 60% Cl wt., ca. 65% Cl wt. and ca. 70% Cl wt.]. For a given chlorine content, the log K_{OW} values increased at an approximately constant rate for every addition of a carbon atom (the average increase in log K_{OW} was estimated to be around 0.29 per carbon).

The Environment Agency noted that the reference substances were aromatic (polar) compounds, and so are not close structural analogues of CPs, which are apolar. Hilger *et al*. (2011) acknowledged that the reference substances were not close analogues and had mainly sourced their log K_{OW} values from academic literature. The mobile phase was methanol/water (90:10 v/v), which could also lead to an

underestimation of log K_{OW} values through the broadening of peaks (although this is likely to be inconsequential). The upper calibration point of the method was equivalent to 7.86 log units. The identified trends are likely to be relatively unaffected because all the values would be expected to be biased in a similar way. The Environment Agency considers that these data are reliable with restrictions (Klimisch 2).

3.3.2 Predicted data

The Environment Agency predicted log K_{OW} values from SMILES codes for a series of hypothetical chlorinated paraffin structures (terminally and evenly chlorinated) with carbon chain lengths of C_{18} to C_{30} and chlorine contents between 42 and 71% Cl wt. using the KOWWIN v1.68 model contained within the EPI Suite™ v4.11 platform (US EPA, 2012; Appendix E). The Environment Agency was able to modify inputs to the software by using experimentally derived melting points which allowed for trends to be identified against chain length and chlorination levels. This is a fragment constant method, and the range of predicted log K_{OW} values was 10.23 to 21.36. Currently, there is no universally accepted definition of the applicability domain of this model. None of the test structures exceed the maximum molecular weight of the training set. The maximum number of chlorine atoms contained in a substance in the training set is 12. Many of the input theoretical structures exceed this. No structural analogues of CPs or homologues of LCCPs were in the training set. Therefore, these predictions should be treated with caution. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

ECHA (2019) compared predicted log K_{OW} values from the KOWWIN model with the experimental data from Hilger *et al*. (2011) for constituents of MCCPs: the difference was 3.29 log units for a C_{18} substance.

In addition, the Environment Agency acquired predicted log K_{OW} values for several of the above hypothetical LCCPs derived using the COSMOtherm modelling software (Personal Communication, J Glüge, ETH Zurich, 2021). The data are presented in Appendix E. This model has previously been shown to have greater predictive accuracy for CPs compared to other commonly used models (Glüge *et al*., 2013; Endo *et al*., 2021). The model suggests an increase in the log K_{OW} value with increasing chain length and degree of chlorination, with the lowest log K_{OW} of 7.636 determined for the randomly chlorinated $C_{18}H_{33}Cl_5$. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

Endo (2021) used COSMO-RS to generate training and validation data for fragment contribution models (FCM) for CPs. A set of CP congener structures (SMILES codes) built using a Monte-Carlo Model were assessed using the FCMs to predict property distributions for CP mixtures. $C_{18\text{-}20}$ LCCP fragments were present in both

the training and the validation sets. The full training and validation set consisted of SCCP, MCCP and LCCP chain lengths at two chlorination levels (53% Cl wt. and 75% Cl wt.). 1 070 CP congeners were included in the training set and 420 congeners were included in the validation set. The median log K_{ow} (25 °C) for $C_{18}Cl_1$ was predicted to be 9.97, decreasing to 8.38 for $C_{18}Cl_7$ and increased to 11.85 for $C_{18}Cl_{19}$. The log K_{OW} for a non-chlorinated C_{18} alkane was 10.48. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

3.3.3 Data from structural analogues

The key study in the EU REACH registrations (ECHA, 2020) is a modern non-GLP OECD TG 123 study (slow stirring method; OECD, 2006) on the structural analogue C_{14} CP, 50% Cl wt. (Unpublished, 2019). This is provided for read-across purposes in a weight-of-evidence assessment. It has been evaluated in detail in ECHA (2019). The average log K_{OW} value was 6.58 ± 0.09 at 19 °C. Variation of log K_{OW} for C_{14} congeners with different chlorine numbers was specifically assessed, and no trend was found. The EU REACH Registrants consider the study to be reliable without restrictions (Klimisch score 1), whereas the Environment Agency rates it reliable with restrictions (Klimisch score 2 – see ECHA, 2019 for details). As LCCP congeners have carbon chains with at least 4 more carbon atoms, they are likely to be more hydrophobic and therefore have greater K_{OW} values (unless the solubility in n-octanol also declines with increasing chain length).

Glüge *et al*. (2013) calculated log K_{OW} values for 29 constituents of MCCPs using COSMOtherm, SPARC and EPI Suite™, and compared the results to experimental data from the literature (this study did not consider LCCPs but provides comparative information). In general, good or very good agreement between calculated and measured data was obtained for COSMOtherm whilst EPI Suite™ showed the largest discrepancies. For C_{17} CPs with 1 chlorine atom, the log K_{OW} was predicted to be around 9.3. Values for higher chlorine contents (up to 15 chlorine atoms) did not change by much, reaching a maximum of 9.8. ECHA (2019) explains how the predicted values for C_{14} congeners with between 4 and 14 chlorine atoms (6.2 to 8.1) were somewhat higher than those measured in a modern non-GLP OECD TG 123 study (6.58 – see above). However, the predictions suggest that log K_{OW} values are relatively independent of chlorine content for a given carbon chain length, up to a chlorine content of 55% Cl wt., which is consistent with the findings of the experimental study for C_{14} congeners.

3.3.4 Summary

LCCPs are difficult to test because of their low water solubility and large number of congeners with a range of intrinsic chemical properties. Chemical analysis is also challenging.

There are no direct measurements of log K_{OW} for LCCP constituents. Studies using chromatographic methods (Renberg *et al*., 1980; Hilger *et al*., 2011) suggest values in the range of 7 to 13, although some of these exceed the highest value of the reference substances, which are either not defined or not structurally relatable to CPs. Nevertheless, the identified trends are relatively reliable because all the values would be expected to be biased in a similar way. Log K_{OW} values are relatively independent of the chlorine content for a given carbon chain length, for chlorine contents between approximately 45 and 55% Cl wt. For higher chlorine contents (up to 70% Cl wt.), the log K_{OW} increases with increasing chlorine content in a non-linear fashion. For a given chlorine content, the log K_{OW} values seem to increase at an approximately constant rate for every addition of a carbon atom.

Predicted values provide some support for these observed experimental trends, although the reliability of the actual values is highly uncertain. Most of the predictions are close to or above 10, where log K_{OW} values cease to be meaningful. COSMOtherm software predicts log K_{OW} values ranging from 7.6 to 14.9, where log K_{OW} values increase with increasing chain length and degree of chlorination.

Accurate determination of representative values for individual or groups of congeners is currently not possible. Ideally, a study of individual LCCP constituents using the OECD TG 123 Slow Stirring Method (2006) should be performed to give more reliable log K_{OW} values. For the purposes of this report, the Environment Agency concludes that LCCP congeners have high log K_{OW} values, many of which are likely to be ≥ 7.5. As chain length increases, the log K_{OW} will become very high.

4 Environmental fate properties

4.1 Degradation

4.1.1 Abiotic degradation

4.1.1.1 Hydrolysis

No hydrolytic data are presented in the EU REACH registrations of LCCPs (ECHA, 2021a). The Environment Agency considers that LCCPs are hydrolytically stable as they do not contain functional groups susceptible to this mechanism of transformation. In addition, they have a very low water solubility (see Section 3.2).

4.1.1.2 Phototransformation

No data about the phototransformation of LCCPs in water or soil are presented in the EU REACH registrations (ECHA, 2021b) or Environment Agency (2009a).

One non-standard study has been reported in the academic literature. Koh and Thiemann (2001) examined the kinetics of the photolytic oxidation of CPs by a combination of ultraviolet light and hydrogen peroxide in aqueous solution with and without co-solvents. The most efficient degradation was found in a 0.1% acetone/water medium (with and without peroxide addition), with half-lives for Hordalub 500 ($C_{10\text{-}13}$ 62% Cl wt.) and Hordaflex LC 50 ($C_{14\text{-}17}$, 52% Cl wt.) of less than 1 hour; the half-life for other products (CP 30 ($C_{17\text{-}24}$, 35% Cl wt.), CP 40 ($C_{17\text{-}20}$, 44% Cl wt.), CP 52 ($C_{12\text{-}18}$, 52% Cl wt.) and CP 56 ($C_{10\text{-}13}$, 56% Cl wt.)) ranged between 2.5 and 5.2 hours. Free chloride was determined using ion chromatography as a function of progressing degradation.

The Environment Agency has assigned a study reliability of ‘not reliable’ (Klimisch 3) for the following reasons:

- Acetone is a known photosensitiser. Under UV-light in an aqueous solution it can promote rapid oxidation and decomposition of organic substances. The authors do acknowledge this. Likewise, the use of hydrogen peroxide-doped media will increase radical concentrations in solution. Therefore, although the modelled kinetics show that under the conditions of the study the substances had the potential to transform quickly, it is not clear how relevant these data are to environmental conditions.
- UV exposures were performed at nominal concentrations of 125 µg/L and 250 µg/L depending on the technical substances. These concentrations are in excess of the water solubility range noted in Section 3.2. The standard

methodology for measuring phototransformation of chemicals in water (OECD TG 316; OECD, 2008) states that the test substance exposure concentration should not be greater than half its aqueous concentration. The best estimates of water solubility for LCCPs and MCCPs are approximately 1/10th of the exposure concentration used in this study. This excess concentration will detrimentally affect the reliability of the results.

- Specific analysis was performed using GC/MS, but interferences were noted due to poor separation and resolution of individual peaks. The authors note that decomposition products were only identified for the resolved peaks. This would only give a partial picture of the transformation of the substances.
- The kinetics were modelled from measured free chloride ion concentrations.
- These data should be treated with caution as no data are presented for non-dosed irradiated control samples.

Data relating to the atmospheric phototransformation of LCCPs were presented in the EU REACH registrations (ECHA, 2021b) and are referenced to Environment Agency (2009a). Atmospheric half-lives were estimated using the AOPWIN model of EPI SuiteTM, based on an atmospheric hydroxyl radical concentration of 5 × 105 molecule/cm3. Values for some representative structures covering the range of constituents present in LCCPs are provided in Table 7. The reliability of these predictions is unknown.

Table 7 Estimated half-lives for LCCP constituents in the atmosphere

Formula	% Cl wt.	K_{CH} (cm^3/ molecules-sec)	Atmospheric half-life (hours)
$C_{18}H_{33}Cl_5$	41.6	1.27×10^{-11}	30.3
$C_{18}H_{30}Cl_8$	53.6	9.83×10^{-12}	39.2
$C_{30}H_{53}Cl_9$	43.6	2.14×10^{-11}	18.0
$C_{30}H_{49}Cl_{13}$	53.0	1.79×10^{-11}	21.5
$C_{30}H_{35}Cl_{27}$	70.8	5.51×10^{-12}	69.9

LCCPs (C_{20+}) with chlorine contents of 70% was estimated using AOPWIN (v. 1.91) to have an atmospheric half-life of around 200 hours by ECCC (Personal communication, D Lee, Environment and Climate Change Canada, December 2021).

The relevance of photodegradation is likely to be low in most natural waters due to depth, turbidity, quenching agents etc. Due to the low vapour pressures and water solubility of LCCP constituents (see Section 3), the Environment Agency does not

expect that LCCPs will degrade significantly in either water or atmospheric compartments via this mechanism.

4.1.2 Biodegradation in water (including sediment)

4.1.2.1 Measured data

Screening tests

The EU REACH registrations contain the following screening studies for biodegradation in water:

- Two studies – Zitko (1974) and Zitko and Arsenault (1977) – assessed ready biodegradability in spiked sediment/water solutions. Environment Agency (2009a) contains additional information that has not been included in the EU REACH registrations. Two CP test substances ($C_{>20}$, 42% Cl wt. and $C_{>20}$, 70% Cl wt.) were examined. The experiment was carried out in flasks containing 25 g of sediment, 300 mL of sea water and 10 mL of a suspension of decomposing organic matter in sea water, at concentrations of 596 and 357 mg/kg dry weight (dw) sediment for the two test substances, respectively. Three flasks were used for both stoppered and aerated exposure scenarios. For each exposure, 2 flasks contained one of the two products tested, and the third was used as a control. All flasks were incubated between 19 and 22 °C for 28 days (the volume of water was kept constant in the aerated flasks by adding distilled water during the test). Samples of sediments were collected at intervals during the experiment and analysed for the presence of the CPs. The GLP compliance of the studies has not been specified, but as these are old academic studies, the Environment Agency assumes they were not performed to GLP. The results are shown in Table 8 Biodegradation in sediment/water (Zitko *et al*., 1974; Zitko and Arsenault, 1977) Concentration of chlorinated paraffin (mg/kg dry weight)Table 8.
- Environment Agency (2009a) provided details of the analytical method, which was based on microcoulometry. This method detects the presence of chlorine and would detect all chlorinated compounds present. Microcoulometry can experience interference from sulfur and nitrogen containing compounds. Interferences occurred in control vessels and those spiked with the $C_{>20}$, 42% Cl wt. product. The interferences were found to be volatile and could be removed by drying the sediment at 46 °C (27 psi; 186 kPa) overnight. The effect of this treatment on the recoveries of the CPs is not given, but the concentrations reported are corrected for overall recovery and background measurements in the control. After 30 days, all the remaining sediments were dried and analysed for CPs and breakdown products using TLC and infra-red spectrophotometry. Only trace amounts of the CPs could be detected, and

there was evidence of more polar metabolites being present. The study authors concluded that primary degradation of LCCPs occurred to some extent in these tests, at a higher rate under anaerobic conditions (stoppered flasks) than aerobic conditions (aerated flasks). However, this interpretation should be treated with caution as no information is given in the paper to show that the stoppered flasks were anaerobic (the flasks had effectively 200 mL of headspace, and the actual oxygen content of the stoppered flasks were not stated).

Table 8 Concentrations of $C_{>20}$ 42% Cl wt. (mg/kg dry weight) in biodegradation tests using sediment/water (Zitko *et al.*, 1974; Zitko and Arsenault, 1977)

Time	Aerated flasks [a]	Aerated flasks [b]	Stoppered flasks [a]	Stoppered flasks [b]
0 days	596	357	596	357
10 days	257	76	80	41
21 days	147	128	194	33
28 days	377	72	98	50

Note: a - Data from ECHA (2021b) and Environment Agency (2009a).
b - Data from Environment Agency (2009a).

The experimental design of this study is not comparable to any currently accepted test guidelines for the determination of ready (enhanced) or inherent biodegradability (i.e. OECD TG 301, 302, 306 or 310). The analytical methodology is not described in enough detail to ascertain what was being measured in the test samples. For example, were only freely soluble LCCPs measured by TLC or were extractions with solvent performed and therefore potentially extractable material included in the extracts? The evident fluctuations in concentration have not been sufficiently explained.

The Registrants interpret the results as indicating that $C_{20\text{-}30}$, 42% Cl wt. CPs are inherently biodegradable. No conclusion was noted for $C_{20\text{-}30}$, 70% Cl wt. The studies are rated as reliable with restrictions (Klimisch 2). The Environment Agency does not agree with this interpretation and considers this study to be unreliable (Klimisch 3).

- Madeley and Birtley (1980) performed three types of tests using a $C_{20–30}$, 42% Cl wt. CP product: a prolonged Biochemical Oxygen Demand (BOD) test; a series of Hach respirometry experiments; and an anaerobic sludge digestion experiment. Only the BOD study is presented in the EU REACH registrations. The results were discussed in detail in Environment Agency (2009a).

In brief, the prolonged BOD test used a concentrated emulsion of the test substance which was prepared in distilled water and left to stand for 24 hours. This was sub-sampled to measure the concentration. Measurements were performed after solvent extraction of the sub-samples using infra-red spectrophotometry. Aliquots of the concentrated emulsion were added to BOD dilution water to give final nominal concentrations of 2, 10 and 20 mg/L. Four BOD bottles were prepared for each test concentration. The vessels were then seeded with microbes. Two microbial populations were used in the study: a culture from soil collected close to a CP production plant that was acclimatised over an eight-week period to a concentration of 20 to 50 mg/L of the CP; and a non-acclimatized culture obtained from the effluent of a laboratory activated sludge unit treating domestic sewage.

The concentration of dissolved oxygen was measured at sampling intervals of 5, 10, 15, 20 and 25 days. Results were based on comparing the BOD to the theoretical oxygen demand (ThOD). After 25 days, 7.5% and 23% biodegradation were measured in the non-acclimated and acclimated bottles, respectively. The results are presented in Table 9, and indicated some potential for degradation with acclimated microorganisms.

Table 9 Biological oxygen demand (g O_2/g substance) concentrations values for $C_{20–30}$ 42% Cl wt. (Madeley and Birtley, 1980)

Substance	Inoculum	Day 10	Day 15	Day 20	Day 25	Percentage biodegradation[a] at day 25
$C_{20–30}$, 42% Cl wt.	Non-acclimated (soil)	0.16	0.18	0.31	0.14	7.5
$C_{20–30}$, 42% Cl wt.	Acclimated (laboratory activated sludge)	0.01	0.14	0.37	0.43	23

Note: a - The approximate % biodegradation was estimated from the BOD/ThOD ratio. The ThOD (theoretical oxygen demand) was estimated (ThOD (g O_2/g substance) = 16[2×c+0.5×(h-cl)]/mw; where c=number of carbon atoms, h=number of hydrogen atoms, cl=number of chlorine atoms and MW = molecular weight) for an example formula of the commercial substance as follows: 42% Cl wt. ($C_{25}H_{45}Cl_7$), ThOD=1.86 g O_2/g substance. Slightly different degradation percentages would be obtained if different formulae were used.

Environment Agency (2009a) also describes the series of experiments performed using non-acclimated micro-organisms in Hach respirometers. The test substance was a ^{14}C-labelled pentacosane ($C_{25}H_{52}$, radiolabelled on the central carbon) mixed with a $C_{20–30}$, 42% Cl wt. CP product. After eight weeks'

incubation, approximately 11% of the applied radioactivity was collected as $^{14}CO_2$, indicating that where degradation had occurred it was extensive enough to release the central carbon atom of the C_{25} chain. From the results presented it was not possible to determine whether the non-labelled chlorinated substance was degrading at the same rate as the non-chlorinated ^{14}C-pentacosane (C_{25}) under aerobic conditions.

The preliminary anaerobic study used anaerobic bacteria obtained from anaerobic sludge digesters as the inoculum. Gas production (methane and carbon dioxide) in the presence of increasing quantities of an emulsion of the CP test substance was determined over 30 days and compared with controls. No significant increase or decrease in bacterial activity was seen at concentrations of the CP up to 10% by weight of dry sludge solids. It was concluded that the substance was not toxic to the bacterial population present and was not actively degraded under anaerobic conditions.

The EU REACH Registrants have rated this study as Klimisch 2 (reliable with restrictions). The Environment Agency notes that the tests performed by Madeley and Birtley (1980) are not comparable to currently accepted test guidelines for assessing either ready or inherent biodegradation, i.e. OECD TG 301, 302, 306 or 310. No data were presented that would allow comparison against standard validity requirements (ECHA, 2017c). Current guidance does not allow for inocula to be pre-acclimated or pre-adapted to a test substance as this provides too favourable an environment for biodegradation, leading to false 'not persistent' conclusions (ECHA, 2017c). Although the results suggest that a $C_{20–30}$, 42% Cl wt. CP can potentially degrade under aerobic conditions, the Environment Agency considers the study to be unreliable (Klimisch 3).

- An unreferenced non-GLP study dated 1972 is referenced in the EU REACH registrations. Environment Agency (2009a) provides further details. Howard *et al*. (1975) reported the results of unpublished biodegradation studies on LCCPs carried out by Hildebrecht in 1972. Degradation (determined by oxygen consumption) was studied over 20 hours using a Warburg respirometer and over 5 days using a BOD method. The sewage seed was acclimated to up to 100 mg/L of the CP test substance before use in the test. The details of the substances tested, and the results are shown in Table 10.

Table 10 Biodegradation results of Hildebrecht (1972)

Chlorinated paraffin	Formulation tested	Warburg respirometry Oxygen consumption (mg/L)	Warburg respirometry Degradation[a]	BOD dilution method BOD (mg/L)	BOD dilution method Degradation[a]
$C_{>20}$, 40–42% Cl wt.	500 mg/L of a mixture containing 75% CP, 5% surfactant and 20% water.	83	17.2%	120	25%
$C_{>20}$, 70% Cl wt.	500 mg/L of a mixture containing 37.5% CP, 37.5% perchloroethylene, 5% surfactant and 20% water.	298	17.2%	30	2%
-	500 mg/L of the surfactant.	377	46.5%	530	65%

Note: a - Degradation was estimated by the authors as the percentage of the theoretical oxygen demand based on the total carbon content of the test solution. Substances other than the CP may have contributed to this total carbon content.

The EU REACH registrations (ECHA, 2021a) contain data for only one of the test substances assessed (C_{20-30}, 40 to 42% Cl wt. (liquid)) and concluded that the test substance is inherently biodegradable. Environment Agency (2009a) noted that $C_{>20}$, 70% Cl wt. degraded more slowly under the conditions of the BOD test.

The extent of degradation was determined by comparing the oxygen consumption in the test with the theoretical oxygen demand (ThOD) based on oxidation to carbon dioxide of the total organic carbon present in the solution from all sources. The Environment Agency notes that the test solutions contained a surfactant (and in some cases other carbon sources) that may have been biodegradable under the conditions of the test. Unidentified nutrients were also added to the test, which may also have contributed to the BOD. Howard *et al*. (1975) indicated that estimation of ThOD by this method is only approximate as it does not account for any oxygen consumed in the formation of water from available hydrogen. Therefore, the results refer to the biodegradability of the formulation tested rather than the actual CP component of the formulation. It is not possible to draw definite conclusions as to the potential degradability of CPs from the data.

The EU REACH Registrants have rated this study as Klimisch 2 (reliable with restrictions). The Environment Agency notes that the tests performed Howard *et al*. (1975) are not comparable to currently accepted test guidelines for assessing either ready or inherent biodegradation, i.e. OECD TG 301, 302, 306 or 310. No data were presented that would allow comparison against standard validity requirements (ECHA, 2017c). Current guidance does not allow for inocula to be pre-acclimated or pre-adapted to a test substance as this provides too favourable an environment for biodegradation, leading to false 'not persistent' conclusions (ECHA, 2017c). Although the results suggest that a $C_{>20}$, 40–42% Cl wt CP can potentially degrade under aerobic conditions, the Environment Agency considers the study to be unreliable (Klimisch 3).

An old study summarised in Environment Agency (2009a) has been disregarded by the EU REACH Registrants. Hoechst AG (1976 and 1977) reported 5-day BOD values for various LCCPs using non-adapted activated sludge. Few details of how the tests were carried out are available. The results are presented in Table 11 and show minimal biodegradation when compared with the measured chemical oxygen demand (COD) values.

Table 11 BOD and COD values for various LCCPs (Hoechst AG, 1976 and 1977)

Chemical	COD (mg O_2/g)	BOD (mg O_2/g)	Biodegradation
$C_{18–20}$, 35% Cl wt.	1,720	12	0.7%
$C_{18–20}$, 44% Cl wt.	820	<10	<1.2%
$C_{18–20}$, 49% Cl wt.	440[a]	<10	<2.3%
$C_{18–20}$, 52% Cl wt.	1,620	<10	<0.6%

Note: a - The COD value was not reproducible.

Although removal was reported to be >90% in all cases, the majority of removal was by adsorption to the sludge solids rather than mineralisation. The Environment Agency considers the reliability of these data to be unreliable (Klimisch 3).

Simulation tests

No standard definitive simulations studies were presented for LCCPs in the EU REACH registrations (ECHA, 2021a). The EU REACH Registrants state that an OECD TG 308 (OECD, 2002) water-sediment simulation study is technically not feasible since the substance is highly insoluble in water. The EU REACH registrations reference Fisk *et al*. (1998) and an un-named publication from 2005 as

supporting evidence, which are rated Klimisch 2 (reliable with restrictions). The GLP compliance was not specified.

Environment Agency (2009a) contains greater detail than the EU REACH registrations. Fisk *et al*. (1998) reported half-lives of 12 days and 58 days in aerobic sediment at 11.6 °C for two MCCPs: ^{14}C labelled $C_{16}H_{30.7}Cl_{3.3}$ (35% Cl wt., labelled in the 1-position) and $C_{16}H_{20.6}Cl_{13.4}$ (69% Cl wt., uniformly labelled). The Environment Agency considers that the study design and analytical methods were not sufficient to address the endpoints required of an OECD TG 308 study (i.e. primary and/or ultimate degradation rate, degradation half-lives ($DegT_{50}$), dissipation half-lives (DT_{50}), route and rate of transformation for substance and associated transformation products and non-extractable residues (NER)). The reported half-lives were calculated from data generated as part of a study investigating the accumulation of MCCPs in the oligochaete *Lumbriculus variegatus* and are summarised in EC (2005). The reported degradation was based on the difference between toluene-extractable ^{14}C-measurements (taken to represent unchanged CPs) and total ^{14}C-measurements in the sediment. Therefore, quoted half-lives depend on the assumption that the non-extractable ^{14}C represent total CPs and potential transformation products. It should also be noted that the study does not differentiate between dissipation half-life and transformation half-life. Data presented are dissipation half-lives. As no elevated temperature/pressure or modified extraction conditions were examined, it must be assumed that any NER or 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 extent. Based on available screening data reported in ECHA (2019), the 35% Cl wt. substance would be expected to be readily biodegradable, but the 69% Cl wt. substance would not. The Environment Agency considers this study to be unreliable (Klimisch 3) for the purposes of deriving relevant sediment half-lives.

4.1.2.2 Predicted data

No estimated data were included in the EU REACH registrations (ECHA, 2021a).

ECHA (2019) noted that almost all the MCCP structures modelled using the BIOWIN v4.10 model in EPI Suite™ are predicted to be persistent, although the predictions may not all be reliable. The REACH Guidance interpretation of the BIOWIN predictions is conservative when compared to the results of the available modified screening tests. This may partly because the guidance is based on the results of standard ready biodegradation tests rather than tests that have been modified to ensure appropriate dosing of the test substance. In addition, several of the modelled compounds contain more chlorine atoms than the maximum number of instances of the fragment in any training set compound for the BIOWIN 2 and 3 models.

Therefore, these constituents are outside the applicability domain of the model and the predictions may not be accurate.

An attempt by the Environment Agency to predict the biotransformation pathways of several congeners of MCCPs using EnviPath (the Environmental Contaminant Biotransformation Pathway Resource; Wicker *et al*., 2015) returned no pathways.

Since the same conclusions would be drawn for LCCPs, no further modelling has been performed for the purposes of this assessment.

4.1.2.3 Data from structural analogues

Data available for MCCPs (ECHA, 2019) indicate that C_{14} CPs, 41.3 and 45.5% Cl wt. meet the criteria for ready biodegradation in a modified ready test (using activated sludge inoculum) using alkylphenol polyalkoxylate to increase availability. C_{14} CP, 50% Cl wt. failed to meet the criteria for ready biodegradation under the same conditions but met the 60% pass threshold after an extended period of 56 days when river water was used as the inoculum. These substances would typically have around 4 to 5 chlorine atoms per molecule on average. The overall level of degradation declined with increasing numbers of chlorine atoms. Both a 55 and 60% Cl wt. C_{14} CP failed to meet the pass threshold even after extended timescales. These substances would typically have around 6 to 9 chlorine atoms per molecule on average. Similarly, C_{15} CP, 51% Cl wt. failed to meet the pass threshold after an extended timescale in river water (although it achieved up to 63% degradation after 60 days using inoculum derived from activated sludge). The alkane chains would typically have around 6 to 7 chlorine atoms per molecule on average. The interpretation of the results for MCCP test substances containing a mixture of alkane chain lengths was complicated by the lack of detail characterising the composition in terms of the varying chain lengths. As a substance, $C_{14\text{-}17}$ chlorinated n-alkane, 45.5% Cl wt. was not readily biodegradable, but more than 60% degradation was seen after extended timescales (i.e. after 28 days) using inoculum derived from activated sludge. No data were available for a river water inoculum.

In conclusion, $C_{14\text{-}17}$ CP, 45.5% Cl wt. may contain a significant proportion of constituents (e.g. C_{14}) that are readily biodegradable, but some constituents with longer chain lengths and/or a greater number of chlorine atoms are clearly less degradable. Both the 51.7 and 63.2% Cl wt. $C_{14\text{-}17}$ chlorinated n-alkane failed to meet the pass threshold after extended timescales using inoculum derived from activated sludge (no data are available using river water as the inoculum), although the former substance only narrowly failed (57% degradation was achieved after 60 days).

Biodegradation simulation studies using OECD TG 308 were performed for SCCPs and the results were summarised in ECHA (2008). A C_{10} CP, 65% Cl wt. (ca. 6 to 7

chlorine atoms per molecule) and a C_{13} CP, 65% Cl wt. (ca. 7 to 9 chlorine atoms per molecule) had degradation half-lives of 335 and 680 days, respectively, in marine sediments and 1 340 and 1 790 days, respectively, in freshwater sediments at 16 °C. The half-lives have been extrapolated beyond the 100-day exposure period and should be treated with caution, but these data were used to conclude that SCCP is a very persistent substance.

ECHA (2019) reports the results of an OECD TG 308 study in two types of aerobic natural freshwater sediment using a non-radiolabelled C_{14} 50% Cl wt. CP with congener specific analyses. The study was conducted over 120 days at 12°C in the dark and in accordance with GLP. Chemical analysis showed no observable biotransformation, and so the sediment half-life was >120 days under the conditions of this study. Both the EU REACH Registrants of MCCPs and the Environment Agency consider the study to be reliable without restriction (Klimisch 1). Although it is possible that there is a long lag period, the fact that there was no significant measurable degradation over 120 days suggests that it is unlikely that ≥50% mineralisation would occur over a subsequent 60-day period. Therefore, the Environment Agency considers that the sediment half-life of C_{14} CP, 50% Cl wt. is likely to exceed 180 days, although there is no empirical evidence to confirm this. The same test substance was found to degrade by 60% after 56 days in a ready biodegradation test using surfactant and a river water inoculum. The negligible degradation rate in aerobic sediment may reflect a reduction in bioavailability caused by adsorption and application in solvent rather than emulsion. Since the water-sediment simulation test is more environmentally relevant than the ready biodegradation test, it must be given more weight in the assessment of persistence.

4.1.2.4 Other information

Environment Agency (2009a) presented data from river system bacterial culture experiments performed by Allpress and Gowland (1999). A bacterium (*Rhodococcus* sp.) was able to utilise CPs as the sole source of carbon and energy, but little or no utilisation occurred for CPs with chlorination levels above 59 to 60% Cl. wt.

4.1.3 Biodegradation in soil

No standard definitive simulations studies were presented for LCCPs in the EU REACH registrations (ECHA, 2021a). Instead, the EU REACH Registrants report the results of a soil bacteria study by Omori *et al*. (1987), which they rate as Klimisch 2 (reliable with restrictions). The GLP compliance is not specified. The study is discussed in detail in Environment (2009). In summary, the degradation of $C_{24.5}$ CP, 40.5, 50 and 70% Cl wt. products was studied by monitoring the release of chloride ion in resting cell cultures of 5 bacterial species. Degradation was consistent with that of other chlorinated substances in that a variety of enzymes were required to

degrade CPs and the most likely mode of degradation involves firstly dechlorination of the terminal methyl groups, with subsequent oxidation to form chlorinated fatty acids, which are then broken down to 2- or 3-carbon chlorinated fatty acids via β-oxidation. The data indicate a potential for LCCPs to degrade under the conditions of the study. However, the Environment Agency does not consider the data to be relevant for the purpose of this assessment as there are no other soil studies to compare them to.

Heeb *et al*. (2019) reported the partial biotransformation of SCCPs by single enzyme cultures extracted from the soil bacterium Sphingomonadacea *Sphingobium indicum* B90A, which was isolated from dump sites of hexachlorocyclohexane (HCH) manufacturers in India, Japan and France. Several strains of the Spingomonadacea isolated from a HCH dump site have evolved to express a dehydrohalogenase LinA enzyme that can transform HCH and hexabromocyclododecane (HBCDD). LinA enzymes are both regio- and stereo-selective, breaking very specific carbon-hydrogen and carbon-halogen bonds. Heeb *et al*. (2019) hypothesised that many isomers present in CP technical mixtures may also be substrates for LinA2 and could be transformed to chlorinated olefins. The study detected *in vitro* conversion of some of the SCCP test material with LinA2. The observed transformation was very slow and not completed. Other CPs present in the test material were not transformed. Modelled half-lives were between 1.4 and 260 hours.

Leading on from the work of Heeb *et al*. (2019), Knobloch *et al*. (2021) examined the transformation of SCCPs with the LinB enzyme. In this study the codon optimised pDEST17 vector with a histidine tagged LinB gene from the same bacterial species as used by Heeb *et al*. (2019) was cloned into *Escherichia coli* BL21-AI bacteria. The LinB enzyme then produced by these modified bacteria catalysed dehalohydroxylation reactions and led to the formation of mono- and di-hydroxylated transformation products within a complex mixture of CP substances. $Cl_{>9}$ substances were observed to accumulate. $Cl_{<8}$ substances were preferentially transformed to mono- and di-hydroxylated substances (chlorinated alcohols). The authors confirmed that CPs with higher degrees of chlorination are more persistent.

The Environment Agency considers the studies of Heeb *et al*. (2019) and Knobloch *et al*. (2021) to be reliable with restrictions (Klimisch 2). However, although they suggest that SCCPs and related homologues have the potential to transform in soils that contain microorganisms with dehydrochlorination or dehalohydroxylation activity, the relevance of this information to LCCPs (which are more hydrophobic than SCCPs) under typical environmental conditions is limited. The half-lives were modelled from data generated using enzyme concentrations in excess of that which is environmentally relevant. A degree of acclimation and adaptation of the soil microorganisms is also likely based on their collection sites, so they may not be representative of species found in typical soils.

4.1.4 Transformation products

Environment Agency (2009a) presented a discussion on the possible degradation products of LCCPs. Degradation to more bioavailable SCCPs and MCCPs in the environment was considered unlikely for the following reasons. Under aerobic conditions, the most likely mechanism for degradation would be ß-oxidation, which would lead to chain shortening by two carbon units each time. This would also lead to oxidation of the terminal carbon, usually forming an acid group. As such these processes progress stepwise in reducing the carbon chain, thereby increasing bioavailability of the transformation product. There is no reason why it would stop at any particular carbon chain length. The co-metabolic degradation experiments carried out by Omori *et al*. (1987; see Section 4.1.3) indicated that ß-oxidation will initially form chlorinated fatty acids which are then broken down to 2- or 3- carbon chlorinated fatty acids. Under anaerobic conditions, most chlorinated compounds appear to degrade by reductive de-chlorination, which removes chlorine from the molecule but would not be expected to alter the carbon chain length. This sort of reaction has been extensively studied for halogenated aromatics, but substances such as tetrachloroethylene and trichloroethylene appear to degrade in a similar way. Again, even if chain shortening did occur as well, there is no reason why the reaction would stop at any particular carbon chain length. From the above studies of Heeb *et al*. (2019) and Knobloch *et al*. (2021) it could be surmised that once LCCPs and MCCPs were degraded to SCCP chain lengths, degradation would continue to the same 2- or 3-carbon fatty acids. However, congeners with different chain lengths, degree of chlorination and position of chlorination are likely to have variable resistance to biodegradation.

Wu *et al*. (2020a) examined soils contaminated with CPs. Their results indicated that soil microbes exposed to CPs and other contaminants may lead to microbial group assemblages with the potential for degradation.

Contradictory data were presented in a study by He *et al*. (2020) (Section 6.9), who investigated metabolism of CPs in human liver microsomes. Enzymatic transformation of LCCPs and MCCPs was reported to lead to increased concentrations of MCCPs and SCCPs, respectively. However, the Environment Agency considers that the results are unreliable (Klimisch 3) given the deficiencies in the data (see Section 6.9 for more details).

4.1.5 Summary and discussion of degradation

No degradation studies are available for LCCPs that meet current regulatory standards. Key studies cited in the EU REACH registrations cannot be considered reliable. However, it is possible to conclude that LCCPs are unlikely to undergo significant abiotic degradation.

There are no environmental simulation studies, but evidence for SCCPs and MCCPs indicates that the rate of biodegradation will vary according to chain length and chlorination level of the substance. Some of their constituents, particularly those with shorter chains and lower degrees of chlorination, meet the criteria for ready biodegradation in modified tests (where surfactants have been used to increase availability or the time period is extended beyond 28 days). However, higher degrees of chlorination lead to reduced biodegradation rates. Longer chain lengths found in LCCPs would be expected to be less water soluble and more adsorptive than $C_{\leq 15}$ CP substances, and therefore rates of degradation are likely to be even lower.

Of greatest relevance to this assessment is the finding that constituents of both SCCPs and MCCPs have long degradation half-lives in sediment. For C_{10} CP, 65% Cl wt. (ca. 6 to 7 chlorine atoms per molecule) and C_{13} CP, 65% Cl wt. (ca. 7 to 9 chlorine atoms per molecule), a half-life of 335 and 680 days, respectively, was determined in marine sediments at 16 °C (with longer half-lives in freshwater sediment). A measured half-life >120 days at 12 °C was reported for a C_{14} CP, 50% Cl wt. substance in two types of aerobic freshwater sediment (with the half-life likely to exceed 180 days since chemical analysis showed no observable biotransformation over the duration of this study).

There is evidence that some adapted microorganisms may be capable of degrading LCCPs in the environment in acclimated or co-metabolic systems. However, it is unclear if the same trend would be observed for LCCPs as MCCPs, where n-alkanes with fewer than 5 chlorine atoms may have the potential to degrade within shorter time frames.

In the absence of reliable measured data to the contrary, the assumption must be that most constituents of LCCPs will have long half-lives in freshwater sediments, most likely exceeding 180 days at 12 °C. It is possible that low chlorine content products (e.g. 30% Cl wt.) might not be as persistent, but definitive data to confirm this are not available.

4.2 Environmental distribution

This section only summarises information that is directly relevant to the PBT assessment.

4.2.1 Adsorption/desorption

No experimental data are available for LCCPs in the EU REACH registrations (ECHA, 2021a), and none were located in the literature search.

Castro *et al*. (2018) studied the partitioning behaviour of five different CP technical mixtures using the water flea Daphnia magna as the organic carbon substrate. This study is not reported in the EU REACH registrations (ECHA, 2021a). Toxicity aspects of this study are discussed in Section 6.1. The calculated organic carbon-water partition coefficient (K_{OC}) values are not comparable to those that would be determined via OECD TG 106 (OECD, 2000), so are not summarised in this report. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

The Environment Agency has predicted log K_{OC} values using the KOCWIN v2.00 model in EPI Suite™ for selected LCCPs that were homogenously chlorinated. These data are presented in Table 12.

Table 12 Predicted organic carbon-water coefficient (log K_{OC}) for selected LCCP constituents (homogenously chlorinated) using EPI Suite™ KOCWIN v2.00

Molecular formula	% Cl wt.	g/mol	Melting point °C	Log K_{ow}	Log K_{oc} (MCI [a])	Log K_{oc} (Log K_{ow} [b])
$C_{18}H_{30}Cl_8$	54%	530	0	10.7	6.9	9.3
$C_{20}H_{33}Cl_9$	54%	593	0	11.9	7.7	10.3
$C_{25}H_{42}Cl_{10}$	51%	697	0	14.5	9.2	12.6
$C_{30}H_{49}Cl_{13}$	53%	871	0	17.6	11.2	15.2
$C_{18}H_{33}Cl_5$	42%	427	-25	10.2	6.4	8.9
$C_{20}H_{36}Cl_6$	44%	489	-25	11.3	7.0	9.8
$C_{25}H_{45}Cl_7$	42%	594	-25	14.0	8.5	12.1
$C_{30}H_{53}Cl_9$	44%	733	-25	16.8	10.2	14.6
$C_{25}H_{29}Cl_{23}$	71%	1145	100	16.8	12.0	14.6
$C_{30}H_{35}Cl_{27}$	71%	1353	100	20.1	14.2	17.4

Note: a - $\log K_{OC} = 0.5213\ MCI + 0.6$ [MCI: Molecular Connectivity Index]
b - $\log K_{OC} = 0.8679 \log K_{OW} - 0.0004$

The predicted log K_{OC} ranges from 6.4 to 17.4. Based on the findings of Glüge *et al*. (2013) that EPI Suite™ did not perform well for calculating log K_{OW} values for 29 constituents of MCCPs (see Section 3.3.4), so these values may not be reliable. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

Predictions of log K_{OC} were therefore also performed using the VEGA KOC Model (IRFMN) v 1.0.0 for the same group of LCCPs. The predicted log K_{OC} value was approximately 11.7 for all substances. The Applicability Domain Index (ADI) values

ranged from 0.47 to 0.66, where 0 is the worst case and 1.0 the best case. No similar compounds with known experimental values were located in the training set.

In addition, the Environment Agency acquired predicted log K_{OC} values for several of the above hypothetical LCCPs derived using the COSMOtherm modelling software (Personal Communication, J Glüge, ETH Zurich, 2021). The data are presented in Appendix E. This model has previously been shown to have greater predictive accuracy for CPs compared to other commonly used models (Glüge *et al*., 2013 & Endo *et al*. 2021). The lowest log K_{OC} was determined as 5.3 for $C_{18}H_{33}Cl_5$ and the highest as 12.3 for $C_{25}H_{29}Cl_{23}$ (the longest chain length modelled). The degree of chlorination had a far greater influence on the predicted log K_{OC} than chain length in this model.

The Environment Agency considers that these predicted values are uncertain as the reliability of these methods is unknown for this type of substance.

Many constituents of LCCPs have low water solubility and are likely to have log K_{OW} values ≥ 7.5 (see Section 3.3.4). This means that they will be highly adsorptive to suspended matter, sediments and soils. This is consistent with the information provided in the EU REACH registrations (ECHA 2021a) and Environment Agency (2009a). Therefore, persistence in the sediment compartment is more relevant than persistence in the water compartment.

4.2.2 Henry's Law constant

The EU REACH registrations (ECHA, 2021a) present calculated Henry's Law constants (HLC) for different fractions of LCCPs, referenced to Environment Agency (2009a). The information is rated Klimisch score 2 (reliable with restrictions) by the EU REACH Registrants. Given the uncertainty in the physico-chemical properties (see Section 3), the Environment Agency considers that these calculated HLC values may be unreliable.

Glüge *et al*. (2013) compared estimated HLCs (water) for SCCPs and MCCPs using EPI Suite™, SPARC and COSMOtherm estimation software against published experimental data. All three calculation programmes and experimental values predict a decrease in HLC with increasing chlorine content and chain length.

In addition, the Environment Agency acquired the predicted HLC values for several of the above hypothetical LCCPs derived using the COSMOtherm modelling software (Personal Communication, J Glüge, ETH Zurich, 2021). The data are presented in Appendix E. This model has previously been shown to have greater predictive accuracy for CPs compared to other commonly used models (Glüge *et al*., 2013; Endo *et al*., 2021). The Henry's Law constants ranged from 1.52 $x10^{-10}$ for

$C_{18}H_{33}Cl_5$ to 3.09 x 10^{-22} for $C_{25}H_{29}Cl_{23}$ in octanol and 3.94 x 10^{-2} for $C_{18}H_{33}Cl_5$ 4.61 x 10^{-7} for $C_{25}H_{29}Cl_{23}$ in water. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

The Environment Agency therefore expects that under environmentally relevant conditions, volatilisation from water is likely to be an insignificant transfer mechanism for most constituents of LCCPs. Adsorption of LCCPs to dissolved organic carbon is likely to be more relevant.

4.2.3 Octanol-air partition coefficient (Log K_{OA})

The octanol-air partitioning coefficient gives an indication of the propensity of a substance to volatilise from organic media and can be used in the determination of the Henry's Law constant. It is also indicative of the potential for bioaccumulation in terrestrial organisms (log K_{OA} > 5, REACH Guidance Document R.11 (ECHA, 2017a)). This is discussed is greater detail in the bioaccumulation summary and conclusion (Section 4.3.3).

The Environment Agency has predicted octanol-air partition coefficients using the KOAWIN v1.10 model in EPI Suite™ for selected LCCPs that were homogenously chlorinated. These data are presented in Table 13.

Table 13 Predicted log K_{OA} values for selected LCCP constituents (homogenously chlorinated) using EPI Suite™ KOAWIN v1.10

Molecular formula	% Cl wt.	Molecular weight g/mol	Melting point (assumed) °C	Log K_{ow}[a]	Log K_{AW}[b]	Log K_{OA}[c]
$C_{18}H_{30}Cl_8$	54%	530	0	10.7	-1.1	11.8
$C_{20}H_{33}Cl_9$	54%	593	0	11.9	-1.3	13.1
$C_{25}H_{42}Cl_{10}$	51%	697	0	14.5	-1.1	15.6
$C_{30}H_{49}Cl_{13}$	53%	871	0	17.6	-1.8	19.4
$C_{18}H_{33}Cl_5$	42%	427	-25	10.2	0.3	9.9
$C_{20}H_{36}Cl_6$	44%	489	-25	11.3	0.1	11.2
$C_{25}H_{45}Cl_7$	42%	594	-25	14.0	0.3	13.7
$C_{30}H_{53}Cl_9$	44%	733	-25	16.8	0.0	16.8
$C_{25}H_{29}Cl_{23}$	71%	1145	100	16.8	-7.0	23.8
$C_{30}H_{35}Cl_{27}$	71%	1353	100	20.1	-8.2	28.3

Note: a - Estimated from the EPI Suite™ KOWWIN™ model.
b - Air-water partition coefficient, estimated using the EPI Suite™ HENRYWIN™ model.
c - Estimated from the EPI Suite™ KOAWIN™ v1.10 model using the ratio of K_{OA} and K_{AW}.

Based on the findings of Glüge *et al*. (2013) that EPI Suite™ did not perform well for calculating log K_{OW} values for 29 constituents of MCCPs (see Section 3), these values may be inaccurate.

Predictions of log K_{OA} were therefore also performed using the VEGA KOA Model (OPERA) v 1.0.0 for the same group of LCCPs. The predicted log K_{OA} value was approximately 11.7 for all substances. The Applicability Domain Index (ADI) values ranged from 0.47 to 0.66, where 0 is the worst case and 1.0 the best case. No similar compounds with known experimental values were located in the training set, so the predicted values may be unreliable.

In addition, the Environment Agency acquired predicted log K_{OA} values for several hypothetical LCCPs (the same as those modelled for K_{OC}) derived using the COSMOtherm modelling software (Personal Communication, J Glüge, ETH Zurich, 2021). These data are presented in Appendix E. Log K_{OA} values are predicted to increase with increasing chain length and degree of chlorination. The degree of chlorination appears to have a greater impact on the log K_{OA} than does chain length. The lowest log K_{OA} of 13.2 was predicted for $C_{18}H_{33}Cl_5$ and the highest of 24.9 for the longest chain length modelled, namely $C_{25}H_{29}Cl_{23}$. The Environment Agency consider these data to be Klimisch 4 (unknown reliability).

Endo (2021) used COSMO-RS to generate training and validation data for fragment contribution models (FCM) for CPs. A set of CP congener structures (SMILES codes) built using a Monte-Carlo Model was passed to the trained FCMs to predict property distributions for CP mixtures. $C_{18\text{-}20}$ LCCP fragments were present in both the training and the validation sets. The full training and validations set consisted of SCCP, MCCP and LCCP chain lengths at two chlorination levels (53% Cl wt. and 75% Cl wt.). 1 070 CP congeners were included in the training set and 420 congeners were included in the validation set. The median Log K_{OA} (25 °C) for $C_{18}Cl_1$ was predicted to be 9.11, increasing to 19.74 for $C_{18}Cl_{19}$. The log K_{OA} for a non-chlorinated C_{18} alkane was 8.15. The Environment Agency considers these data to be Klimisch 4 (unknown reliability).

4.2.4 Long-range transport potential

4.2.4.1 Measured

No measured atmospheric half-lives are available for CPs with $C_{18\text{-}30}$ chain lengths.

4.2.4.2 Predicted

The Environment Agency has used AOPWIN v1.91 (US EPA, 2021) to make predictions of the hydroxyl radical rate constant (K_{OH}) to estimate atmospheric half-

lives for LCCP constituents in the vapour phase. Data are presented Table 14. The SMILES codes relating to these molecules are presented in Appendix E.

Table 14 Predicted atmospheric half-lives, and hydroxyl radical rate constant (K_{OH}) for several theoretical LCCP constituents

Chemical formula	% Cl wt.	Molecular weight	Terminal chlorination Overall K_{OH} rate constant (cm^3/ molecule-sec)	Terminal chlorination Half-life (days)[a]	Non-terminal chlorination Overall K_{OH} rate constant (cm^3/ molecule-sec)	Non-terminal chlorination Half-life (days)
$C_{18}H_{30}Cl_8$	53.6	530.06	14.713×10^{-12}	0.727	10.06×10^{-12}	1.063
$C_{18}H_{33}Cl_5$	41.6	426.73	18.655×10^{-12}	0.573	15.30×10^{-12}	0.699
$C_{25}H_{29}Cl_{23}$	71.3	1144.93	13.369×10^{-12}	0.800	3.031×10^{-12}	3.528
$C_{25}H_{42}Cl_{10}$	50.9	697.14	21.969×10^{-12}	0.487	13.518×10^{-12}	0.791
$C_{25}H_{45}Cl_7$	41.9	593.81	25.922×10^{-12}	0.413	18.997×10^{-12}	0.563

Note: a - 12-hour day; 1.5×10^6 OH/cm^3

The model is based on a training set of 667 organic chemicals, of which 1-chlorohexane is the closest analogue to the chlorinated $C_{18\text{-}30}$ structures. Five LCCPs have been modelled. The C_{18} congener was selected based on minimal laboratory data for persistence and bioaccumulation, and a C_{25} congener was selected as they are widely detected in field monitoring samples. Using a hydroxyl radical concentration of 1.5×10^6 OH/cm^3, varying atmospheric half-lives were calculated. No distinct trend was observed in the likelihood of atmospheric photodegradation. These estimates should be treated with caution, as the closest chlorinated alkane in the model training set is a C_6 alkyl substance with a single chlorine atom, and there are no measured data with which to directly compare the current estimates. For a given chain length, increasing the chlorination level decreases the rate constant as fewer C-H bonds exist for reaction with the hydroxyl radicals.

In addition, the Environment Agency acquired predicted second order rate constants for degradation in air with hydroxyl radicals (25 °C) using the COSMOtherm modelling software (Personal Communication, J Glüge, ETH Zurich, 2021). The data are presented in Appendix E. Values ranged from 8.9×10^{-13} cm^3/sec ($C_{18}H_{22}Cl_{16}$) to 1.17×10^{-12} cm^3/sec ($C_{25}H_{29}Cl_{23}$). No clear trend with regards to chain length or chlorination level could be discerned.

CPs are only likely to be present in the atmosphere on particulate material, due to their very low vapour pressure and high estimated K_{OC} values. The relevance of vapour phase reaction rates with hydroxyl radicals is therefore likely to be low.

4.2.4.3 Data on structural analogues

Li *et al*. (2014) reported predicted hydroxyl rate constant values and atmospheric half-life values for 9 SCCP congeners. They developed a density functional theory (DFT) method for predicting k_{OH} values for 6 CPs through comparison with experimental values. The Environment Agency notes that the k_{OH} values reported by Li *et al*. (2014) are lower than those predicted from AOPWIN v1.92 for 6 of the SCCPs, higher for 2 SCCPs and similar for 1. For the 6 SCCPs where AOPWIN v1.92 predicted a lower value than Li *et al*. (2014), the difference in the two methods broadly increased with percentage chlorination. The biggest difference between predictions was noted for 1,1,1,2,3,9,11,11,11-nonachloroundecane ($C_{11}H_{15}Cl_9$; 68.4% Cl wt.). This comparison suggests that AOPWIN v1.92 may potentially over- or under-predict atmospheric half-life values for some LCCP congeners, although as noted above, the relevance of these values is likely to be low

4.2.4.4 Modelling of long-range transport potential

The long-range transport potential for the structural analogue MCCPs is currently under review by the United Nation's Persistent Organic Pollutants Review Committee (UN POPRC). Further work for LCCPs should await the conclusions of that assessment, and clarification of key physico-chemical and PBT properties. In addition, further information on monitoring in remote environments would be valuable.

4.2.4.5 Detection in remote locations

LCCPs have been detected in lake sediments in remote locations (see Section 4.2.5.1).

4.2.5 Field monitoring

The following studies were identified in the targeted literature search (Appendix A) as relevant to the persistence assessment of LCCPs. These studies are not referenced in the current EU REACH registrations (ECHA, 2021). As discussed in Section 2, there are considerable analytical challenges associated with the detection and quantification of LCCPs. Therefore, especially for studies conducted before 2012, the detection of LCCPs in environmental matrices should be treated as qualitative only, unless specified otherwise. Field monitoring studies generally include a range of CPs, and information is provided on MCCPs and SCCPs to provide additional context where appropriate. Further data on MCCPs have previously been reviewed

in UK Gov (2021) and ECHA (2019), so are not discussed here. Studies published since the Substance Evaluation of MCCPs (ECHA, 2019) which have not been included in this report due to limited relevance or time constraints are presented in Appendix B.

4.2.5.1 Sediments

Sediment systems are good indicators of temporal deposition and spatial distribution of substances. Sediment cores capture the sequential deposition of organic and particulate matter. Lake sediments are often better preserved due to limited turnover of material when compared to coastal or benthic marine sediments and can therefore be considered a regional snapshot of spatial distribution and temporal change of a substance's input and distribution. Caution should still be applied due to influences such as bioturbation and geophysical factors when interpreting the data.

Zhang *et al*. (2019) determined concentrations of SCCPs, MCCPs and LCCPs in lake sediment core and surface samples from 9 lakes in China, which varied in terms of geographical location and degree of urbanisation. Two are remote from areas of industry: Lake Qinhgai in the Tibetan Plateau and Lake Bosten in the Mengxin lake region of north-western China. Samples were collected between 2006 and 2019. Sediment cores were generally collected from the deepest location of the lakes' centre. The Environment Agency considers the reported methods for collection, extraction, storage and analysis of the sediment samples are robust and reliable. In brief, multiple cores were taken at each sampling location. One core was used for sediment dating (^{137}Cs and $^{239/240}$Pu, or ^{210}Pb analysis) and characterisation (i.e. total organic carbon, bulk density and solid content data). Characterisation data were used to estimate sedimentation rates. A second core was used for analysis of CPs.

Extraction recoveries calculated against procedural blanks and spiked samples (100 ng/g commercial mixtures) were in the range of 96 to 107%, 64 to 98%, and 67 to 88% for SCCPs, MCCPs and LCCPs, respectively. No significant variation in extraction recoveries were observed between the different sediment types from the 9 lakes. The internal quantification standard $^{13}C_{10}$-anti-Dechlorane Plus (DP) recoveries ranged from 62 to 108% (n = 123). Analyses of the extracts were performed using Ultra High Performance Liquid Chromatography-Quadrupole Time of Flight-Mass Spectrometry (UPLC-QTOF-MS). Method detection limits (MDLs) were calculated as 3 times the standard deviation of the procedural blanks. MDLs were reported to be 6.2, 5.0 and 4.1 ng/g dw for total SCCPs, MCCPs and LCCPs, respectively. Concentration data for the cores and surface samples from each lake are presented in detail in Appendix G.

CP concentrations in surface sediments from 2006 were compared to study spatial distribution. SCCPs, MCCPs and LCCPs concentration in the surface sediment

samples from the 9 lakes ranged from 28 to 400 (median 160 ng/g dw), 25 to 2 700 (median 270 ng/g dw), and 36 to 650 ng/g dw (median 130 ng/g dw), respectively. The authors propose that these variations in concentrations are due to the proximity of some of the lakes to large cities and manufacturing industries.

The temporal distribution of CPs with depth and 'calculated year' showed an increase in concentration with decreasing sediment depth for all lakes. The rate of increase of SCCP, MCCPs and LCCPs was greater for lakes in industrial and populated areas, with trends correlating to both up-scaled production and changes in use patterns. SCCPs and MCCPs were detected in pre-industry sedimentary layers, which is proposed to result from bioturbation or leaching. This same flux was not observed for LCCPs.

Homologue profiles were used to infer the temporal trends of CPs. They indicated that usage and/or production of chemicals shifted to a maximum from the 1980s to the late 2010s; thus, the average homologue patterns of CPs were obtained based on the average concentrations in sediment slices with dated years after the 1980s. These profiles are unique to each sampling site, with the relative contributions in the range of 8.8 to 36%, 14 to 73%, and 11 to 57% for SCCPs, MCCPs and LCCPs, respectively. The authors highlight that the relative contribution of SCCPs is lower than expected but consistent in each lake. Sediment cores from 4 lakes were dominated by MCCPs which accounted for 43 to 73% of the total CP burden (LCCPs contributed 10 to 21%). In contrast, sediment cores from 5 of the lakes were dominated by LCCPs, accounting for 35 to 57% of the total CP burden. For all lakes LCCP concentrations are increasing in concentration in the upper sediment layers and reflects an increase in their production and usage.

Dominant congener groups of LCCPs were consistent in all sediment core profiles: C_{18} (10 to 27%) > C_{23} (11 to 14%) > C_{22} (7 to13%) > C_{24} (8 to 12%) > C_{25} (7 to 16%), and > C_{19} (7 to 13%), with 8 or 9 associated chlorine atoms (19 to 27% and 18 to 26%, respectively). This equates to LCCPs of 48 to 54% Cl wt. Zhang *et al*. (2019), proposed that the presence congeners of C_{18} and C_{23} CPs in the homologue profile are associated with the commercial products CP-52 and CP-70, respectively.

Zhang *et al*. (2019) presented fluxes to all 9 lakes for the year 2006, and to 7 lakes for the year 2013/2014. For 2006, the fluxes ranged from 0.77 to 158, 1.3 to 1153 and 1.9 to 137 ng/cm^2/year, for total SCCPs, total MCCPs and total LCCPs, respectively. For the year 2013/2014, the fluxes ranged from 0.86 to 111, 1.8 to 132 and 2.3 to 172 ng/cm^2/year, for total SCCPs, total MCCPs and total LCCPs, respectively. The spatial distribution of the ranges reflect that observed for the surface sediment concentrations, i.e. the highest fluxes were observed for lakes in close proximity to industrial bases for the production of steel and iron. From these

data the loading rates, inventories, and total burden of CPs to the sediments were estimated. These data are presented in Table 15.

Table 15 Range of loading rates, inventories and total burden of CP groups in Chinese lake sediments

	Total SCCPs	Total MCCPs	Total LCCPs
Loading rates[a] (kg/year)	7.0 to 700	32 to 890	12 to 230
Inventories (ng/cm^2)	41 to 1 390	27 to 3 260	35 to 1 620
Total burden	0.26 to 5 100	0.29 to 21 000	0.07 to 4 300

Note: a - The exception was a remote tibetan lake, where loading rates of 0.007 kg/year, 0.005 kg/year and 0.005 kg/yr for total SCCPs, MCCPs and LCCPs were calculated.

The authors have also calculated the increase in total burden between 2006 and 2013 to be 1.2 to 1.8, 1.3 to 1.6, 1.5 to 2.2 -fold for SCCPs, MCCPs and LCCPs, respectively, reflecting the rapid increase in production and changing use of CPs in this time frame.

These data indicate that LCCPs can be detected after years of burial and under changing redox conditions associated with burial at depth in sediment systems. Degradation may have been inhibited by a lack of availability due to hydrophobicity or a lack of competent degraders. The Environment Agency considers that this study can be used as supporting information to inform the persistence assessment of LCCPs and consider the data to be reliable with restrictions (Klimisch 2). These restrictions include cautious comparison between studies that have used alternative technical products to build external calibrations for the reconstruction of congener groups in samples. This is not questioning the accuracy of the data but reflects the difference in CP products produced across China and Western Europe.

Yuan *et al*. (2017b) describes temporal trends over the last 80 years of CPs in Swedish coastal sediment cores located in the proximity of three potential sources (sewage treatment plant, wood related industry and a steel factory). Sweden does not manufacture CPs and therefore the presence of CPs detected is entirely due to import. The cores were collected using gravity corers, sliced into 1.5 to 2.5 cm sections and stored at -20 °C. The Environment Agency considers the methods for extraction and analysis of the sediment samples were robust and reliable. Sediment core dating was performed using radioisotope and stable isotope analyses. The Environment Agency notes that there were a few small discrepancies between data presented in the main text and in the supporting information. Data reported in the supporting information were given preference.

Extraction recoveries calculated against procedural blanks and spiked samples (250 ng/g of selected commercial mixtures) were 107 ± 11%, 95 ± 21% and 112 ± 18%, for SCCPs, MCCPs and LCCPs, respectively. The internal quantification standard ($^{13}C_{10}$-anti-DP) recoveries were 91 ± 26%. Analyses of the extracts were performed using Atmospheric Pressure Chemical Ionisation- Quadrupole Time of Flight-Mass Spectrometry (APCI-qTOF-MS). CP congener patterns from C_8Cl_3 to $C_{36}Cl_{15}$ were included for reconstructing congener profiles of the samples. A goodness of fit (R^2) of 0.88 ± 0.09 was calculated. LOQs for SCCPs and MCCPs were 1.4 and 6.5 ng/g dw, respectively. The instrumental LOQ of LCCPs was used as blank concentrations were below the LOD (0.067 ng, signal:noise 10:1).

Total SCCPs, MCCPs and LCCPs in sediments receiving discharge from a sewage treatment plant (STP) ranged from <LOQ to 5.4 ng/g dw, <LOQ to 15.0 ng/g dw, and <LOQ to 30 ng/g, for SCCPs, MCCPs and LCCPs, respectively. Relative contributions of SCCPs, MCCPs and LCCPs ranged from 7 to 17%, 30 to 77% and 7 to 63%, with mean values of 10%, 50% and 40%, respectively. All CPs first appeared above the LOQ in the same sediment section representing the year 1960. Total LCCPs had a maximum concentration of 30 ng/g dw in the section dated 1985, decreasing fractionally to 28 ng/g dw in the slice dated 1991. A decrease of 88% in total LCCP concentration from the peak years until 2015 was calculated. The measured chlorination degree associated with LCCPs remained fairly constant in the core slices, ranging from 46 to 48% Cl wt. The dominant chain length observed for LCCPs was C_{24} until 1991, after this C_{18} was predominant. The shortest and longest chain lengths detected within this core were C_8 and C_{35}. The oldest sediment section contained chain lengths from C_8 to C_{28}.

Total SCCPs, MCCPs and LCCPs in sediments receiving discharge from a wood related industrial area ranged from <LOQ to 14.0 ng/g dw, <LOQ to 93.0 ng/g dw, and 1.8 to 110 ng/g dw, respectively. Relative contributions of SCCPs, MCCPs and LCCPs ranged from 4 to 28%, 18 to 88% and 8 to 74%, with mean values of 12%, 51% and 37%, respectively. All CPs first appeared above the LOQ in the ‘oldest’ sediment section representing the year 1954. Total LCCPs had a maximum concentration of 110 ng/g dw in the 1993 section, decreasing rapidly to 8.1 ng/g dw in the 2015 section. A decrease in total LCCP concentration from the peak years until 2015 of 93% was calculated. The measured chlorination degree associated with LCCPs remained fairly constant in the core slices, ranging from 46 to 48% Cl wt. The dominant chain length observed for LCCPs was C_{18}. The shortest and longest chain lengths detected within this core were C_8 and C_{36}. The oldest sediment section contained C_8 to C_{34} chain lengths.

Total CPs in sediments sampled near a steel factory ranged from 6.7 to 14 000 ng/g dw, increasing from the 1930s up to the maximum concentration in the surface sediment dated 2015. Total SCCPs, MCCPs and LCCPs in sediments ranged from

2.0 to 140.0 ng/g dw, <LOQ to 12 000 ng/g dw, and 0.9 to 200 ng/g dw, respectively. Relative contributions of SCCPs, MCCPs and LCCPs ranged from 1 to 61%, 16 to 85% and 13 to 57%, with mean values of 24%, 41% and 35%, respectively. Total LCCPs reached maximum concentrations of 200 ng/g dw in the 1950s and 2015, with concentrations fluctuating between 80 and 200 ng/g dw in the interim period. The measured chlorination degree associated with LCCPs remained fairly constant in the core slices, ranging from 46 to 49% Cl wt. The dominant chain length observed for LCCPs was C_{18}. The shortest and longest chain lengths detected with this core were C_8 and C_{36}. The oldest sediment section (1930) contained C_8 to C_{34} chain lengths.

Temporal and spatial trends of CP concentrations measured in the three cores correlate to emission sources. The authors propose that this closely reflects the imported quantities (e.g. the highest annual import was 4 800 tonnes in 1991). Decreases in emissions to the sediments receiving the sewage treatment waste are proposed to correlate to a reduction in the industries that were previously using the CPs.

These data indicate that LCCPs can be detected after years of burial and under changing redox conditions associated with burial at depth in sediment systems. Degradation may have been inhibited by a lack of availability due to hydrophobicity or a lack of competent degraders. The Environment Agency considers that this study can be used as supporting information to inform the persistence assessment of LCCPs and consider the data to be reliable with restrictions (Klimisch 2). These restrictions include cautious comparison between studies that have used alternative technical products to build external calibrations for the reconstruction of congener groups in samples. This is not questioning the accuracy of the data but reflects the difference in products produced in Western Europe and China.

4.2.5.2 Soils

Wu *et al*. (2020b) measured CPs in soil at a brownfield site where former production of CPs had ceased. The authors were looking for effects on soil microbial community structures. Soil samples were collected 6 months after the plant had been closed. Soil had been covered by a hardened layer (50 cm, no further details were given). Seven core columns were collected from which 33 soil samples were isolated, freeze dried and stored at -80 °C until analysis. An internal standard ($^{13}C_{10}$-anti-DP) was added to samples after which they were ultrasonically extracted with dichloromethane (DCM); this was repeated twice with hexane. Extracts were concentrated and clean-up was carried out using silica gel and aluminium oxide columns. Eluents were concentrated and reconstituted in acetonitrile. The Environment Agency considers the reported methods for collection, extraction, storage and analysis of the sediment samples are robust and reliable. Analysis was

carried out using HPLC-ESI-QTOF-MS with method detection limit of 0.1 µg/g dw. Concentrations measured ranged from <LOD to 5 090 µg/g dw, <LOD to 6 670 µg/g dw, and <LOD to 1 450 µg/g dw for SCCPs, MCCPs and LCCPs, respectively.

All CPs were detected in most samples with a CP hotspot at 10 metres' depth indicating downward migration of the substances. The Environment Agency notes that due to limited details on the land usage (i.e. soil deposition, burial and overturning) and temporal environmental factors such as weather, no correction for downward migration of CPs in soil is possible. LCCPs is expected to have a high degree of adsorption to soil organic matter. Therefore, movement would be influenced more by the mobility of organic matter/soil solids than leaching via aqueous media. However, the data indicates that LCCPs are detectable as intact substances after burial over a number of years. No conclusions can be made on the influence of the chain length and level of chlorination from these data. Due to the limited details presented in this study the Environment Agency has assessed the reliability as Klimisch 4 (unknown reliability).

4.2.5.3 Surface water

The Environment Agency notes that due to the hydrophobicity, low solubility and low vapour pressure of LCCPs, significant freely dissolved concentrations would not be expected to be detected in surface waters.

4.2.5.4 Atmospheric monitoring

No national programmes have been identified by the Environment Agency where LCCPs are being monitored for in the atmospheric compartment. Only one academic publication has presented concentration data for LCCPs in the atmospheric compartment. Li *et al*. (2018) collected 28 samples of air originating from 6 sites over a 1-year period (September 2013 to August 2014) in Shenzhen, China. Concentrations of total LCCPs were calculated to be in the range of 0.25 to 8.38 (mean 2.32 ± 1.91) ng/m^3. For comparison, total MCCPs and total SCCPs were estimated to be in the ranges of 0.70 to 12.2 ng/m^3 (mean 3.53 ± 2.93 ng/m^3) and 1.11 to 39.8 ng/m^3 (mean 5.06 ± 7.59 ng/m^3), respectively. No differentiation between gas- or particulate-phase concentrations were presented by the authors. This publication has not been considered in detail for the purposes of this evaluation.

4.3 Bioaccumulation

The studies described in this section were identified in the targeted literature search (Appendix A) as relevant to the bioaccumulation assessment of LCCPs. These studies are not referenced in the current EU REACH registrations (ECHA, 2021). They generally include a range of CPs, and information is provided on MCCPs and

SCCPs to provide additional context where appropriate. Further data on MCCPs have previously been reviewed in UK Gov (2021) and ECHA (2019), so are not discussed here. Studies published since the Substance Evaluation of MCCPs (ECHA, 2019) which have not been included in this report due to limited relevance or time constraints are presented in Appendix B.

As discussed in Section 2, there are considerable analytical challenges associated with the detection and quantification of LCCPs. Therefore, especially for studies conducted before 2012, the detection of LCCPs in biota and environmental matrices should be treated as qualitative only, unless specified otherwise. Environment Agency (2009a) summarised several old studies that are not reported in the EU REACH registrations (ECHA, 2021a), and these are also referenced in Appendix B. Even concentration data from recent studies should only be considered semi-quantitative. Evaluation of available data were performed in conjunction with the relevant guidance text from ECHA R.11 and R.7.c (ECHA 2017 a and d).

4.3.1 Aquatic bioaccumulation

4.3.1.1 Measured data

The EU REACH registrations (ECHA, 2021b) do not contain experimental data relating to bioaccumulation.

Aqueous exposure studies

Environment Agency (2009a) presented the following data for fish:

- Bengtsson *et al*. (1979) studied the bioaccumulation of a C_{18-26}, 49% Cl wt. CP by Bleak (*Alburnus alburnus*) (a saltwater fish) in a non-guideline study. Exposure was performed at 10 °C using a semi-static procedure in which the test solutions containing 125 μg/L of the test substance were renewed every 2 to 3 days over a 14-day exposure period. This was followed by a 7-day depuration period. Very little uptake occurred during the 14-day exposure period, with whole body levels of around 1 to 2 mg/kg fresh body weight determined at the start of the 7-day depuration phase. From this value a bioconcentration factor (BCF) of around 8 to 16 L/kg was estimated. The analytical method (neutron activation analysis) was not substance-specific and therefore could have led to an overestimate of concentrations if metabolism were occurring. On the other hand, the aqueous concentration exceeded the solubility limit in pure water (see Section 3.2), so it is possible that not all the test substance was present in true solution in the experiment. Since BCFs should be based on dissolved concentrations, the BCF might have been higher than reported by at least an order of magnitude. Also, the

exposure period was relatively short and so it is not certain that equilibrium had been reached. The Environment Agency considers this study to be unreliable (Klimisch 3).

- Madeley and Maddock (1983a & 1983b) studied accumulation in Rainbow Trout (*Oncorhynchus mykiss*) over 60 days. The investigations were carried out as part of a long-term toxicity test carried out at 12±1 °C in accordance with GLP, although BCFs were only determined at the end of the study. Two commercial CP products were tested ($C_{22–26}$, 43% Cl wt. and $C_{>20}$, 70% Cl wt.) mixed with ^{14}C-n-pentacosane-13 (C_{25}) that had been chlorinated to a similar degree. A flow-through system was used for each test and the CP concentrations were measured by both radioactivity measurements and parent compound analysis (using a TLC method). No depuration period was involved. No treatment-related mortalities occurred (although some behavioural effects were seen in both the control and exposed populations during the test with the higher chlorine content substance).
  For the C_{22-26}, 43% Cl wt. substance (Madeley and Maddock, 1983a), two nominal exposure concentrations of 1.0 and 3.2 mg/L were prepared with acetone as a solvent at a concentration of 500 ppm (0.5 mL/L). The Environment Agency have been unable to verify the number of fish per treatment and how many fish comprised a sampling group. Mean measured concentrations were 0.97 and 4.0 mg/L, respectively, based on frequent ^{14}C-measurements. Parent substance analyses were carried out on 5 occasions, giving a mean measured concentration of 0.76 and 2.2 mg/L, respectively. The BCFs in whole fish were 17.9‑37.6 L/kg based on ^{14}C measurements and 3.6‑9.0 L/kg based on parent compound analysis, with the higher BCF values corresponding to the higher exposure concentration.
  For the $C_{>20}$, 70% Cl wt. substance (Madeley and Maddock, 1983b) three nominal exposure concentrations of 1.0, 2.1 and 4.2 mg/L were prepared with acetone at a concentration of 500 ppm for the two lower concentrations or 1 000 ppm (1 mL/L) for the highest concentration. Mean measured concentrations were 0.84, 1.9 and 3.8 mg/L, respectively, based on frequent ^{14}C-measurements. Parent compound analyses were also carried out on 5 occasions, giving a mean measured concentration of 0.6, 1.0 and 2.1 mg/L, respectively. The BCFs in whole fish were 5.7 to 53.8 L/kg based on ^{14}C measurements and 1.0 to 42.8 L/kg based on parent compound analysis, with the higher BCF values occurring at the lowest exposure concentration.
  The maximum whole fish concentrations were 36 or 150.2 mg/kg wet weight (ww) (parent and ^{14}C analysis, respectively) for the C_{22-26}, 43% Cl wt. product, and 120 or 124 mg/kg ww (parent and ^{14}C analysis, respectively) for the $C_{>20}$, 70% Cl wt. product. As steady state was not confirmed it is possible that the concentrations could become higher with exposures beyond 60 days. Corrections for fish lipid content or growth were not performed.

The Environment Agency notes that the reported exposure concentrations exceeded the solubility limit in pure water (see Section 3.2) by up to 2 orders of magnitude, so it is likely that not all the test substance was present in true solution in the experiments. Direct ingestion of undissolved test substance could therefore have occurred, which complicates interpretation. Since BCFs should be based on dissolved concentrations, the BCF might have been higher than reported by at least 2 orders of magnitude. No characterisation data were presented for the composition of the commercial products combined before or after addition of the radiolabel. It is also unclear how the analysis of the 'parent' substance was performed using TLC and whether this was also combined with radio-detection via phosphorimaging. The differences in the values obtained by the 2 TLC methods could be the result of the sensitivity of the extraction, separation and detection method (all of which are unknown) rather than metabolism. The variation between the concentrations measured via the two techniques were hypothesised to be the result of metabolism in the original Environment Agency (2009a) report. However, the Environment Agency notes that this could also be due to a lack of sensitivity in the TLC analysis. The extraction method and type of tissue being extracted can result in interferences. Co-extracted material that contains adsorbed radioactivity will interact with the stationary phase of the TLC plate, leading to a non-resolved smearing and a concentrated point on the origin of the TLC plate. Due to the reduced resolving power of TLC in comparison to other methods this can underestimate concentrations, even if a defined region of radioactive interest is observed that corresponds to the parent compound.

The Environment Agency considers these studies to be unreliable (Klimisch 3).

Environment Agency (2009a) presented the following data for invertebrates:

- Madeley and Thompson (1983a & 1983b) determined bioaccumulation in mussels (*Mytilus edulis*) at the end of 60-day flow-through toxicity studies performed in accordance with GLP using the same substances as used in the *O. mykiss* studies summarised above. BCFs were only determined at the termination of the study. The mussels were exposed via the water phase, but algae were continuously added to the in-flowing dilution water as food at a rate of 1.0 - 1.1 x 10^9 cells/day. No treatment-related mortality occurred during the test, although reduced filter feeding behaviour compared with control organisms was consistently observed at the higher exposure concentration from day 7 onwards for the lower chlorine content substance.
  For the $C_{22\text{-}26}$, 43% Cl wt. substance (Madeley and Thompson, 1983a), two nominal test concentrations of 0.32 and 3.2 mg/L were prepared using acetone at a concentration of 500 ppm (0.5 mL/L). The highest test concentration was reported to be cloudy in appearance, and some fine white deposits were observed occasionally on the surface. This indicates that

solubility in the test system was exceeded. The mean measured exposure concentrations were 0.12 and 2.18 mg/L, respectively, based on frequent ^{14}C-measurements, or 0.09 and 2.85 mg/L, respectively, based on parent compound (TLC) analyses on 4 occasions. The BCFs in whole mussels (ww) were 261 to 1 158 L/kg based on ^{14}C measurements and 87.2 to 1 000 L/kg based on parent compound analysis, with the higher BCF values occurring at the lower exposure concentration.
For the $C_{>20}$, 70% Cl wt. substance (Madeley and Thompson, 1983b), two nominal concentrations of 0.56 and 1.8 mg/L were prepared using the same concentration of acetone as the first study. Some deposition of the test substance was observed at the higher concentration tested, indicating that solubility in the test system had been exceeded. The mean measured exposure concentrations were 0.46 and 1.33 mg/L, respectively, based on frequent ^{14}C-measurements, or 0.51 and 0.9 mg/L, respectively, based on parent compound (TLC) analysis on 4 occasions. The BCFs in whole mussels were 223 to 341 L/kg (ww) based on ^{14}C measurements and 105 to 167 L/kg based on parent compound analysis, with the higher BCF values occurring at the lower exposure concentration.
There was no indication that steady state had been reached. Please see the earlier comments on the robustness of the 2 analytical methods. Although the results are reported as BCFs, it is highly likely that dietary exposure was involved since mussels' process large volumes of water and the CPs will have adsorbed to the algal food, making the values bioaccumulation factors (BAFs) rather than BCFs.

The Environment Agency notes that the reported exposure concentrations exceeded the solubility limit in pure water (see Section 3.2) by up to 2 orders of magnitude, so it is likely that not all the test substance was present in true solution in the experiments (as indicated by the presence of cloudy material or deposits). Direct ingestion of undissolved test substance could therefore have occurred, which complicates interpretation. Since BCFs should be based on dissolved concentrations, the BCF/BAF might also have been higher than reported by at least 2 orders of magnitude.

The Environment Agency considers these studies to be unreliable (Klimisch 3).

Additional invertebrate bioconcentration data were located by the Environment Agency as part of this evaluation:

- Castro *et al*. (2019) investigated bioaccumulation potential in the cladoceran water flea (*Daphnia magna*). Five “commercially available” products[5] were used, including 2 that contained congeners that are present in LCCPs: CP-42 ($C_{10-14,}$ C_{21-31} 42% Cl wt.) and CP-52 (C_{9-30} 52% Cl wt.). The daphnids were cultured in M7 media with a stock density of approximately 10 individuals per litre and fed a mixture of green algae (*Pseudokirchneriella subcapitata* and *Scenedesmus spicatus*) 3 times per week. A passive dosing device was prepared to generate stable solutions in water, by loading medical grade silicone with 1.0 or 2.5 g (±1%) of the test substance (to give a final concentration of each technical substance of 1 mg per g silicone). The dosed silicone was added to water in test vessels and equilibrated for 48 hours to create the test solutions. The experiments were conducted under static conditions at a constant temperature of 22 °C and a 16:8 h light/dark cycle. Blank controls were also prepared (no silicone or substance, n = 10). Daphnia neonates (<24 h old) were exposed to dosed water alone (aqueous exposure) or dosed water with food (dietary exposure) for a 48-hour period, followed by a depuration period of 24 hours (using clean water and food). The density of animals in the tests were 2 mL per neonate in accordance with OECD TG 202 (OECD, 2004b). The food concentration (when added) was 4 µg/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 hours with the loaded silicone, to measure a freely dissolved concentration (avoiding sorption to organic matter). Liquid−liquid extractions were performed twice with iso-hexane in glass tubes, the solvent evaporated, and 20 ng of dechlorane-603 added prior to analysis as a volumetric standard. Juvenile daphnids (3 and 4 days’ old after the uptake or depuration phase, respectively) were collected, and dead animals discarded. The samples were freeze-dried. Exoskeletons shed by unexposed adult daphnids were also

[5] In response to a request from the Environment Agency, the study authors confirmed that most of the test substances were obtained from the manufacturers in the late 1980s, Cereclor 42 having been obtained from Imperial Chemical Industries, UK. This product has a much wider carbon chain length range than current commercial products. Castro *et al.* (2018) performed semi-quantitative mass fraction analysis on the Cereclor 42 product, and determined that SCCP, MCCP and LCCP congeners comprised 28, 4 and 67% of the total mass, respectively. For details of CP-52, see Section 1.1 (Personal communication, M Castro, University of Stockholm, September 2020).

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 were added to the vials as a volumetric standard. Quantification was carried out with APCI-qTOF-MS. The recovery of the internal standard was determined using GC-ECNI-LRMS. The LOD in the water and daphnid samples was 0.39 µg/L and 0.13 ng/µg dw, respectively, based on the amount measured in the blank plus 3 times the standard deviation (SD). The limit of quantification (LOQ) in the water and daphnid samples was 0.47 µg/L and 0.25 ng/µg dry weight, respectively, based on the amount measured in the blank plus ten times the SD.
Recoveries were on average 130 ± 0.2 and 101 ± 0.1% for daphnid and water samples, respectively. The high average recoveries for Daphnia were thought to be caused by interferences in either the internal or the volumetric standard. This due to the high number of congeners present in the technical substance and their overlapping isotopic mass patterns.
The average lipid content of the daphnids was determined by extraction followed by gravimetric analysis. The lipid content was 5 and 7% of the dry weight (w/w) for starved and fed daphnid juveniles, respectively. The ratio between lipid content and dry weight determined in control individuals was used to estimate the lipid content for the remaining samples, where only the dry weight was known. Lipid content was not expected to change much over the short duration of the experiment.
Mortality did not exceed 10% in any of the controls (no information is provided for the treatment groups). BCF and BAF values were calculated using the freely dissolved water concentration of CP-42 and CP-52 (1.4 µg/L for both substances). Kinetic data were derived using the concentration at the end of the uptake and of the depuration phases, assuming first-order kinetics. The results are provided in Table 16.
BCF/BAFs for CP-42 and CP-52 were in the range 540 000 to 590 000 L/kg dw (which was the same order of magnitude as measurements for Cereclor S45 (570 000 to 590 000 L/kg dw; 97% of congeners by mass were MCCPs). Lipid corrected BCF/BAFs for CP-42 and CP-52 were in the range 650 000 to 710 000 L/kg lipid. The paper only presents the results in terms of the total product composition, so it is not clear what contribution the LCCP chain lengths made to the reported BCF/BAF values. However, the deconvoluted spectra of the extracted Daphnia magna samples did contain long chain congeners.

Table 16 Bioaccumulation data for *Daphnia magna* (Castro *et al*., 2019)

Parameter	Results for CP-42	Results for CP-52
Log BAF	5.4 ± 0.13 L/kg dw	5.7 ± 0.08 L/kg dw
Log BAF	6.5 ± 0.13 L/kg lipid	7.0 ± 0.11 L/kg lipid
Log BCF	5.4 ± 0.23 L/kg dw	5.9 ± 0.17 L/kg dw
Log BCF	6.7 ± 0.23 L/kg lipid	7.1 ± 0.17 L/kg lipid
Uptake rate constant for fed daphnids, k_u	2.5 x 10^5	1.7 x 10^5
Uptake rate constant for unfed daphnids, k_1	3.0 x 10^5	3.0 x 10^5
Depuration rate constant, K_d	0.097 (fed)	0.072 (fed)
Depuration rate constant, K_d	0.072 (unfed)	0.074 (unfed)
Depuration half-life ($t_{1/2}$)[a]	7 h	10 h
Time to 95% to steady state (t_{95})	31 h	41 h

Note: 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).

In response to a request from the Environment Agency the study authors advised against calculating BCF or concentrations of the LCCP congeners in daphnids due to large uncertainties in the calculation resulting from the semi-quantitative aspect and selectivity of the analytical method. The method used does not allow for quantification of single congeners and generates a substance concentration based on the sum of selected congener signals.

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

Concentrations in daphnids were generally higher after aqueous exposure than after simultaneous aqueous and dietary exposure, again indicating that passive diffusion is the dominant uptake process. It is possible that when food is available during the uptake phase, elimination processes such as growth, metabolism and faecal

egestion might be increased, although this was not indicated by the depuration rates. The Environment Agency notes that bioavailability might be reduced by adsorption to uneaten food.

The depuration half-life was 7 days. The authors noted that there was an increase in the depuration rate of approximately 35% when food was added for the "C_{10-14}, C_{21-31}" 42% Cl wt. product. It was speculated that this could have been explained by metabolism of low chlorine content congeners and that this supports the hypothesis that passive diffusion may be the dominant removal pathway for CPs in *D. magna*. Increasing levels of chlorination appear to increase both BCF and BAF values, whereas changes in carbon chain length did not appear to affect uptake significantly.

The Environment Agency notes the following points for this study:

- There is no standard internationally recognised test guideline for bioaccumulation in *D. magna*. The study appears to have been performed well, but in the absence of a ring-test, the reliability and reproducibility of the method are unknown. The results are expressed in terms of dry weight, but for fish studies they are wet weight. Wet weight concentrations would be lower.
- The data are based on analysis of non-radiolabelled test substances in tissues with no measure of the efficiency or effectiveness of the extraction method, which affects the study interpretation. If identical to the data presented in Castro *et al*. (2018) then extraction efficiencies and recoveries should have been acceptable. The study did not provide information for specific chain lengths, just total values for the technical products. This may give a misleading impression of adsorption for some chain lengths. It would have been preferable to have used a radiolabel allowing the total radioactive residue associated with ingested/biomass-related test substance to be calculated.
- The dissolved concentration of LCCPs measured for CP-42 and CP-52 was 1.4 µg/L, which is below the water solubility range noted in Section 3.2. It is not known whether 48 hours gave sufficient time for all soluble congeners to fully dissolve. Only a single water concentration value is presented in the paper, which was derived in the absence of test organisms. It is not clear how this differs from the actual exposure concentration, or how variable this might have been over the duration of the test.
- Steady state was claimed to have been achieved after 48 hours. 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 magna* are very small organisms, so it is likely that a steady state can be achieved in a shorter time than for fish, especially if passive diffusion is the dominant process (as suggested by the data). However, the Environment Agency cannot be certain that the organisms had reached steady state because only the concentration at the end of uptake was measured. On the other hand, if steady state had not been reached, the final concentration over a longer time frame may have been higher. The Supporting Information shows the equilibration time for three sampling intervals for the CP-52 product in *D. magna*. To have confidence in the 48-h value, further detailed information should have been provided for a minimum of five intervals.

- The Environment Agency questions the use of the terms 'equilibration' and 'steady-state' by the authors relating to the use of solid-state passive dosing methods. It is not known whether the CPs were evenly distributed in the test systems prior to addition of food and the neonates within the timeframe of the exposure periods. Data presented in an earlier paper (Castro *et al*., 2018) show that a good number of variables had been assessed, but that a longer time period was probably required for the longer chain length substances. This might also have influenced the distribution of congeners observed in the analysis.
- It is likely that some daphnids died (at least in the vessels without food) as the dissolved concentrations are only a factor of 5 below the 48-h EC_{50} of 5.9 µg/L for MCCPs (ECHA, 2019). Although the paper mentions that dead daphnids were discarded, there is no further information about the number. Bioaccumulation tests are normally carried out at a concentration that avoids adverse effects and causes less than 10% mortality in the treatment groups.
- Daphnia are very small organisms, and the amount of sample collected for each measurement is not stated. This could affect the reliability of concentration measurements, which would also have been affected by the analytical recovery rate exceeding 100%. Only two measurements were used to derive the kinetics and hence the BCF and BAFs. The sensitivity of the results to variations in the measured concentrations is unclear. In addition, the depuration kinetics are based on an LOD value, and since the actual concentration in the organisms may have been lower, the depuration rate constant could have been higher. The depuration rate is used directly to estimate the uptake rate, so influences the final result. As noted by the authors, since static conditions were used, the concentration of LCCPs in water after 24-h depuration would not have been zero, which complicates the interpretation of depuration.

- Overall, the Environment Agency considers that the results of this study suggest very high BCF/BAFs for *Daphnia*, but there are major uncertainties in the numerical values which make them unreliable for regulatory decision making for LCCP congeners (Klimisch 3).

Dietary exposure studies

No standard definitive data for dietary accumulation in fish (OECD TG 305; OECD, 2012a) were presented in the EU REACH registrations (ECHA, 2021b).

Environment Agency (2009a) presented the following data for dietary studies with fish:

- The accumulation of a C_{18}, 49% Cl wt. CP was studied in juvenile Rainbow Trout (*O. mykiss*) by Fisk *et al*. (2000). The study design does not follow that recommended in the OECD TG 305 (OECD, 2012a) and was not GLP compliant. A radiolabelled test substance was synthesised by the authors and had an average molecular formula of $C_{18}H_{30.3}Cl_{6.7}$, which equates to 48% Cl wt. The position of the radiolabel was on the first carbon of the chain. Radio-purity of the test substances was calculated to be >99% and the specific activity was 17.1 dpm/ng. Chemical purity was determined to be 99% using a gas chromatography-electron capture detector. Data were matched to gas chromatography – negative ion mass spectrometry data for verification. ^{14}C analysis was performed using fraction collection or known volume aliquots in conjunction with liquid scintillation counting (LSC), correction was performed via a quench curve. No limits of detection or quantification were presented for the analysed media. Residue analyses were performed via combustion using a standard model oxidiser prior to total radioactivity determination via LSC. The food used during the test was a commercial fish food (41% protein, 14% lipid and 3% fibre). The test substance was added to the food as a suspension in hexane followed by evaporation of the solvent. No confirmatory analysis of either the radioactive content or homogeneity of the food were presented.
  Each treatment group was held in separate 100 L aquaria. The systems were flow-through with the dilution water comprising ultraviolet and carbon dechlorinated tap water. Two nominal substance exposure concentrations (1.5 and 15 mg/kg ww food) and a control exposure tank (non-spiked food) were prepared. Each tank contained 36 juvenile fish in flow-through tanks (initial weight 1 to 5 g, final weight 23 to 69 g). Fish contained in the exposure tanks were fed spiked food at a daily feeding rate of 1.5% of mean weight of fish over a 40-day period, followed by a 160-day depuration period using clean food. Fish contained in the control tank were fed at the same rate with a

non-spiked food. The mass of food to be fed was re-calculated after every sampling interval.
Three fish per exposure were removed for analysis at each sampling interval. No indication of when sampling was performed in relation to feeding or tank husbandry were presented by the authors. OECD TG 305 (OECD, 2012a) states that all uneaten food and faecal matter should be siphoned from the tanks within 30 to 60 minutes of feeding to keep organic carbon contents as low as possible and prevent secondary uptake. As such, sampling time in relation to feeding time was not specified in the paper. Sampling was performed on days 5, 10, 20, 30 and 40 of the uptake period, and days 5, 10, 20, 40, 80 and 160 of the depuration period (equating to days 45, 50, 60, 80, 120 and 200 of the total study length). Sampled fish tissues were separated into liver, gastrointestinal tract, adipose fat tissue associated with the organs, and carcass. At all sampling intervals fish carcasses were freeze dried and extracted with toluene. For two sampling intervals, i.e. day 40 (end of uptake phase) and day 120 (mid-depuration phase), the amount of non-toluene-extractable ^{14}C-label present in the carcass was determined via combustion of the residual toluene extracted fish tissue. Lipid content of each extract was determined by gravimetric determination on 1 mL of the toluene supernatant. All measured concentrations were corrected for growth dilution and lipid content in line with the OECD TG 305 (OECD, 2012a) text. No effect on body and liver growth rates or liver somatic indices were seen between exposed and control populations during the test. Results indicated that a steady state had not been reached by day 40 and so the BMF was determined kinetically. The assimilation efficiencies (based on lipid corrected concentrations in fish carcass and food) were determined to be 13 to 22%, and the depuration rate constants estimated to be 0.0076 to 0.0088 d^{-1} (depuration half-life ca. 79 to 91 days; growth and lipid corrected; six sampling intervals). The calculation can be considered equivalent to that recommended in the OECD TG 305 (OECD, 2012a) Based on the measured kinetic parameters, the BMF (concentration in fish (lipid normalised)/concentration in food (lipid normalised) was calculated to be in the range 0.81 to 0.93.

Environment Agency (2009a) performed a correction of the Fisk *et al*. (2000) study data for the lipid content of the fish food (~14%). The lipid content of the food was higher than that of the fish (6 to 11%). These calculations led to accumulation factors expressed in terms of a whole fish and whole food basis that were lower by around a factor of 1.3 to 2.3. It could be argued that in the environment the food for a predatory species would be generally of lower lipid content than found in laboratory fish food (and may be of lower lipid content than the predatory species itself). It is therefore not possible to infer from these results (or other laboratory-based results using proprietary food of high lipid content) that the accumulation factor on a whole

body and food basis would be lower in the environment than found in the laboratory studies. Environment Agency (2009a) therefore estimated that non-growth-corrected fish accumulation factors from the study would be in the range 0.10 to 0.11 on a lipid basis. It should be noted, however, that since the original raw concentration-time data were lacking in the paper (only the derived kinetic parameters were reported) the reanalysis is only approximate and may be subject to errors.

The Environment Agency notes the following points for this study:

- Many details required for assessment against the validity criteria set out in the standard OECD guideline (OECD, 2012a) were not reported. These include the exposure temperature and monitoring to show that variation greater than ±2 °C did not occur; measurements of the dissolved oxygen concentration to demonstrate that it did not fall below 60% saturation during the whole study; the lipid determination method was not detailed further than a gravimetric method; and details of maintenance and husbandry of the test system were omitted. OECD TG 305 also states that all uneaten food and faecal matter should be siphoned from the tanks within 30 to 60 minutes of feeding to keep organic carbon contents as low as possible and prevent secondary uptake. However, the sampling time in relation to feeding time was not specified in the paper. The accuracy, precision and sensitivity of the analytical methods were not documented; data relating to specific analysis via GC/MS are presented with limited details. The LODs and LOQs of specific analyses and radio analysis have not been presented. All data are based on the radioactive measurements in the toluene extracts of the carcass tissues after freeze drying. It is unclear from the text why freeze drying was performed prior to extraction as this can lead to increased binding of substance to the carcass tissues. Recoveries in fish and food have not been presented. This information is especially important when freeze drying has been performed as part of the extraction procedure. The data would be more robust if internal procedural standards had been used.
- The Environment Agency also notes that the determination of total accumulation in the fish was not reported. The authors propose that the toluene extraction is representative of the non-bio-transformed substances and that the remaining non-extractable radioactivity was representative of bio-transformed substances. The Environment Agency does not completely disagree with the hypothesis, but the extraction is likely to be compromised due to increased sorption to organic material promoted by the freeze-drying process. In addition, the use of only one apolar solvent at ambient temperatures should not be used to make such a conclusion. One solvent will only allow extraction and removal via a specific mechanism, such as disruption of van der Waals electronic interactions between the substance and

the tissues. More than one interaction is likely to be involved and therefore a greater distribution of polarities and potentially amended solvents would need to be investigated to give a realistic picture of biologically incorporated substance material.

- The lack of substance determination in liver and adipose tissues also raises concern that the bioaccumulation potential of the substance has been underestimated.
- The Environment Agency has accessed the full text of the study and the calculations have been checked. The Environment Agency considers the reliability of this study to be Klimisch 4 (unknown reliability). Given the shortcomings in the chemical analysis, the Environment Agency considers that the fish accumulation factors may have been higher than reported (e.g. if all fish tissues had been included and an appropriate range of solvents used).

The following studies investigate uptake and accumulation of LCCPs in fish and invertebrates:

- The uptake and accumulation of a $^{14}C_{25}$ - $C_{20\text{-}30}$ 42% Cl wt. product was studied in both juvenile Rainbow Trout (*O. mykiss*), and mussels (*M. edulis*) by Madeley and Birtley (1980). The Environment Agency has not been able to access the publication and is therefore relying on the summary provided in Environment Agency (2009a). The mussel experiment is described separately below. The study was performed prior to the inception of GLP and the revision of OECD TG 305 to include dietary exposure (OECD, 2012a). The test substance was a ^{14}C-pentacosane (radiolabel on the central carbon atom of the C_{25} chain) which had been chlorinated to 42% wt. This was then mixed with a commercial $C_{20\text{-}30}$, 42% wt. product before use. The food used in the test was a commercial trout diet. The food was dosed prior to feeding of the organisms. No details can be located for the preparation of the food or its composition in terms of lipid or protein contents.
  Three groups of 40 fish were fed diets containing the test substance at nominal exposure concentrations of 0, 47 or 385 mg/kg dry food for 35 days. After the 35-day exposure period, all three groups were fed the control diet for a further 49-day depuration period. The number of fish sampled at each interval was not specified. The temperature during the experiment was maintained at 12 ± 3 °C. No treatment related adverse effects were seen in any of the fish during the experiment. The Environment Agency have not been able to confirm whether the test system was semi-static or flow through or details of the feeding schedule. In addition, the feeding and husbandry details with respect to sampling are unavailable. The feeding rate has not been detailed (% body weight) or whether adjustments were made after the removal of fish from the tanks.

Tissue concentrations of the fish determined by ^{14}C measurements are presented (Table 17). The uptake of radioactivity was found to be highest in the liver and gut, with concentrations approaching those of the administered food. The Environment Agency notes that depending on the feeding/sampling schedule the radioactivity in the gut could reflect the concentration of undigested food.

The levels in all tissues were found to increase with time during the exposure phase but were all approaching a plateau level by day 35 of the exposure. During the depuration phase, the ^{14}C-activity in both gut and liver was found to rapidly diminish. Based on the ratio of the concentration in fish at day 35 and the concentration in food, the BMF can be estimated to be 0.22 to 0.26 on a dry weight basis. The original data were not lipid or growth corrected.

In addition to the ^{14}C-analyses, some fish in the 385 mg/kg dry food dose group were analysed for parent chlorinated paraffin by a TLC method at the end of the depuration phase. These results are also shown in Table 17 for comparison with the ^{14}C measurements. The levels measured by this direct method were lower than those obtained by the ^{14}C-method. Environment Agency (2009a) proposed that this could be the result of metabolism. However, the Environment Agency hypothesise that this could also be due to a lack of sensitivity in the TLC analysis. The extraction method and type of tissue being extracted can result in interferences. Co-extracted material that contains adsorbed radioactivity will interact with the stationary phase of the TLC plate, leading to a non-resolved smearing and a concentrated point on the origin of the TLC plate. Due to the reduced resolving power of TLC in comparison to other methods this can under-estimate concentrations even if a defined region of radioactive interest is observed that corresponds to the parent compound.

Table 17 Tissue concentrations, based on ^{14}C-radioisotope methods, mg/kg dry weight, from fish fed a diet of $^{14}C_{25}$-$C_{20\text{-}30}$ 42% Cl wt. (Madeley and Birtley, 1980)

Dose	Exposure phase	Liver	Gut	Flesh	Remains	Total body burden (TBB)[b]	TBB minus gut[c]
47 mg/kg dry food	End of 35-day uptake period	29.5	36.4	2.5	6.8	10.3	5.3
47 mg/kg dry food	End of 49-day depuration period	2.8	4.8	1.4	3.1	3.3	2.0
385 mg/kg dry food	End of 35-day uptake period	263	353	23.1	66.3	100.6	50.3

Dose	Exposure phase	Liver	Gut	Flesh	Remains	Total body burden (TBB)[b]	TBB minus gut[c]
385 mg/kg dry food	End of 49-day depuration period	21.8 (6.5)[a]	47.3 (5.4)[a]	17.2 (3.7)[a]	29.8 (5.7)[a]	31.6	18.7

Note: a - Concentration of CP determined directly by TLC analysis.
b - No details for TBB calculation were presented in Environment Agency (2009a).

c - Normalised as a percentage to give the values corrected without the gut concentrations.

An indicative depuration (elimination) rate constant (k_2) has been cautiously estimated by the Environment Agency using the data presented (Table 17). In the absence of growth correction this may be unreliable. For each exposure concentration, the natural log of concentrations in tissues and the total body burden (TBB) and TBB minus gut (TBB-gut) – to account for residual spiked food present in the gut, which would lead to an overestimate of the starting concentration for depuration – were plotted at the two time points using Microsoft® Excel. Undigested food present in the gut of the fish during sampling could also account for the observed rapidly diminishing radioactivity in the gut tissues. Linear trend lines were plotted to model pseudo-first order kinetics:

- Estimated depuration rate constants for $^{14}C_{25}$ - $C_{20\text{-}30}$ 42% Cl wt. CP were 0.081 d^{-1} (TBB) and 0.070 d^{-1} (TBB-gut) for the 47 mg/kg dosed feeds, respectively.
- Estimated depuration rate constants for $^{14}C_{25}$ - $C_{20\text{-}30}$ 42% Cl wt. CP were 0.083 d^{-1} (TBB) and 0.071 d^{-1} (TBB-gut) for the 385 mg/kg dosed feeds, respectively.
- These are equivalent to a depuration half-life of approximately 8.5 days (TBB) and approximately 9.8 days (TBB-gut).

The results should be treated with caution as only two data points were available, the reliability of the analytical method for parent compound is unknown and lipid normalisation/growth corrections were not performed. The results should also be considered to apply only to the radiolabelled C_{25} chain length as the plotted data relate to measured radioactivity rather than parent substance. The Environment Agency has not been able to ascertain whether spiked food was still present in the gut, so the TBB-gut data may be more relevant. Overall, the Environment Agency considers the study data should be used with caution and therefore considered of unknown reliability (Klimisch 4).

- Zitko (1974) studied the dietary uptake of two LCCPs in juvenile Atlantic Salmon (*Salmo salar*) over 181 days uptake and 74 days depuration. The study also investigated uptake from suspended silica particles over shorter durations, however these data are not summarised in this report. This study was performed prior to the inception of GLP. Seven exposure scenarios were prepared for the test substances ($C_{>20}$ 42% Cl wt. and $C_{>20}$ 70% Cl wt. products), a positive control (polychlorinated biphenyl - Aroclor 1254) and negative control. The tanks were flow-through and maintained between 10 and 15 °C. The nominal concentrations of the test and positive control substances in the fish food were 10 and 100 mg/kg, and control fish were fed non-dosed food. Each tank contained 20 fish. The number of tanks per exposure were not reported in the paper. Fish were fed manually several times a day over 5 days per week. There is no information about the timing of feeding versus sampling. The feeding rate was reported as 8 g per tank per week (1 140 mg/day). The Environment Agency has estimated that this was 0.95% of the fish body weight at the start of exposure (the percentage at later times cannot be estimated due to the absence of growth data over the uptake and depuration period). In addition, the authors did not state whether the feeding rate was adjusted after the removal of fish from the tanks. One fish was sampled for each sampling interval. Concentrations in the fish were expressed on a whole-body weight basis as chlorine. No details of the analytical method are presented in the paper. Mortalities occurred in the exposed fish and also in the control group during the feeding studies. These findings are discussed further in Section 5.1.1. The results are shown in Table 18.
  Very little uptake of the CPs occurred in comparison to the mass fed during the uptake period, although it is unfortunate that additional sampling was not performed between days 33 and 109. The highest reported concentration in fish (0.51 mg Cl/kg at 33 days for the $C_{>20}$ 70% Cl wt. substance) is only 10 times the limit of quantification (0.05 mg Cl/kg). The origin of the chlorine measured in the blank control fish was not known.

An important aspect of any bioaccumulation study is that the selected exposure levels should be below that which can cause toxic effects. This aspect was not addressed by the authors. The significantly lower lipid content of CP-exposed fish compared to those exposed to Aroclor 1254 raises concerns that a detrimental effect may have occurred. The observed mortalities were also unexplained. In addition, the fish would have been expected to grow significantly over the length of the study, but no details are provided. Together with the uncertainty in the measured concentrations, the Environment Agency considers that this study is unreliable (Klimisch 3), and further interpretation of the data is not meaningful.

Table 18 Dietary uptake of LCCPs by juvenile Atlantic Salmon (Zitko, 1974)

Substance	Exposure concentration	Exposure time (d)	Fish lipid content	Fish concentration mg Cl/kg	Fish concentration mg/kg[a] substance
Control		33	1.03%	0.30	
Control		109	0.65%	<0.05	
Control		181	0.47%	<0.05	
$C_{>20}$, 42% Cl wt.	10	33	1.30%	0.11	0.262
$C_{>20}$, 42% Cl wt.	10	109	0.69%	<0.05	< LOQ
$C_{>20}$, 42% Cl wt.	10	181	0.49%	<0.05	< LOQ
$C_{>20}$, 42% Cl wt.	100	33	1.22%	0.51	1.214
$C_{>20}$, 42% Cl wt.	100	109	0.49%	<0.05	< LOQ
$C_{>20}$, 42% Cl wt.	100	181	0.34%	<0.05	< LOQ
$C_{>20}$, 70% Cl wt.	10	33	1.13%	0.29	0.415
$C_{>20}$, 70% Cl wt.	10	109	0.40%	<0.05	< LOQ
$C_{>20}$, 70% Cl wt.	10	181	0.29%	<0.05	< LOQ
$C_{>20}$, 70% Cl wt.	100	33	1.30%	0.49	0.701
$C_{>20}$, 70% Cl wt.	100	109	0.56%	<0.05	< LOQ
$C_{>20}$, 70% Cl wt.	100	181	0.92%	<0.05	< LOQ
Positive control (Aroclor 1254)	10	33	5.09%		3.86
Positive control (Aroclor 1254)	10	109	3.10%		3.80
Positive control (Aroclor 1254)	10	181	2.07%		3.80
Positive control (Aroclor 1254)	100	33	5.30%		13.9
Positive control (Aroclor 1254)	100	109	2.73%		24.0
Positive control (Aroclor 1254)	100	181	2.69%		30.0

Note: a – Zitko *et al*. (1974) state that the chlorine concentration can be converted to concentration of CP by multiplying by 2.38 and 1.43 for the $C_{>20}$, 42% Cl wt. and $C_{>20}$, 70% Cl wt. substance, respectively. No further details or explanation were provided.

- Bengtsson and Baumann Ofstad (1982) examined the uptake of LCCPs in a non-standard feeding study using Bleak (*A. alburnus*). The Environment Agency has not been able to access the publication to obtain further details and is therefore relying on the summary provided in Environment Agency (2009a). The fish were exposed to a $C_{18–26}$, 49% Cl wt. CP product via food for 91 days, followed by a 316-day depuration period. The exposure temperature ranged broadly from 3.5 to 16 °C, following the natural fluctuations from the brackish intake water (around 7 parts per thousand salinity). The fish used had a body weight of ~4 g at study initiation. Test substance was added to the fish food (flakes) at a concentration of 3 400 mg/kg food, and this was added to the glass exposure tank (containing 30 fish) in 0.25 g portions twice daily on weekdays and once daily at weekends. At study initiation this equated to 0.5 g per 120 g fish/day (0.42% body weight). It is not known whether this feeding rate was adjusted for removal of fish from the tanks and recalculated for potential growth. Fish in 3 further tanks were fed non-contaminated food at the same rate and acted as the control groups for the experiment. Throughout the test, the dissolved oxygen was measured to be above 90 percent of saturation. Fish were sampled on days 14, 28, 56 and 91 of the exposure phase and on days 7, 35, 133 and 316 of the depuration phase. These fish were starved for two days (to avoid contributions of CP from undigested food) prior to whole body analysis for levels of total chlorine using neutron activation analysis. No significant increase in mortality was seen in the exposed fish during the experiment.
  The estimated concentration of chlorine (assumed to be CP) in fish reached 24 mg/kg at the end of the 91-day exposure period (the BMF was calculated from this value to be 24/3400 = 0.007). The authors estimated that the uptake efficiency was around 2%. The total chlorine levels in the fish reduced by around 50% during the first 4 to 5 weeks of depuration, after which the level appeared to remain constant for the remainder of the depuration period (40 weeks).
  The concentration of CP achieved at the end of the 91-day exposure period is around the same order of magnitude as that reported by Madeley and Birtley (1980) after 35 days' exposure using *O. mykiss*, where exposure concentrations were 725 times lower. The Environment Agency notes that the concentration in feed appears to be relatively high and cannot comment further without access to full descriptions of the extraction and analyses that were performed on the fish tissues. These data should be treated with caution as the analytical method was not specific for CPs. In addition, no correction for lipid content or growth was performed.

The Environment Agency considers that this study is unreliable (Klimisch 3) and further interpretation of the data is not meaningful.

There is one dietary bioaccumulation study of invertebrates:

- Madeley and Birtley (1980) studied the uptake and accumulation of a $^{14}C_{25}$ - $C_{20–30}$, 42% Cl wt. CP product in mussels (*M. edulis*). The Environment Agency has not been able to access the publication and is therefore relying on the summary provided in Environment Agency (2009a). Details of the test substance and temperature are provided above for the parallel experiment with *O. mykiss*. The food used in the test was dry yeast cells, dosed at a concentration of 524 mg/kg dw prior to feeding of the organisms. The exposure period was 47 days, followed by a depuration period of 56 days. Tissue concentrations in the mussels were measured at various sampling intervals covering the uptake and depuration phases of the study. In addition to the ^{14}C analysis, some mussels were analysed for the parent compound directly by a TLC method at the end of both the exposure and depuration phases. The results are presented (Table 19). The levels measured by this direct method were generally in agreement with those obtained by the ^{14}C method. However, as per earlier comments, the TLC methods should be treated cautiously. Co-extracted material that contains sorbed radioactivity will interact with the stationary phase of the TLC plate, leading to a non-resolved smearing and a concentrated point on the origin of the TLC plate. Due to the reduced resolving power of TLC in comparison to other methods this can underestimate concentrations even if a defined region of radioactive interest is observed that corresponds to the parent compound.
  Please see the earlier comments about the robustness of the 2 analytical methods. During the test, 7 control and 10 exposed mussels died. The total number of mussels used in the study was not given in the paper but was at least 84, so the difference in death rate is probably not significant.
- The Environment Agency has estimated an indicative depuration rate constant using these data (day 7 to day 56 of depuration which equate to day 54 and day 103 of the study). For both exposure concentrations, concentrations in tissues and the total body burden and total body burden (TBB) minus the digestive gland (TBB - gut) were plotted at the relevant time points using Microsoft® Excel. The correction for total body burden was performed to account for residual spiked food present in the digestive gland, which would lead to an overestimate of the starting concentration for depuration, and subsequently the calculated k_2 (d^{-1}) value. Linear trend lines were plotted to model pseudo-first order kinetics. There is no guidance on how to take growth rate into account for mussels. Please note that it is not

clear from the text of Environment Agency (2009a) whether lipid correction had been performed on the data.

Table 19 Tissue concentrations (mg/kg dry weight, based on ^{14}C-radioisotope methods) during the uptake and depuration of $^{14}C_{25}$ - $C_{20\text{-}30}$ 42% Cl wt. by mussels (Madeley and Birtley, 1980)

Time (day)	Digestive gland	Foot	Gonad	Gill	Remaining tissues	TBB	TBB-minus gut
5^U	-	-	-	-	-	1.8	-
9^U	-	-	-	-	-	2.4	-
12^U	-	-	-	-	-	4.2	-
19^U	-	-	-	-	-	5.1	-
26^U	155.2	2.6	2.8	3.5	1.8	4.3	-
33^U	36.6	1.3	1.9	5.3	2.9	5.9	-
42^U	100.7	2.2	3.5	4.4	4.6	6.6	-
47^U	80.5	5.4	1.9	7.0	6.8	11.2 (3-16) [a]	-
7^D (54)	35.1	1.8	1.4	3.3	1.7	5.5	1.0
21^D	37.0	3.3	2.0	3.1	1.7	2.9	0.6
28^D	42.2	3.1	1.0	1.9	1.5	2.0	0.3
39^D	15.8	2.9	2.0	3.6	1.7	2.2	0.9
49^D	11.3	1.7	1.5	2.5	1.3	3.1	1.2
56^D (103)	7.0	0.9	0.9	1.5	0.6	1.2 (<1-7) [a]	0.4

Note: a - Concentration of chlorinated paraffin determined by TLC analysis.
U - Uptake phase
D - Depuration phase

Assuming pseudo-first order kinetics, an exponential trend line gave a first-order exponential rate constant of 0.0298 d^{-1} with an R^2 value of 0.73 for the TBB. This equates to a half-life of 23.3 days. The first-order exponential rate constant for TBB minus gut was 0.0026 d^{-1}, with an R^2 values of 0.0192. This equates to a half-life of 266 days. Due to the lack of details available, the Environment Agency considers this study to be Klimisch 4 (unknown reliability).

Discussion of dietary studies

- Dietary exposure tests are the recommended method for bioaccumulation assessment of highly hydrophobic substances like LCCPs. However, all of the available studies were performed prior to the revision of OECD TG 305 (OECD; 2012) which provided detailed guidance for fish dietary exposure studies for the first time following an international ring test. Many details required to assess them against the guideline are unavailable. There is no standard guidance for the determination of BMFs in invertebrates. In addition, none of the studies were performed in accordance with GLP. This is a major drawback for large and complex experiments such as these, and they are generally of unknown reliability. Studies with some other highly hydrophobic substances such as decabromodiphenyl ether (Mörck *et al*., 2003a and 2003b; Sandholm *et al*., 2003) also suggest that the presence of undissolved microcrystals can affect the degree of absorption across the gut and the nature of the food may also have an influence. This may also be applicable to LCCPs.
- Although the available studies should be given a low weighting as part of the assessment of bioaccumulation potential due to their uncertain reliability, they still provide some relevant insights. For example, the Environment Agency has performed a rudimentary benchmarking exercise for depuration half-life to provide further context. There may be significant variability in measuring this half-life between and within species (e.g. due to differences in lipid content and metabolic profiles, age of fish, etc.). However, advantages of using this metric as a key indicator for bioaccumulation assessment are that it is relatively easy to determine and not so dependent on other variables within a particular study.
- It was only possible to estimate depuration rates from the dietary fish studies of Fisk *et al*. (2000), Madeley and Birtley (1980) and the mussel study of Madeley and Birtley (1980) (calculations could be performed for the Bengtsson and Baumann Ofstad (1982) study but as it is considered unreliable this information is not reported here).
- Two approaches were used:
    - Environment Agency (2012), OECD TG 305 and its associated guidance documents (OECD, 2012c and 2017 have analysed depuration rate constants (k_2) from a large number of available BCF studies. A k_2 value ≤ 0.065 d^{-1} (95% confidence interval: 0.062 to 0.068) or a lipid-normalised k_2 ≤0.085 d^{-1} (95% confidence interval: 0.083 to 0.086) was found to be consistent with a BCF of ≥5 000 L/kg (normalised to a 5 % lipid content). A k_2 value ≤ 0.178 d^{-1} was found to be consistent with a BCF of ≥ 2 000 L/kg (normalised to a 5% lipid content).

- The reported 'growth-corrected lipid-normalised' k_2 range for a C_{18}, 49% Cl wt. CP product was 0.0076 to 0.0088 d^{-1} (Fisk *et al*., 2000). The low rate of depuration suggests that the BCF could exceed 5 000 L/kg. The way that the k_2 was derived by the study authors is consistent with the approach used in the OECD TG 305 guidance (OECD, 2012).

- Estimated k_2 values for a $^{14}C_{25}$ - $C_{20\text{-}30}$, 42% Cl wt. CP product were 0.081 and 0.083 d^{-1} for 2 different feed doses (Madeley and Birtley, 1980). These rates are borderline in terms of indicating a BCF exceeding 5 000 L/kg. Estimated k_2 values corrected for substance in the gut were 0.070 and 0.071 d^{-1}. These rates indicate a BCF exceeding 5 000 L/kg. These values were not growth corrected or lipid normalised.
- The estimated k_2 value in mussels for a $^{14}C_{25}$ - $C_{20\text{-}30}$, 42% Cl wt. CP product was 0.0298 d^{-1} (Madeley and Birtley, 1980). The estimated k_2 value corrected for substance in the gut was 0.0026 d^{-1}. These rates indicate BCFs exceeding 5 000 L/kg. These values were not growth corrected or lipid normalised.
- Data for LCCPs can be compared with other substances that are generally agreed to be very bioaccumulative under the REACH Regulation. For example, polychlorinated biphenyls (PCBs) data have been used to support the identification of perfluorohexane-1-sulfonic acid (CAS no. 355-46-4) as a Substance of Very High Concern (ECHA, 2017e). Information on depuration half-life has been transcribed from ECHA (2012) and is summarised in Table 20, with additional data on MCCPs from ECHA (2019).

Table 20 Depuration half-lives and BCF values for chemicals that are considered to be very bioaccumulative

Substance	Depuration half-life, days	BCF value, L/kg
SCCPs	39 to 87	7 273
MCCPs (C_{14} 50% Cl wt.)[a]	86 (from k_2)	55 524 to 125 952
MCCPs (C_{14} 50% Cl wt.)[a]	108.9 (from lipid & growth corr. k_2)	55 524 to 125 952
Musk xylene	2.8 to 4.2	3 730 to 10 500
D4	3.8, 105	≥11 495
D5	24 to 39	≥ 5 860
D5	19 to 22	12 600
Arochlor 1248 (commercial PCB mixture)	>28	>>5 000

Arochlor 1260 (commercial PCB mixture)	>42, 50	>>5 000
PCB-52	>974	>>5 000

Note: a - ECHA (2019)

> Therefore, with one exception (musk xylene), very bioaccumulative substances generally have a relatively long depuration half-life of 20 days or more in at least one fish species[6]. A depuration half-life above around 8 to 10 days is also suggestive of a lipid-normalised and growth-corrected BCF above 5 000 L/kg according to the analysis in EA (2012). The depuration half-life of LCCPs in fish from the estimated depuration rate constants discussed above are average 9.2 days ($^{14}C_{25}$ - $C_{20\text{-}30}$, 42% Cl wt.) and 347 days ($C_{18\text{-}26}$ 49% Cl wt.).

This information therefore suggests that LCCPs with chain lengths between C_{18} and C_{25} and chlorination levels of 42 to 49% may have a significant level of bioaccumulation, equivalent to exceeding a BCF of 5 000 L/kg. However, a definitive conclusion is not possible given the limitations of the data available.

4.3.1.2 Predicted data

CPs are neutral organohalogen compounds. Bioaccumulation would traditionally be expected to involve simple partitioning to lipid storage tissues, although this may not be a straightforward assumption for LCCPs. The degree of bioaccumulation of the constituents will depend on their hydrophobicity and metabolism potential; the BCF can therefore be predicted using QSAR correlations with log K_{OW} or aqueous solubility. Other methods depend on theoretical quantum mechanical descriptors, which require expert interpretation. Standard prediction methods include:

- Non-linear equation from REACH Guidance R.7c (ECHA, 2017c).
- log K_{OW} >7 regression equation and Arnot and Gobas (2003) method in BCFBAF v3.01 in EPI Suite™ (US EPA, 2012).
- COMPTox Dashboard (US EPA, 2021).

[6] Goss *et al*. (2013) also consider the use of elimination half-life data in bioaccumulation assessment, taking a first principles approach without considering actual data. The proposed half-life corresponding to a BMF of 1 is 70 days assuming 100% assimilation efficiency (longer if the assimilation rate goes down).

- VEGA (IRCCS, 2020 and 2021).
- CASE Ultra (MultiCASE); and
- CATALOGIC (LMC).

CASE Ultra and CATALOGIC are commercial platforms which are not available to the Environment Agency at this time. In addition, no relevant information was located in the COMPTox dashboard (US EPA, 2021). Consequently, no data originating from these models and platforms will be discussed in the following text.

The EU REACH registrations (ECHA, 2021a) present predicted BCFs using a log K_{OW} of 9.7 in accordance with the pre-REACH technical guidance documents (ECB, 2003a and b). These values were originally derived in Environment Agency (2009a). A single value is not appropriate for PBT assessment given the complexity of the substance (some congeners will have a log K_{OW} around 7.5). Estimation methods have also been refined, so these earlier predicted values are not included in this report.

LCCPs congeners have high log K_{OW} values, many of which are likely to be ≥ 7.5 (see Section 3.3.4). While there is a lack of empirical bioaccumulation data for LCCPs, the results provided in a Canadian government report using a Modified Gobas BAF Model suggested that of all the LCCPs congeners only liquid $C_{18\text{-}20}$ LCCPs have significant bioaccumulation potential (EC & HC, 2008). The Environment Agency has not been able to assess the reliability of this information in the absence of data on applicability domain, etc.

For the purposes of this assessment, some standard methods (ECHA, 2017c) were used to predict the following fish BCF values using log K_{OW} as predicted by the software, with the exception of:

- where a log K_{OW} of 7.5 was selected.
- Bi-linear equations Bintein (1983) and modified Connell and Hawker (1988) from REACH Guidance R.7c (ECHA, 2017c): ≥ 9 195 L/kg (the value declines as log K_{OW} values increase).
- The Environment Agency determined the BCF/BAF of a range of hypothetical LCCPs using both EPISuite v4.1 (US EPA, 2012), and VEGA QSAR v1.2.8 (IRCCS, accessed 2021) software packages. The VEGA platform contains 3 different models: Arnot-Gobas v1.0.0, CAESAR v2.1.14, and Meylan v1.0.3. EPISuite contains the BCFBAF v3.01 model. These data are presented (Table 21).

Table 21 Estimated BCF values of selected LCCPs using EPISuite™ (US EPA, 2012) and VEGA v 1.2.8 (IRCCS, 2021)

Chemical formula	% Cl wt	Molecular weight	EPISUITE v4.1 BCFBAF (v3.01) (L/kg ww)	VEGA v1.2.8 Arnot Gobas v1.0.0 (L/kg)	VEGA v1.2.8 CAESAR v2.1.14 (L/kg)	VEGA v1.2.8 Meylan v1.0.3 (L/kg)
$C_{18}H_{30}Cl_8$	53.6	530.06	51.9	10	1	205
$C_{18}H_{33}Cl_5$	41.6	426.73	87.99	17	4	348
$C_{20}H_{33}Cl_9$	53.9	592.56	13.98	2	4	55
$C_{20}H_{36}Cl_6$	43.6	489.23	25.75	3	13	102
$C_{25}H_{29}Cl_{23}$	71.3	1144.93	3.16	0.93	1	3
$C_{25}H_{42}Cl_{10}$	50.9	697.14	3.16	0.94	3	3
$C_{25}H_{45}Cl_7$	41.9	593.81	5.2	0.94	5	5
$C_{30}H_{35}Cl_{27}$	70.8	1352.84	3.16	0.93	0.77	3
$C_{30}H_{49}Cl_{13}$	53	870.61	3.16	0.93	1	3
$C_{30}H_{53}Cl_9$	43.6	732.83	3.16	0.93	3	3

Note: a - SMILES codes associated with these data are presented in Appendix D.

There is clearly a major difference between the output of these models (which all suggest a relatively low degree of bioconcentration) and the value estimated using the method recommended in the REACH Guidance. However, given the uncertainty and breadth of log K_{OW} values attributed to LCCPs (see Section 3.3.4), all predictions should be considered with caution.

The VEGA program flagged that the values generated using CAESAR and MEYLAN models should be considered unreliable with predictions outside of the applicability domains. No related substances with associated experimental values were included in the training sets. The accuracy of predictions for similar molecules in the training sets were not optimal i.e. experimental values disagree with the predicted data, or experimental variability is observed. The descriptors for the substances had values inside the descriptor range of compounds in the training set and atom centred fragments were found in compounds of the training set. In addition to these previous points, the reliability of logP predictions in the Gobas-Arnot Model was also flagged as not adequate.

In addition, the QSARs themselves are based on assumptions and in some cases very small data sets. It is also relevant to note that the BCFBAF program estimates the BCF (and BAF) based on the total concentration in water rather than the dissolved concentration in water (EA, 2013). The freely dissolved concentration of

LCCP congeners may be very low and so predictions from this model could be misleading (i.e. under-estimating the actual BCF).

The Environment Agency has also screened LCCP congeners against the criteria used in the REACH guidance (ECHA, 2017a) to indicate substances that may have limited absorption and distribution potential via passive transport (the screening criteria are used to indicate the potential for a substance to exceed a BCF of 2 000 in aquatic species). The criteria are:

- an average maximum diameter greater than 17 Å (1.7 nm), plus a molecular weight greater than 1 100 g/mol; or
- a measured octanol solubility (in mg/L) below 0.002 times the molecular weight, as an indicator of lipid solubility (without observed toxicity or other indicators of bioaccumulation).

Average maximum diameters of LCCPs with chlorination levels between 51 and 53% were calculated to be 18.9 to 27.4 nm for $C_{18}H_{31}Cl_7$ to $C_{30}H_{49}Cl_{13}$ using OASIS Basic, version 1.06 (Environment Agency, 2009b). Chain lengths from 18 to 21 carbon atoms would need to have between 17 and 20 chlorine atoms to achieve a >70% chlorination level (the highest degree of chlorination for commercial products). The majority of LCCP constituents would therefore meet the first part of the first criterion. However, no LCCP congener in this range has a molecular weight exceeding 1 100 g/mol. For LCCP congeners with 22 to 32 carbons, the molecular weight cut-off occurs at chlorination levels of 19 to 21 chlorine atoms (equivalent to 61 to 72% Cl wt.). On the basis of this information, the first criterion is only fulfilled for the highly chlorinated congeners (> 60% Cl wt.) with greater than 22 carbons. These data are tabulated in Appendix E.

Octanol solubility data are not available for LCCPs. Subsequently, the second criterion cannot be assessed.

4.3.1.3 Data from structural analogues

ECHA (2019) and UK Gov (2021) provide up-to-date summaries of the information available for MCCPs.

Two reliable aquatic fish BCF studies are available. A growth-corrected and lipid-normalised kinetic BCF of 10 500 to 14 600 L/kg was obtained for a C_{14}, 45% Cl wt. substance (without growth correction, the BCF is 3 230 to 4 460 L/kg). The highest growth-corrected kinetic BCF for a C_{15}, 51% Cl wt. substance is 2 164 L/kg (lipid normalisation was not possible). There are no definitive fish BCF data for C_{14} CPs with chlorine contents above 50% Cl wt., C_{15} chlorinated n-alkanes below 50% or ≥55% Cl wt., or longer chain length substances. However, the EU REACH Registrants concluded that a "C_{14}, 50% Cl test material will include the same

congener groups as in this [C_{14}, 45% Cl wt.] test material". Therefore, C_{14}, 55-60% Cl wt. products will also have a BCF above 5 000 L/kg.

Evidence from enhanced ready biodegradation studies suggest that some constituents (particularly those with low chlorine contents) are susceptible to microbial transformation under the conditions of those tests. However, there is no information about metabolic rate constants in fish for different constituents. Given the large number of constituents, their low water solubility, and difficulties associated with accurate chemical analysis, it is likely to be very difficult to generate more data on fish metabolism.

A reliable fish dietary bioaccumulation test with a C_{14}, 50% Cl wt. substance gave a growth-corrected depuration half-life of 108.9 days and growth-corrected and lipid-normalised BMF of 0.448. Calculated BCFs using the 15 models within the OECD TG 305 BCF estimation tool significantly exceed 5 000 L/kg. This is consistent with the findings of the aqueous tests. The evidence from this study suggests that metabolism is not sufficiently quick to prevent high levels of bioaccumulation.

The available fish dietary bioaccumulation data from a series of studies by Fisk *et al*. (2000, 2001, 2004) show a generally similar pattern of accumulation, with the potential for uptake (as measured by assimilation efficiency) decreasing with increasing carbon chain length and increasing chlorine content. Depuration from the fish is relatively slow and dietary BMFs above 1 are estimated for C_{14} CPs with 4 to 6 chlorine atoms per molecule (corresponding to chlorine contents of approximately 42 to 53% by weight). Calculated BCFs from these studies using the 15 models within the OECD TG 305 BCF estimation tool significantly exceed 5 000 L/kg for C_{14} (42 to 55% Cl wt.) and C_{16} (32 to 68% Cl wt.) CPs. The structure of the substance tested had terminal and adjacent chlorine atoms. NMR analysis presented in the publications of van Mourik *et al*. (2021) and Sprengel *et al*. (2019) have shown that terminal and adjacent chlorination occurs in commercial products. BMFs are estimated to be close to 1 for C_{16} CPs with 3 chlorine atoms per molecule (chlorine content approximately 32% by weight). At higher chlorine contents than these, the BMF is below 1 for both the C_{14} and C_{16} substances.

A high degree of accumulation has been observed in aquatic invertebrates in laboratory studies using $C_{14\text{-}17}$, 52% Cl wt., C_{13}-C_{18}, 45% Cl wt. and C_{16}, 34% Cl wt. substances, with BCFs and BAFs exceeding 2 000 L/kg, although there are significant uncertainties in the reliability of these studies, there may be some under-estimation due to the nominal exposure concentrations exceeding the water solubility limits.

A Biota Sediment Accumulation Factor (BSAF) of 4.4 on a lipid normalised basis was determined for a C_{16} chlorinated n-alkane, 35% Cl wt. in a study using Lumbriculus

variegatus; the BSAF for a C_{16} chlorinated n-alkane, 69% Cl wt. substance was 0.6. The Environment Agency considers this study to be unreliable (Klimisch 3).

4.3.1.4 Monitoring data for aquatic biota

The studies described in this section are also tabulated in Appendix F.

Environment Agency (2009a) included brief summaries of various studies that were available at the time:

- Kemmlein *et al*. (2002) reported the results of a study looking at the levels of CPs in marine mussels and crabs from an area close to a CP manufacturer in Australia. The levels of total CPs found were 25 mg/kg (µg/g) lipid in mussel and 109.5 mg/kg (µg/g) lipid in crabs. LCCPs were found to make up around 27% of the total CPs in mussel and 13% of the total in crabs (i.e. approximately 6.75 and 14 mg/kg lipid, respectively). Identical results were presented in OSPAR (2000), which were referenced to an unpublished study by Rotard *et al*. (1998).
- Details of an unpublished study (Froescheis, 1997) were also reported by OSPAR (2000). This study detected CPs (including chain lengths above C_{17}) in the deep-sea fish *Sebastolobus altivelis*, but it was not possible to quantify the levels found. $C_{10–20}$ and C_{20-30} CPs were measured in seals, marine shellfish and salt and freshwater fish from around the United Kingdom (Campbell and McConnell, 1980). Environment Agency (2009a) suggested that the $C_{10–20}$ levels were likely to be dominated by contributions from SCCPs and MCCPs.
- The results of an unpublished survey of levels of LCCPs (average carbon chain length C_{24}) in biota, carried out by Baldwin and Bennett (1974) were reported by Zitko (1980). In all of the 52 samples that were analysed, covering eggs from 4 species of aquatic bird, 6 species of fish and 2 species of shellfish. LCCPs were detected only once, at 0.06 mg/kg, which was close to the detection limit of the method used. Few other details (for example location, analytical methods used) of this study are available.
- Jansson *et al*. (1993) reported the occurrence of CPs (of unspecified chain length, with 6 to 16 chlorine atoms/molecule) at levels of 570 to 1 600 µg/kg lipid in fish and 130 to 280 µg/kg lipid in seals from Sweden. In addition, they also reported levels of CPs of 2 900 µg/kg lipid in rabbit muscle, 4 400 µg/kg lipid in moose muscle, 140 µg/kg in reindeer fat and 530 µg/kg in osprey muscle in pooled samples from the same area. It is not known what contribution LCCPs made to these levels.
- Levels of total $C_{10–24}$ CPs in food, fish and marine animals were reported by Greenpeace (1995). LCCPs were thought to make up between 53.5 and 94% of the total CPs found. The concentrations of LCCPs present can be

estimated from the data as 225 µg/kg in mackerel, 50 µg/kg in fish oil, 58 µg/kg in margarine, 13 to 107 µg/kg in porpoise, 819 µg/kg in Fin Whale, 37 µg/kg in pork, 43 µg/kg in cow's milk and 35 µg/kg in human breast milk (on a lipid weight basis). The average chlorine content of the CPs detected was around 33%.

- CPs (of unspecified type) were not found in any of the 108 Japanese fish samples analysed (detection limit 500 µg/kg ww in the early 1990s (Environment Agency Japan, 1991). This is surprising given the known bioaccumulative behaviour of SCCPs and MCCPs, and evidence from Europe.

These studies suggest that LCCP congeners may be present in a wide variety of species, including organisms at the top of the food chain such as porpoise and Fin Whale, and also in human breast milk. However, given their age and generally limited background information, the reported numerical concentrations may not be reliable, and the Environment Agency considers that they provide qualitative evidence of detection only.

Several studies have been published since Environment Agency (2009a) and these are summarised below. They generally include a range of CPs, and information is provided on MCCPs and SCCPs to provide additional context where appropriate. Further data on MCCPs have previously been reviewed in UK Gov (2021) and ECHA (2019), so are not discussed here. Studies published since the Substance Evaluation of MCCPs (ECHA, 2019) which have not been included in this report due to limited relevance or time constraints are presented in Appendix B.

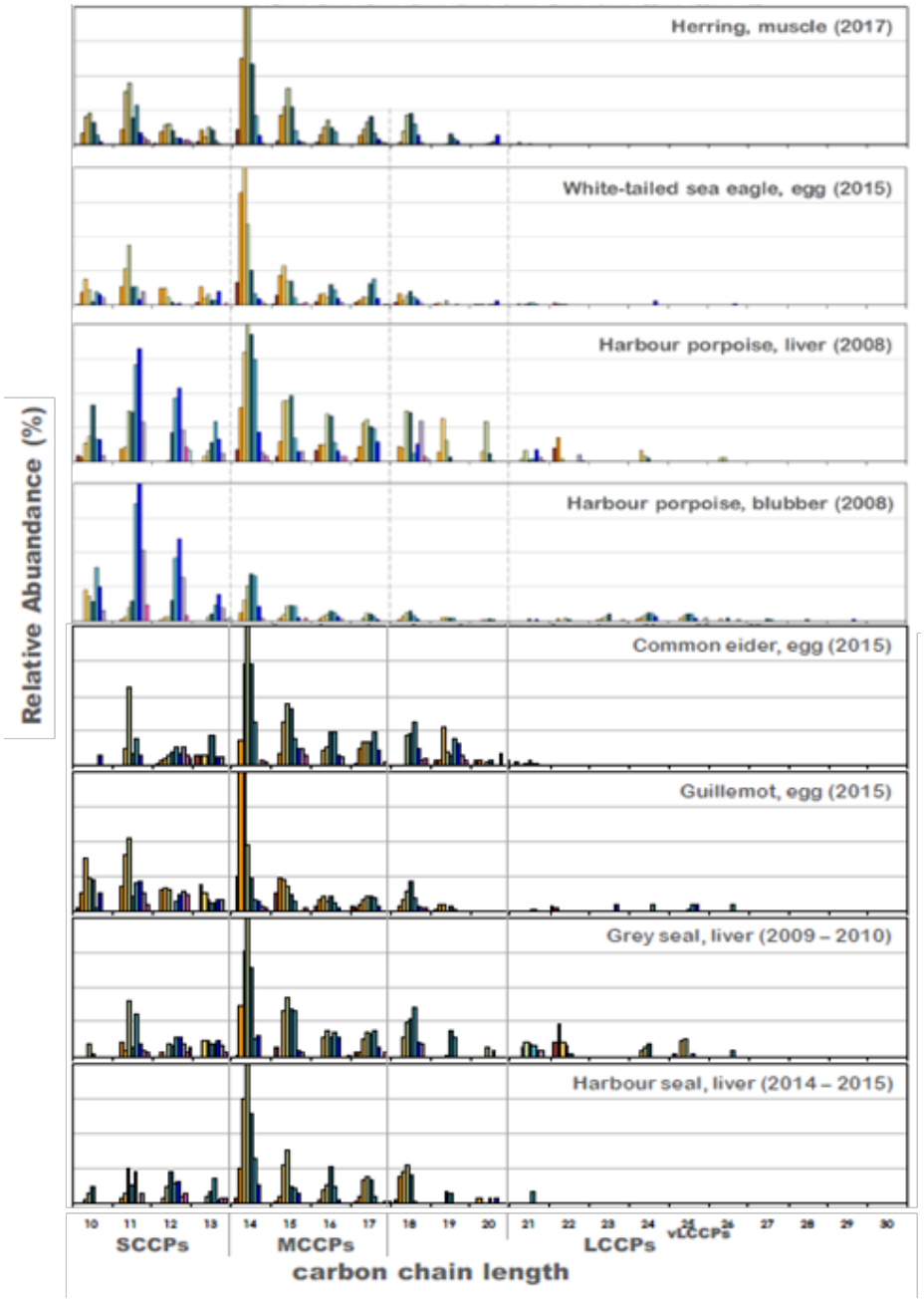
- As part of an analytical method development exercise Yuan *et al*. (2018) analysed fillet samples from Herring, Common Dab, Salmon, Flounder and Blue Mussel collected between 2008 and 2016 from water bodies in Sweden, The Netherlands, the Atlantic Ocean and Chile. Apart from Herring (n=10), more than 10 individuals were sampled for each species, and pooled for analysis. Extract and clean-up of the tissues were performed using the method described in Yuan *et al*. (2019) (described below). Analyses were performed using APCI-qTOF-MS using bromine and chlorine enhanced detection methods. For bromine enhanced detection, procedural LOQs of LCCPs, MCCPs and SCCPs were calculated to be 2.7 ng/g lipid, 36 ng/g lipid and 45 ng/g lipid, respectively. CPs were detected in all biota above their LOQs. The highest LCCP concentrations were measured in Blue Mussel from Chile and The Netherlands at 650 ng/g lipid and 440 ng/g lipid, respectively. Corresponding concentrations of MCCPs and SCCPs were approximately 1 to 3 times higher. Further details are presented in Appendix H.
- Yuan *et al*. (2019), (originally published as Yuan and de Wit, 2018b), investigated the presence of LCCPs, MCCPs and SCCPs in samples of 7

aquatic species collected from several locations in the Baltic Sea between 2006 and 2017, including fish, seabirds and marine mammals. All samples were produced from a pool of 2 to 40 individuals and contained tissues from both sexes. Paired samples of different tissues (liver/muscle, liver/blubber, liver/egg) were produced from the same individual or the same colony in which the individual lived. All samples were from adult organisms, except for Grey and Harbour Seals (for which only juvenile samples were available). Sampling, processing and analysis are well documented, with methods adapted from those widely used in the CP academic community (i.e. Zhou *et al*., 2016 and Yuan *et al*., 2017). To summarise, sample processing and extractions were optimised to take account of tissue water content. The water content of marine organisms and egg samples meant that extractions were performed without freeze drying, using accelerated solvent extraction (ASE) [DCM and n-hexane (1:1 v/v)]. All extracts were taken to almost dryness and cleaned using solid-phase extraction. Resulting eluents were re-constituted in polar solvents, and 20 ng of Dechlorane-602 was added as a volumetric standard. Chemical analyses were performed using DCM enhanced APCI-qTOF-MS. Quantification and qualification of CPs in the tissues were performed using CP technical mixtures sourced from different European manufacturers. Relative instrumental responses of CP congener groups from $C_{10}Cl_3$ to $C_{30}Cl_{12}$ comprised a C_nCl_m fingerprint of the analyte. The m/z ratios used were previously published in Yuan *et al*. (2017). The C_nCl_m of each analyte was reconstructed from the technical mixtures using the linear combination method (as per Bogdal *et al*., 2015). Lipid determination was performed using the standard sulphuric acid method (Jensen *et al*., 2009). The Environment Agency notes that rigorous quality control methods were applied throughout the laboratory study and data processing. For the specific aquatic tissues, LOQs for LCCPs, MCCPs and SCCPs ranged from 1.5 to 6.1 ng/g lipid, 10 to 41 ng/g lipid and 9.3 to 37 ng/g lipid, respectively. These are presented in detail in the supporting information of the publication. SCCP, MCCP and LCCP congeners in all of the samples were above the calculated LOQs. Representative relative abundance of CP congeners in the aquatic tissues are presented in Figure 4. A table of species, tissue samples, sampling location, lipid contents and concentrations are presented in Appendix H.

Concentrations across all aquatic samples ranged from 6 to 130 ng/g lipid, 32 to 140 ng/g lipid and 26 to 330 ng/g lipid, for total LCCPs, MCCPs and SCCPs, respectively. On average LCCPs contributed to 15% of the total CP concentrations across all species, with MCCPs accounting for 47%. Median concentrations of total LCCPs observed in fish, sea birds and sea mammals were 24, 35 and 50 ng/g lipid, respectively. The highest concentration of LCCPs was detected in the liver of Harbour Porpoise (n=11)

(130 ng/g lipid); the paired blubber samples contained LCCPs at a concentrations of 25 ng/g lipid. The highest concentrations of LCCPs in marine birds were measured in two pooled Common Eider (n=5/n=5) samples. These were 120 ng/g lipid (liver) and 18 ng/g lipid (egg), and 34 ng/g lipid (liver) and 52 ng/g lipid (egg). The concentrations of LCCPs in the pooled egg samples of Guillemot (n=4/n=5) and White-tailed Sea Eagle (n=4/n=5) were 36/18 ng/g lipid, and 34/76 ng/g lipid, respectively. Concentrations of LCCPs in Herring muscle ranged from 14 to 27 ng/g lipid.
Muscle/liver paired analyses comprised of two sample pools (n=38 and n=40) Concentrations of LCCPs were 44 ng/g lipid (liver) and 24 ng/g lipid (muscle), and 14 ng/g lipid (liver) and 27 ng/g lipid (muscle) in each of the pools, respectively. Corresponding concentrations of SCCPs and MCCPs were approximately 2 to 4 times higher (the liver samples from juvenile Harbour Seals contained the highest concentration of MCCPs at 540 ng/g lipid). LCCPs were found in lower proportions in the aquatic organisms compared to the terrestrial organisms sampled in the same study (see Appendix D). C_{18} CPs were generally more abundant than C_{19} and C_{20} congeners in most species. The authors note that unexpected concentrations of $C_{>20}$ CPs were detected in all samples and were predominantly $C_{24/25}$ congeners in 11 out of 38 samples. (For MCCPs, the C_{14} chain lengths were identified as the dominant congener group in most samples). Congener fingerprints in these samples are shown (Figure 4).

Figure 4 **CP congener fingerprints in marine wildlife samples (adapted from Yuan *et al*., 2019; copyright © 2019. Published by The American Chemical Society)**



Note: The vertical axis shows relative abundance of each congener group; the most abundant are expressed as 100%.

- De Wit *et al*. (2020) reported the sampling and analysis of two additional species from several locations in the Baltic Sea: Blue Mussel and Viviparous Eelpout. CP analyses were performed using a modified method following Yuan *et al*. (2020). Mussels (n=100) and fish (n=47, male and female,

approximately 2 years old) were collected in 2015. The soft body tissue of the mussel and the muscle tissue of the fish were extracted for CP analysis. Lipid contents (analysed following the method of Jensen *et al*., 2009) of the soft body and muscle tissues were 1.40% and 1.52%, respectively.

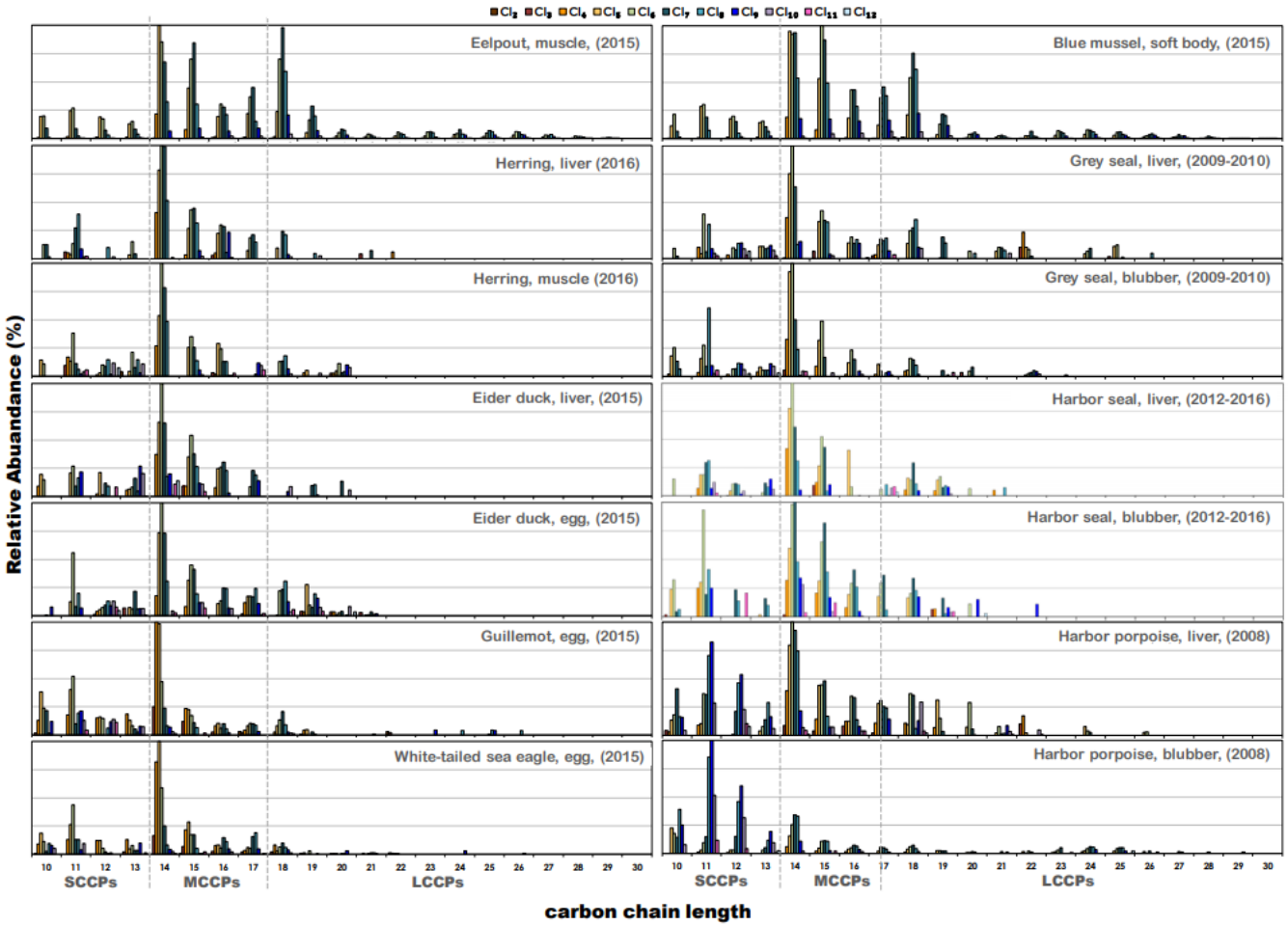
The LOQs of CPs extracted from mussel and fish tissues were calculated as 3 times the instrumental blank. In mussel tissue these were 6.3, 98 and 63 ng/g lipid for LCCPs, MCCPs and SCCPs, respectively. In fish tissues these were 3.4, 52 and 34 ng/g lipid for LCCPs, MCCPs and SCCPs respectively. The recoveries of the internal standard (^{13}C-labelled CP) were 86% for both species.

The concentrations of total CPs in the mussel and fish muscle samples were 400 and 310 ng/g lipid, respectively (single pooled samples). Average total LCCPs, MCCPs and SCCPs concentrations in the mussels were 120, 210 and 72 ng/g lipid, respectively. Average total LCCP, MCCP and SCCP concentrations in the fish muscle were 130, 130 and 52 ng/g lipid, respectively.

De Wit *et al*. (2020) noted the distribution of CPs was similar across all species, with total CPs comprising 13 to 15% LCCPs, 48 to 54% MCCPs and 31 to 38% SCCPs. Concentrations of LCCPs were an order of magnitude higher on a lipid weight basis in mussel soft tissues and Viviparous Eelpout muscle tissue than those measured in Herring muscle tissues reported by Yuan *et al*. (2019), although there is no information indicating whether the samples were collected at the same locations between studies. The dominant homologue and congener patterns were not presented in the publication, although a graphic representation was provided in the Supporting Information (Figure 5). This graphic visually indicates, assuming an identical consistent y-axis range, that chain lengths and congeners between C_{18} and C_{30} are present in a greater abundance in the mussel soft tissues and the Viviparous Eelpout muscle tissues than the other biota.

Using data from Yuan *et al*. (2019), De Wit *et al*. (2020) estimated the biomagnification potential for CPs where they were definitively measured in predator-prey species sourced from identified spatial areas. Predator-prey ratios were calculated using lipid normalised concentrations. Pairs were identified as seal/herring, porpoise/herring, guillemot/herring, sea eagle/guillemot or eider. A calculated ratio above 1 was proposed to be indicative of biomagnification potential.

Figure 5 **Congener group fingerprints of CPs in Baltic wildlife (from De Wit *et al.*, 2020 Figure S1 in the Supporting Information; copyright © 2020 The Authors (s). Published by Elsevier Ltd.)**



For LCCPs, the CP ratio of mean lipid weight concentrations for proposed predator-prey pairs ranged from 0.9 to 3.3 (Table 22). The highest ratios were seen for marine mammal/fish and eagle/Guillemot pairs, with calculated ratios from 2.7 to 3.3 and 2.0, respectively.

Table 22 Lipid weight concentration ratios of CP groups (liver, eggs/liver) between proposed Baltic Sea predator-prey species pairs (adapted from De Wit *et al.*, 2020)

Predator-prey pair	LCCPs	MCCPs	SCCPs
Grey Seal liver - Herring liver	2.7	1.4	3.2
Harbour Seal liver - Herring liver	3.0	2.4	3.9
Harbour Porpoise liver - Herring liver	3.3	1.8	5.0
Guillemot egg - Herring liver	0.9	0.4	1.5
White-tailed Eagle egg - Guillemot egg	2.0	3.1	2.5
White-tailed Eagle egg - Eider egg	1.6	1.1	1.8

The Environment Agency has the following observations on the studies of Yuan *et al.* (2019) and De Wit *et al.* (2020):

- Reported concentrations may be semi-quantitative for the reasons outlined in Section 2. The extraction efficiencies calculated from the recoveries of the internal standard were above 80%, but it is likely that concentrations were still slightly underestimated because not all CPs will have been accounted for within the biological tissues. The Environment Agency therefore considers the concentration data to be reliable with restrictions (Klimisch 2).
- The longest CP chain lengths detected were up to C_{24} in Herring, and similar or slightly longer in sea birds ($C_{24/25}$ were predominant in the White-tailed Sea Eagle) and marine mammals (C_{24} predominant, and shorter than C_{26} in general but up to C_{30} in Harbour Porpoise blubber). The occurrence of $C_{>20}$ CP congeners (with a calculated chlorine content of 52 to 59% Cl wt.) in all of the sampled species indicates that these large molecules are capable of crossing biological membranes in aquatic species. As noted in Section 4.3.1.2, highly chlorinated LCCP congeners (> 60% Cl wt.) with greater than 22 carbons meet the screening criteria for substances considered unlikely to cross biological membranes via passive diffusion (such that they would not be considered “significantly bioaccumulative” – it does not mean that some level of accumulation will not occur).

Caution should be taken in interpreting the calculated lipid weight concentration ratios for proposed predator-prey relationships for several reasons:

- Individual tissue concentrations that have been lipid normalised may not be representative of an organism’s total body burden. This can be due to distribution

differences of a substance within an organism due to uptake route, substance physicochemical properties and influence of the biochemistry of a tissue type. Variations between lipid- and protein-rich tissues were not investigated (for example via a normalisation process to total protein content).

- Comparison of lipid-normalised tissue concentrations within and between species may also be misleading, especially where there are significant differences in lipid content. For example, Mackay *et al*. (2018) presented a modelling perspective for quantifying metrics of bio-uptake of organic chemicals in fish and examined the sensitivity of biomagnification relative to lipid content. For substances that are very hydrophobic (log K_{OW} > 8), such as LCCPs, where diet is responsible for 99.8% of the input, wet weight concentrations were considered more insightful for determining accumulation metrics, especially when estimating trophic magnification. Normalising for lipid content may therefore introduce unnecessary variability. This highlights the need for data to be reported as both wet weight and lipid normalised concentrations.
- The number of samples for some species was as low as 2, so the representativity of the data is unknown. Comparisons between individual species is complicated by the fact that they were sampled from different locations and at very different times (the samples were collected over the course of a decade). The paper does not indicate whether concentration trends were apparent with time, and calculations for the predator-prey species pairs by De Wit *et al*. (2020) involved samples collected from unconnected locations. As well as concentration gradients at specific localities, the presence of other anthropogenic substances might also affect the uptake, storage, and metabolism of CPs, and this will vary geographically.
- The seasonal condition of individual organisms could also be a factor in terms of the CP load they carry (i.e. comparing concentrations between species collected at different times of the year might be inappropriate). The statistical confidence in the comparison is unclear.
- As discussed in Section 2, the standard deviation is not the best measure of accuracy or central tendency, and a median or modal average and range could better reflect the breadth and variance of the data sets.

These 2 studies therefore provide strong evidence that LCCP constituents can accumulate in a wide range of aquatic species and are found in tissues of organisms at the top of the food chain. However, the data are not sufficient to indicate that biomagnification is occurring in specific food chains.

Four related studies by Du and co-workers (Du *et al*., 2018; Du *et al*., 2019; Zhou *et al*., 2019; and Du *et al*., 2020) present information on the levels of LCCPs in a variety of biota (both aquatic and terrestrial) sampled from artificial wetland ecosystems in China (Jinshan rice paddies and Dianshan Lake of the Yangtze River Delta (YRD)). The paddy fields and lake are the receiving environments of CPs discharged from industrial facilities in this region.

- Du *et al*. (2018) analysed for LCCPs, MCCPs and SCCPs in 4 species (2 fish – Pond Loach and Rice Field Eel – and 2 semi-aquatic reptiles – Red-backed Rat Snake and Red-banded Snake) from paddy fields in the YRD, China. Between 4 and 6 individuals (or pooled samples) were available for each species, except for the Red-banded Snake, where only one individual was available. The sample site was adjacent to an industrial park located close to Hangzhou Bay, on the border of Jinshan District (Shanghai) and Jiaxing City (Zhejiang Province). This study reports the re-analysis of samples from Zhou *et al*. (2016) using APCI-qTOF-MS and presents relative contributions of LCCPs, MCCPs and SCCPs to total CP concentrations; CP fingerprints in the wildlife species; and addresses factors that have the potential to influence accumulation of CPs in wildlife. The species, tissue samples, sampling location, lipid contents and concentrations are presented in Appendix H.
  Whole muscle samples were sampled from the fish and snakes. Approximately 2 g dw of each sample or pooled sample was pre-fortified with $^{13}C_{10}$-1,5,5,6,6,10-hexachlorodecane) and freeze dried. Samples were Soxhlet extracted with DCM/hexane (1:1; v/v) for 24 h and lipid content determined gravimetrically. CPs were separated from contaminants such as polychlorinated biphenyls (PCBs) using two silica column-based methods. The presence of PCBs was confirmed in the previous study of Zhou *et al*. (2016). Dechlorane-603 was used to fortify specific fractions prior to analysis. Analysis for CPs was performed using APCI-qTOF-MS. Analysis of the internal standard was performed using gas chromatography-negative chemical ionisation-mass spectrometry (GC-NCI-MS). CPs were quantified using a pattern deconvolution algorithm developed by Bogdal *et al*. (2015), with a CP pattern that comprised 240 CP congeners from $C_{10}H_{19}Cl_3$ to $C_{31}H_{52}Cl_{12}$. The m/z ratios are referenced to Yuan *et al*. (2017). Isotopic analysis of $\delta^{13}C$ was used to identify terrestrial food sources according to methodology set out in Jardine *et al*. (2006). The Environment Agency notes that rigorous quality control methods were applied throughout the laboratory study and the data processing. The LOQs for LCCPs, MCCPs and SCCPs were species specific and reported to range from <0.7 to <1.3 ng/g dw, <12 to <28 ng/g dw and <25 to <52 ng/g dw, respectively. The extraction efficiencies calculated from the recoveries of the internal standard were above 80%.
  LCCPs, MCCPs and SCCPs were detected in all species examined in this study, at concentrations ranging from 14 to 10 000 ng/g lipid (median 950 ng/g lipid), 96 to 33 000 ng/g lipid (median 2 500 ng/g lipid), and <91 to 43 000 ng/g lipid (median 2 300 ng/g lipid), respectively.
  Median concentrations of LCCP congeners detected in decreasing order were 4 200 ng/g lipid in the Red-banded Snake, 1 600 ng/g lipid (range: 730 to 2 900 ng/g lipid) in Rice Field Eel, 1 100 ng/g lipid (range: 930 to 1 800 ng/g lipid) in Red-backed Rat Snake, and 610 ng/g lipid (range: 480 to 1 300 ng/g lipid) in Pond Loach. The highest concentration of LCCP congeners was detected in muscle samples of Red-banded Snake (4 200 ng/g lipid).

LCCP congeners with carbon chain lengths between 18 and 26 were detected in the muscle samples of all species; the breakdown of detection frequency was C_{18-21} 100%, C_{22} 92%, C_{23} 83%, C_{24} 83% and C_{25} 30% and C_{26} 13%. C_{27} CP congeners were detected in the Red-backed Rat Snake at a frequency of 4.3%. C_{28-31} CP congeners were not detected in any samples. The LCCP congener group patterns were dominated by C_{18} CPs (48.4%), followed by C_{19} and C_{20} CPs (18.7% and 13.6%, respectively).
For comparison, the highest concentrations of MCCPs were detected in the muscle samples of Red-backed Rat Snake (median 3 800 ng/g lipid; range: 820 to 3 700 ng/g lipid. MCCPs were the dominant CPs detected in all samples and contributed 44.2 ± 6.9% of the total extracted CP burden. SCCP concentrations correlated significantly (Spearman and Pearson's correlation; $p < 0.01$) to those of MCCPs.
Principal component analysis of $\delta^{13}C$, chain length and chlorination level allowed 3 clusters of correlating biota to be identified. One of these included aquatic/semi-aquatic organisms: Pond Loach, Rice Field Eel, Red-backed Rat Snake, Red-banded Snake (and Peregrine Falcon) (n=23, mean±standard deviation (sd): $\delta^{13}C$ -25.5±1.7, and 52.0±0.4 Cl wt.). It contained a higher proportion of MCCPs, as well as LCCP chain lengths. Two further clusters involved terrestrial organisms only (reported in Section 4.3.2.4).

The Environment Agency considers that the data should be considered reliable with restrictions (Klimisch 2). The same observations are generally applicable as for the Yuan *et al*. (2019) study.

- Du *et al*. (2019) is a continuation of the work reported by Du *et al*. (2018). The Black-spotted Frog was chosen for this study as it is a widespread amphibian species living in the paddy fields of the YRD, China, and is a food source for the 2 species of semi-aquatic snake sampled by Du *et al*. (2018). The sampling site for all biota was the same as that described in Du *et al*. (2018). No details with regards to duration of sampling or time of year were presented. Sixty-nine frogs were collected, and their body weight, length and sex recorded. The species, tissue samples, sampling location, lipid contents and concentrations are presented in Appendix H.
Pooled muscle and liver samples were generated for each sex and unfertilised eggs were collected and pooled from the ovaries of female frogs. CPs were difficult to measure in the muscle tissue, which was thought to be due to the low lipid content. Extraction, chemical analyses and data processing were performed using the same methods as Du *et al*. (2018). LOQs for LCCPs, MCCPs and SCCPs were reported to range between <0.18 to <1.7 ng/g ww, <0.64 to <6.0 ng/g ww and 4.9 to <46 ng/g ww, respectively, and were sample dependent. No variation in LOQs were observed between samples generated from different sexes.
Detection frequencies of LCCPs, MCCPs and SCCPs in all samples were 85%, 100% and 97%, respectively. Total CP concentrations in frog liver, muscle and egg samples ranged from 6.8 to 300 ng/g ww, 6.3 to 97 ng/g ww and 35 to 1

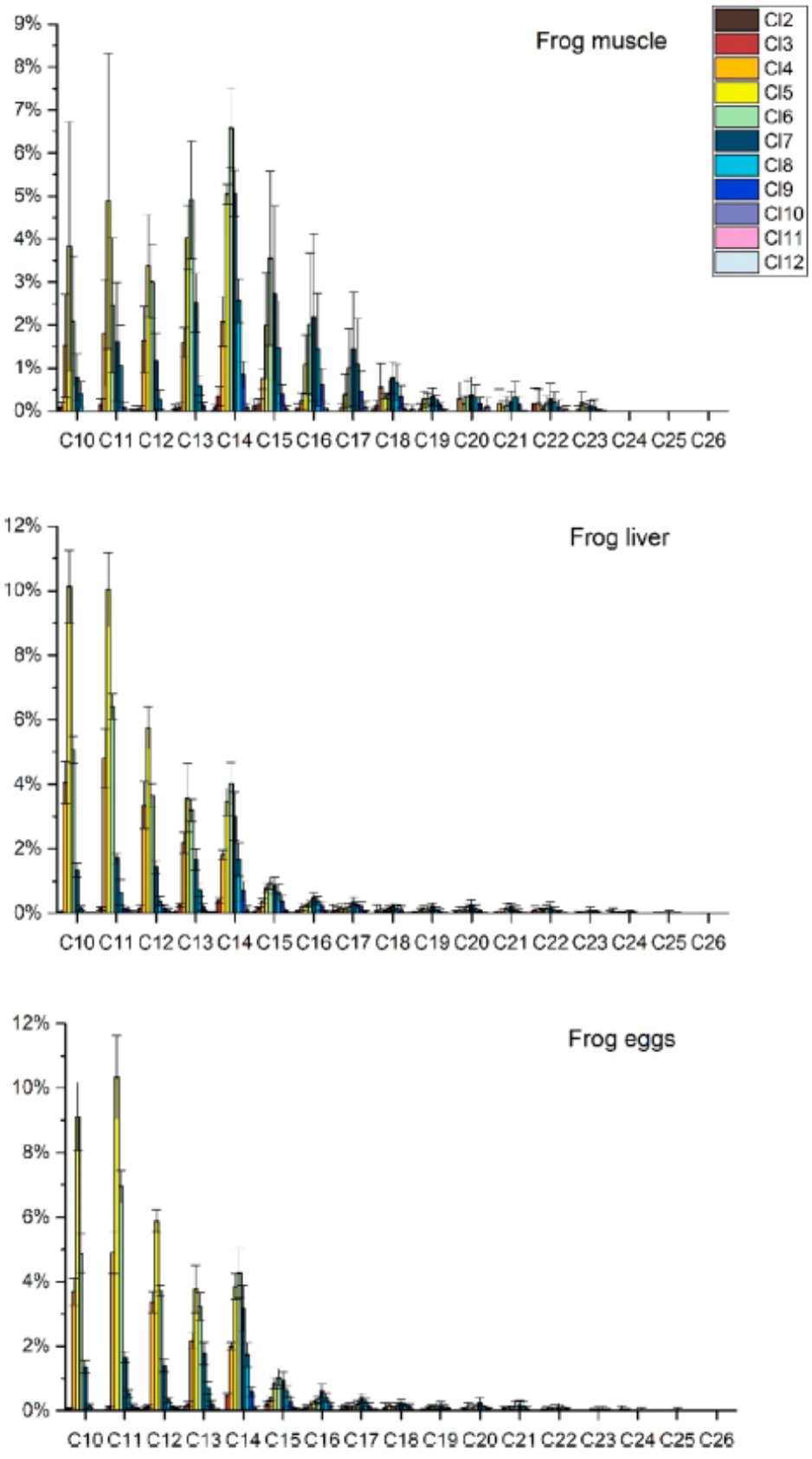
200 ng/g ww, for LCCPs, MCCPs and SCCPs, respectively. In frog liver and egg samples concentrations decreased in the order SCCPs (79%) > MCCPs (18%) > LCCPs (3%). In the pooled muscle samples, concentrations decreased in the order MCCPs (43%) > SCCPs (41%) > LCCPs (16%). The concentrations of CPs detected in the extracts of the different tissues are presented in Table 23. The extraction efficiencies calculated from the recoveries of the internal standard were above 80%. The congener fingerprint of CPs in the different tissues are presented in Figure 6.

Table 23 Concentrations and range of chlorinated paraffins (mean ± standard deviation, ng/g wet weight) in Black-spotted Frog tissues (adapted from Du *et al.*, 2019).

Tissue	Sex	SCCPs	MCCPs	LCCPs
Liver	Female	360 ± 240 (190 to 910)	69 ± 47 (31 to 190)	8.5 ± 6.9 (<LOQ to 26)
Liver	Male	320 ± 300 (28 to 910)	68 ± 59 (5.5 to 180)	28 ± 34 (ND to 110)
Egg		62 ± 64 (ND to 220)	16 ± 14 (<LOQ to 52)	2.9 ± 5.7 (ND to 20)
Muscle[a]	Female	6.9 ± 4.8	5.0 ± 3.0	2.6 ± 2.1
Muscle[a]	Male	14 to 31	25 to 50	7.6 to 16

Note: a - pooled samples; ND – not detected. The Environment Agency does not know why there is a differentiation between 'not detected' and '< LOQ' in this table.

Figure 6 **Chlorinated paraffin congener group profiles in frog tissues (adapted directly from Du *et al*., 2019; American Chemical Society Publishing)**



The measured mean (± standard deviation) lipid contents of liver, muscle and egg tissues were 22.63 ± 8.18%, 0.56 ± 0.06% and 9.87 ± 2.26%, respectively. The authors note that they did not find a significant relationship between total CP loads and lipid contents and that this was unexpected because the physicochemical properties of CPs would generally be expected to lead to a hypothetical distribution within the lipid-rich tissues of an organism (see Section 4.3.3 for further discussion). Concentrations normalised to mean lipid content are presented in Table 24).

Table 24 Concentrations and range of chlorinated paraffins (mean ± standard deviation, ng/g wet weight, lipid normalised) in Black-spotted Frog tissues (adapted from Du *et al.*, 2019).

Tissue	Sex	SCCPs	MCCPs	LCCPs
Liver	Female	1420 (749 - 3588)	272 (122 – 749)	34 (<LOQ – 103)
Liver	Male	1705 (149 - 4848)	362 (29 – 959)	133 (ND – 586)
Egg		324 (ND -2229)	162 (<LOQ – 527)	29 (ND – 203)
Muscle[a]	Female	1302	377	491
Muscle[a]	Male	(2276 – 5041)	(4065 – 8130)	1236 (2602)

Note: a - pooled samples; ND – not detected. The Environment Agency does not know why there is a differentiation between 'not detected' and '< LOQ' in this table.

No significant differences ($p > 0.05$) between hepatic CP levels were observed between male and female frogs, whilst a similar congener pattern distribution was observed. However, the male liver samples appeared to contain higher concentrations of LCCP congeners than egg and pooled muscle samples. The higher accumulation of CPs in liver was proposed by the authors to be driven by lipid enrichment and/or hepatic sequestration resulting from the induction of hepatic microsomal binding proteins. This was supported by the finding of Cranshaw and Winkle (2000), who determined that temperate amphibian species store large amounts of glycogen and fat in their liver tissue in the autumn as energy sources for brumation. The Environment Agency notes that this seasonal retention of glycogen and fat in the liver could be a relevant factor, but there is no information about timing of sampling.

92.4% of the CP congener groups detected in female frog liver tissue were simultaneously detected in the corresponding egg samples. The authors used paired CP concentrations measured in eggs and liver to evaluate the transfer of the substances from the liver to the eggs (E/L ratio). In frogs, and other species, the liver is important for the production of egg yolk as it produces a protein pre-cursor (the lipo-protein vitellogenin). The E/L ratio for LCCPs was 0.14 to 1.6 (mean: 0.71). This was higher than the ratios for SCCPs (0.0086 to 1.0; mean: 0.35) and MCCPs (0.077 to 0.83; mean: 0.52). Additionally, a positive linear relationship was found between E/L ratios and carbon chain lengths in the range $C_{10\text{-}20}$. When $C_{21\text{-}25}$ carbon chains lengths were examined, a scattering was

observed in the data. A parabolic relationship was observed between the E/L ratio and degree of chlorination, with the breakpoint noted at Cl_{6-7}. A significant positive relationship between the E/L ratio of the CPs and log K_{OW} was noted. The presence of LCCP congeners in eggs suggests that they will be transferred to the next generation of frogs at a sensitive stage of their life cycle, and the authors concluded that this is likely to be directly related to their lipophilicity (LCCPs with higher log K_{OW} values are likely to have a higher affinity to lipo-proteins).
Significant differences in concentration were observed for pooled muscle samples between the two sexes. For male frogs mean concentrations of 23, 38, and 12 ng/g ww were measured for SCCPs, MCCPs and LCCPs, respectively. These values are 3.3 to 7.6 times higher than those in females. The authors speculated that this might be a result of maternal transfer to eggs. Female muscle samples were enriched with C_{10-12} CPs and male muscles were enriched with C_{13-17} CPs.
For the LCCPs detected in this study, C_{18} was the most abundant chain length (23.6%) followed by C_{20} (20.4%). With regard to chlorination levels, Cl_5 was dominant in most fractions (31.9% total CPs), with decreasing percentages observed for Cl_6 (25.8%) and Cl_4 (15.4%). The dominant congener was Cl_6 in muscle tissue. For comparison, MCCP patterns in the majority of samples were dominated by C_{14} (63.9%), followed by C_{15} (19.0%). The congener group patterns observed in frog liver and eggs were similar (possibly explained by yolk components being processed in the liver), whilst distinct differences were observed in the muscle samples.
The authors noted that there were similarities in congener patterns between the frog muscle tissue samples and the muscle samples from the Collared Scops Owl and Common Cuckoo reported in Du *et al*. (2018) (Section 4.3.2.4). These bird species are mainly insectivorous, and insects are also the chief food item of the frogs. It is therefore possible that the observed congener pattern similarity could come from ingestion of similar food sources.
The study also reported the relationship between CP burden in liver and physiological parameters. This is briefly discussed in Section 5.1.5 CP concentrations in the frog muscle samples on a wet weight basis were much lower than those reported for reptiles and mammals in Du *et al*. (2018). See Appendix H.

The Environment Agency considers that the data presented in this report should be considered reliable with restrictions (Klimisch 2). The same observations are applicable as for the Yuan *et al*. (2019) study.

- Du *et al*. (2020) is a continuation of the work reported by Du *et al*. (2018) and Du *et al*. (2019). CPs were analysed in pooled muscle, liver and adipose tissues sampled from the semi-aquatic Red-backed Rat Snake (6 females and 3 males, n=9)) collected from paddy fields in October 2011 (data for a terrestrial snake species are summarised in Section 4.3.2.4). Methodology and sampling location

were identical to those summarised in Du *et al*. (2018). A single, Black-spotted Frog (the major prey of the Red-backed Rat Snake) was collected during the same time period. Data from this individual was compared and then combined with that of 69 other frogs as reported in Du *et al*. (2019). The species, tissue samples, sampling location, lipid contents and concentrations are presented in Appendix H.

Concentrations of total LCCPs, MCCPs and SCCPs in liver, muscle and adipose tissues are presented in Appendix H. Concentrations of very short chain chlorinated paraffins (vSCCPs), defined as CPs with chain lengths between 6 and 9 carbons were also measured. Concentrations of LCCPs were highest in the muscle tissues of the snake species (810 to 5 900 ng/g lipid), followed by liver (57 to 1 800 ng/g lipid) and adipose (12 to 380 ng/g lipid). CP levels decreased in the order SCCPs > MCCPs > LCCPs > vSCCPs in liver samples for the snake (contributing 79, 13, 4.4, and 3.8% of the total CP level, respectively). SCCPs (37 to 46%) and MCCPs (43 to 49%) were the two predominant CP groups in the snake muscle samples. For adipose samples, MCCPs and LCCPs were the two most abundant CP groups contributing to 45−58% and 28−34% of total CPs, respectively. An emerging pattern was observed going from liver to muscle to adipose tissues, with shorter chain, lower chlorinated congeners predominant in liver tissues, longer chain lengths and a higher chlorination degree observed in muscle, and increased chlorination levels in adipose. The LCCP congener patterns for all snake tissues were dominated by C_{18} (contributing to 32% of total LCCPs in muscle and adipose tissues) followed by C_{19} (18%). Snake liver samples were distinctly different, with the LCCP group pattern dominated by C_{20} (21%) and C_{21} congeners (20%). These levels were similar to those found in another snake species sampled at the same time (the semi-aquatic Red-tailed Rat Snake; see Section 4.3.2.4) although homologue and chlorine patterns for the liver and muscle of each species were different (chlorination degrees were generally lower in the Red-backed Rat Snake).

Stable isotope analyses were performed to elucidate the trophic level of Red-backed Rat Snake and their potential prey species (Black-spotted Frog, Pond Loach and Rice Field Eel) in the local environment (Table 25). The authors reported a difference of 1.07‰ in the measured $\delta^{13}C$ values for Red-backed Rat Snake and the Black-spotted Frog, which indicated that these two species were feeding in the same food web. A difference of 3‰ is desired between $\delta^{15}N$ values to confirm a predator-prey relationship. For the Red-backed Rat Snake and the Black-spotted Frog a difference of 1.97‰ was measured. The Pond Loach and Rice Field Eel were not in the same food web as the Red-backed Rat Snake, since this had significantly lower ($p < 0.05$) $\delta^{13}C$ value differences indicative of a different carbon food source.

Table 25 Stable isotope ratios measured in the Red-backed Rat Snake and associated candidate prey species (adapted from the Supporting Information of Du *et al.*, 2020)

Species	$\delta^{15}N$ (‰)[a]	$\delta^{13}C$ (‰)[a]
Red-backed Rat Snake	9.33±0.62	-23.76±0.89
Black-spotted Frog	7.36±1.21	-24.83±0.41
Pond Loach	10.22±1.34	-27.66±0.60
Rice Field Eel	10.82±0.66	-26.49±0.99

[a] mean±standard deviation

Biomagnification factors were calculated from the Black-spotted Frog to the Red-backed Rat Snake using the following equation:

$$\mathrm{BMF} = \frac{C_{\mathrm{predator}}}{C_{\mathrm{prey}}}$$

Where C_{predator} and C_{prey} were the lipid normalised CP concentrations in muscle tissues for predator and prey, respectively.
Mean (and maximum) BMFs were calculated as 1.7 (4.5), 1.8 (2.8), 1.9 (3.7) and 2.2 (3.4), for LCCPs, MCCPs, SCCPs and vSCCPs, respectively. The maximum BMF corresponds to the following individual congeners: $C_{18}Cl_{10}$ (59% Cl wt.) for LCCPs), $C_{15}Cl_{11}$ for MCCPs, $C_{13}Cl_9$ for SCCPs, and C_9Cl_9 for vSCCPs. For individual LCCP congener groups the percentage of BMF values greater than 1 was 78%. For MCCPs, SCCPs and vSCCPs the corresponding percentage was 97%, 88% and 53%, respectively.

In response to questions from the Environment Agency, the lead researcher of the paper provided additional information, as follows (Personal communication, X Du, Shanghai Ocean University, 2021):

- Some LCCP congener groups were observed to have a relatively low instrumental response, which in combination with small sample size may lead to uncertainty for some specific congener groups.
- Snakes have two different types of muscle tissue and several thousand individual muscles. All muscle tissue from a snake was treated as one sample for extraction and analysis. Therefore, any variation in CP concentration between the different muscle types could not be distinguished. Muscle fibre density as well as lipid, water and protein content of the different muscle types may affect the distribution of chemicals.
- Previous work with persistent organic pollutants and organohalogens in wild turtles and frogs indicated that summed total substance concentrations detected in muscle, liver and adipose tissues could be used as a proxy for the total body burden (although precise concentrations varied between sexes, sample location and substance). However, the total body burden of CPs in wildlife is unknown.

- According to the observations of the research group, the tissue distribution pattern of CPs is different to other organohalogens, with the highest CP concentration in muscle rather than adipose tissues. Therefore, BMFs were calculated using the muscle concentrations (lipid normalised) rather than a total body burden.
- As part of the work, food items in the stomachs of the snakes were identified and analysed. Isotopic data from the frog samples yielded the closest values to that of the corresponding snakes and frog data were therefore used in the BMF calculations. However, seasonal variation in available food for the snakes should be expected.

The Environment Agency considers that the data presented in this study should be considered reliable with restrictions (Klimisch 2). The same observations are applicable as for the Yuan *et al*. (2019) study.

- Zhou *et al*. (2019) analysed pooled muscle and soft tissue samples of 9 species (7 fish, 1 bivalve and 1 gastropod) from the freshwater ecosystem of Lake Dianshan, China. Concentrations of LCCPs ranged from below the LOQ to 55 ng/g lipid in fish muscle and between 88 and 380 ng/g lipid in mollusc soft tissue (further details are presented in Appendix H). LCCPs contributed between 0.4% and 15% of the total CP burden on average (MCCPs contributed 45% on average). Due to limited sample numbers (only 1 or 2 individuals were sampled for 6 of the fish species), and in the absence of stable isotope data to confirm the congener level relationship proposed by the authors, the Environment Agency considers these data indicate qualitative detection only.

4.3.2 Terrestrial bioaccumulation

Evaluation of available data were performed in conjunction with the relevant guidance text from ECHA R.11 and R.7.c (ECHA 2017 a and d).

4.3.2.1 Measured data

The EU REACH registrations (ECHA, 2021a) do not contain experimental data relating to bioaccumulation in terrestrial species.

There are no standard studies for terrestrial bioaccumulation in the context of a PBT evaluation. Mammalian toxicokinetic data can be useful as part of a weight of evidence assessment, and the limited available data are discussed in Section 6.1. Absorption via the oral route may be significant (about half of the administered dose). Excretion (between 60 and 95% of the dose, depending on the degree of chlorination) is mainly through the hepatobiliary pathway in faeces. The majority of excretion occurs in the first few days following exposure, but some of the dose remains within the body for more than 7 days, where it accumulates in liver and is then gradually distributed to fatty tissues and organs. Excretion via breast milk could therefore occur, and this is confirmed by biomonitoring (see Section 6.8). It is possible that there will be some metabolism of LCCPs, although this may

become slower as carbon chain length and degree of chlorination increase, resulting in a lower elimination rate. Half-lives for a C_{18-30} CP, 42 to 52% Cl wt. product were estimated to be 4.5 days in rats and 0.6 years in humans, respectively.

4.3.2.2 Predicted data

The potential for accumulation in air-breathing organisms can be screened using simple physico-chemical parameters according to REACH Guidance Document R.11 (ECHA, 2017a). The log K_{OA} of LCCPs is above 9 (see Section 4.2.3) and the log K_{OW} is above 7.5 (see Section 3.3). These exceed the screening thresholds of log K_{OA} >5 and log K_{OW} > 4.5, suggesting some constituents of LCCPs may have a high bioaccumulation potential in air-breathing organisms (see Appendix D). However, as LCCPs contains constituents with much higher predicted log K_{OA} and log K_{OW} values, it is unlikely that the screening criteria are appropriate for the whole substance.

4.3.2.3 Data from structural analogues

ECHA (2019) and UK Gov (2021) provide up-to-date summaries of the information available for MCCPs.

An earthworm-soil accumulation factor of 2.4 for adults and 2.3 for juveniles was determined for a C_{15} chlorinated n-alkane, 51% Cl wt. in a 56-day study using *Eisenia fetida* (Thompson *et al*., 2001d). This is assessed to be reliable with restrictions.

Yuan and de Wit (2018b) and Yuan *et al*. (2019b) analysed for CPs with a chain length up to C_{30} in the Swedish environment using APCI-QToF-MS. For the terrestrial species sampled between 2012 and 2017, Bank Voles (*Myodes glareolus*) were found to contain the lowest amounts of C_{14-17} congeners. The detected concentrations of C_{14-17} congeners in muscle were comparable in Eurasian Lynx (*Lynx lynx*) and Grey Wolf (*Canis lupus*) (0.75 to 0.83 mg/kg lipid), whilst Moose (*Alces alces*) muscle contained the highest concentrations (1.6 mg/kg lipid). C_{14-17} congeners were also detected in muscle or eggs of terrestrial birds of prey (Tawny Owl (*Strix aluco*), Eagle Owl (*Bubo bubo*), Marsh Harrier (*Circus aeruginosus*), Golden Eagle (*Aquila chrysaetos*) and Peregrine Falcon (*Falco peregrinus*)) up to 0.72 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 other dietary concentrations. It is therefore not possible to draw firm conclusions about trophic magnification from the data collected in this study.

4.3.2.4 Monitoring data for terrestrial biota

The studies described in this section are also tabulated in Appendix H.

- Yuan *et al*. (2019), (originally published as Yuan and de Wit, 2018b) investigated the presence of CPs in samples of 11 terrestrial bird and mammal species, collected between 2012 and 2017 in Denmark and Sweden. Muscle samples were produced from a pool of 3 to 10 adult

individuals with the exception of Starlings, where samples originated from fledglings.

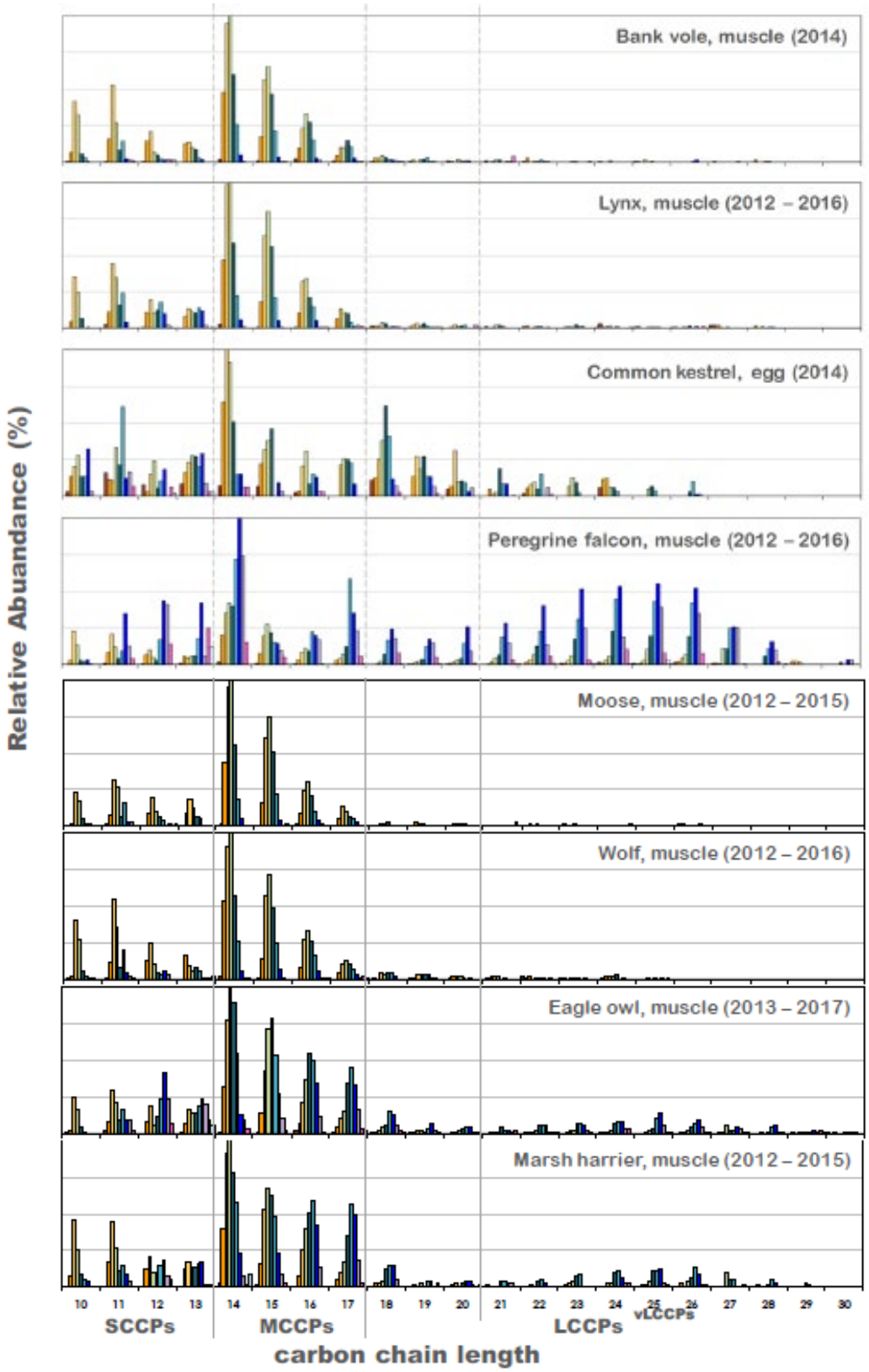
- Samples were extracted and analysed for CPs and lipids (methods are described in Section 4.3.1.4). In the terrestrial samples LOQs for LCCPs, MCCPs and SCCPs ranged from 0.4 to 12 ng/g lipid, 3.0 to 78 ng/g lipid and 2.7 to 70 ng/g lipid, respectively. The lowest LOQ was always observed for Tawny Owl muscle samples and the highest for Moose muscle samples.
- LCCPs, MCCPs and SCCPs were detected at concentrations above the LOQ in all wildlife samples. Representative relative abundance of CP congeners in the wildlife samples are presented in Figure 7. The species, tissue samples, sampling location, lipid contents and concentrations are presented in Appendix H.
- LCCP, MCCP and SCCP concentrations across all samples ranged from 25 to 1 200 ng/g lipid (mean 220 ng/g lipid), 85 to 1 600 ng/g lipid (mean 518 ng/g lipid) and 85 to 1 500 ng/g lipid (mean 578 ng/g lipid), respectively.
- The mammal muscle samples contained concentrations of LCCPs, MCCPs and SCCPs ranging from 36 to 180 ng/g lipid, 370 to 1 600 ng/g lipid and 400 to 1 500 ng/g lipid, respectively, with LCCPs contributing 5% of total CPs. LCCP concentrations in wolf (n=10) and lynx (n=10) were similar, and higher than in voles (n=10), at 100, 92 and 36 ng/g lipid, respectively. The same concentration pattern was also observed for MCCPs and SCCPs. The highest concentration of LCCPs (180 ng/g lipid) was observed in moose muscle (n=10), and the longest chain lengths in all samples exceeded C_{24} (C_{28} was the longest, in lynx). The degree of chlorination for all congeners was around 51% Cl wt. For comparison, the highest concentrations of other CPs were found in muscle tissues of moose (SCCPs 1 500 ng/g lipid; MCCPs 1 600 ng/g lipid), wolf (SCCPs 1 100 ng/g lipid; MCCPs 830 ng/g lipid) and lynx (SCCPs 800 ng/g lipid; MCCPs 750 ng/g lipid).
- The raptor muscle samples contained concentrations of LCCPs, MCCPs and SCCPs ranging from 100 to 1 200 ng/g lipid, 180 to 720 ng/g lipid and 220 to 730 ng/g lipid, with LCCPs contributing around 23 to 55% of total CPs. In contrast, Starling muscle samples were 25, 320 and 350 ng/g lipid for LCCPs, MCCPs and SCCPs, respectively, possibly due to limited dietary exposure compared to adult birds. The highest LCCP concentration (1 200 ng/g lipid) was measured in pooled Peregrine Falcon (n=10) muscle tissues (contributing 55% of the total CP burden; corresponding concentrations of SCCPs and MCCPs were 540 ng/g lipid and 410 ng/g lipid, respectively). Concentrations of LCCPs detected in other birds of prey were 51 ng/g lipid (Common Kestrel, egg, n=3), 49 ng/g lipid (Tawny Owl, egg, n=4), 380 ng/g lipid (Eagle Owl, muscle, n=10), 100 ng/g lipid (Marsh Harrier, muscle, n=10), and 210 ng/g lipid (Golden Eagle, muscle, n=10). For comparison, the highest concentrations of other CPs were found in Eagle Owl muscle tissues (SCCPs 730 ng/g lipid; MCCPs 720 ng/g lipid). The longest chain lengths observed in birds were above C_{25}, and up to C_{30} in Golden Eagle and

Peregrine Falcon muscle. C_{18} CPs were generally more abundant than C_{19} and C_{20} congeners in most species, with the exception of Peregrine Falcon. The authors noted that unexpected concentrations of $C_{>20}$ CPs were detected in all samples and were predominantly $C_{24/25}$ congeners in 11 out of 38 samples.

The Environment Agency's observations made in the study description in Section 4.3.1.4 are applicable to the terrestrial samples. In addition:

- The longest CP chain lengths were up to $C_{25\text{-}30}$ in terrestrial birds. These results suggest that terrestrial species are more likely to accumulate longer, larger molecular weight CPs than aquatic species, although the amounts are small.
- Higher concentrations of LCCPs in terrestrial raptors compared to mammals may be due to differences in diet, metabolism, sex, and/or the influence of different exposures during migration, of the individuals and/or their prey. For example, Peregrine Falcons mainly consume other birds, whereas predatory mammals such as wolf and lynx mainly feed on other mammals. The authors noted that further work is needed to examine concentrations of LCCPs through structured food webs.

Figure 7 **CP congener fingerprints in terrestrial wildlife samples from Scandinavia (adapted from Yuan *et al*., 2019; American Chemical Society Publishing)**



Note: The vertical axis shows relative abundance of each congener group; the most abundant are expressed as 100%.

- Du *et al*. (2018) analysed for CPs in 5 terrestrial species (1 snake (Short-tailed Mamushi), 1 mammal (Yellow-tailed Weasel) and 3 birds (Peregrine Falcon, Collared Scops Owl and Common Cuckoo) from paddy fields in the YRD, China. The details of the sampling site, analysis and total CP concentrations are described in Section 4.3.1.4. The species, tissue samples, sampling location, lipid contents and concentrations are presented in Appendix H.
  The LOQs for LCCPs, MCCPs and SCCPs were species specific, and ranged from <27 to <40 ng/g dw, <13 to <28 ng/g dw and <0.7 to 1.5 ng/g dw, respectively. C_{18-26} CP congeners were detected in the muscle samples of all species; the breakdown of detection frequencies were C_{18-21} 100%, C_{22} 92%, C_{23} 83%, C_{24} 83%, C_{25} 30% and C_{26} 13%. C_{27} CP congeners were detected in Short-tailed Mamushi at a frequency of 4.3%. C_{28-31} CP congeners were not detected in any samples. The highest concentration of LCCP congeners was detected in muscle samples of Peregrine Falcon (10 000 ng/g lipid), followed by Short-tailed Mamushi (5 200 ng/g lipid) (similar to that found in a semi-aquatic snake species – see Section 4.3.1.4). The LCCP congener group patterns were dominated by C_{18} CPs (48.4%), followed by C_{19} and C_{20} CPs (18.7% and 13.6%, respectively). An exception occurred for Common Cuckoo samples, in which percentage contributions of 20.3%, 20.1% and 22.9% were noted for C_{18}, C_{19} and C_{20} congeners, respectively.
  For comparison, the highest concentrations of MCCPs were detected in the muscle samples of Yellow-tailed Weasel, Peregrine Falcon and Short-tailed Mamushi, with values of 33 000 ng/g lipid, 29 000 ng/g lipid and 19 000 ng/g lipid, respectively. MCCPs were the dominant CPs detected in the samples and contributed 44.2 ± 6.9% of the total extracted CP burden. SCCP concentrations correlated significantly to those of MCCPs.
  Principal component analysis of $\delta^{13}C$, chain length and chlorination level allowed 3 clusters of correlating biota to be identified. One cluster included Collared Scops Owl and Common Cuckoo (n=12, mean±sd: $\delta^{13}C$ -26.5±0.5 and 52.5±0.5 Cl wt.), for which CPs were detected in relatively low concentrations in muscle, with predominantly lower chain lengths. These two bird species prefer forested habitats and mainly feed on insects, and are most likely to be exposed to CPs via the atmosphere. A second cluster included the Yellow Weasel and the Short-tailed Mamushi (n=11, mean±sd: $\delta^{13}C$ -23.0±0.7 and 57.2±1.5 Cl wt.). This cluster contained the highest total MCCP concentrations and congeners with the greatest degrees of chlorination, as well as longer CP chain lengths (C_{16+}). These species live exclusively in dry terrestrial environments and have common dietary items such as rodents. A third cluster involved aquatic/semi-aquatic organisms (reported in Section 4.3.1.4).
  The authors proposed two hypotheses that may explain the observed pattern of accumulation in the different species:
  - Terrestrial species have a greater capacity for metabolising lower halogenated congeners; or
  - High K_{OA} values associated with highly chlorinated CPs and those of longer chain lengths result in association with airborne particles or plant surfaces,

and reduces their propensity for respiratory elimination, resulting in greater accumulation in terrestrial species (see Section 4.3.2.2).

The Environment Agency considers these data should be considered reliable with restrictions (Klimisch 2). The same observations are generally applicable as for the Yuan *et al*. (2019) study.

- Du *et al*. (2020) analysed for CPs in pooled muscle, liver and adipose tissues in the terrestrial Short-tailed Mamushi (5 females and 2 males, n=7) (as well as other CP chain lengths) collected from paddy fields in the YRD, China in October 2011. Methodology and sampling location were identical to those summarised in Du *et al*. (2018). The study is summarised in Section 4.3.1.4 as it focussed mainly on aquatic species. Concentrations of LCCPs were highest in the muscle tissues (980 to 5 100 ng/g lipid), followed by liver (95 to 2 300 ng/g lipid) and adipose (44 to 270 ng/g lipid). CP levels decreased in the order SCCPs > MCCPs > LCCPs > vSCCPs in liver samples (65, 23, 9.2, and 2.6% of the total CP level, respectively). SCCPs (37 to 46%) and MCCPs (43 to 49%) were the two predominant CP groups in the snake muscle samples, with higher lipid weight concentrations of both CP groups in muscle. For adipose samples, MCCPs and LCCPs were the two most abundant CP groups contributing to 45 to 58% and 28 to 34% of total CPs, respectively. An emerging pattern was observed going from liver to muscle to adipose tissues, with shorter chain, lower chlorinated congeners predominant in liver tissues, longer chain lengths and a higher chlorination degree observed in muscle, and increased chlorination levels in adipose. These levels were similar to those found in another snake species sampled at the same time (the semi-aquatic Red-tailed Rat Snake; see Section 4.3.1.4) although homologue and chlorine patterns for the liver and muscle of each species were different (chlorination degrees were generally higher in Short-tailed Mamushi). The LCCP congener patterns for all tissues were dominated by C_{18} (contributing to 32% of total LCCPs in muscle and adipose tissues) followed by C_{19} (18%). Liver samples were distinctly different, with the LCCP group pattern dominated by C_{20} (21%) and C_{21} congeners (20%).

The Environment Agency considers that the data presented in this study should be considered reliable with restrictions (Klimisch 2). The same observations are applicable as for the Yuan *et al*. (2019) study.

Human biomonitoring studies are summarised in Section 6.8. LCCPs have been detected in samples of human blood and breast milk from China and Scandinavia (but not blood from Australia at a detection limit of 0.16 ng/mL). Levels are generally higher in China than in other countries, likely due to high production volumes and greater exposure. Concentrations generally follow the order SCCPs > MCCPs > LCCPs. Concentrations were higher in first time mothers compared to second, suggesting that expression of milk is a significant depuration mechanism. This may also lead to maternal transfer resulting in exposure during sensitive developmental windows. LCCP concentrations in both blood and human milk can be in the region of 10 to 500 ng/g lipid weight.

4.3.3 Summary and discussion of bioaccumulation

LCCPs is a highly complex substance with a very large number of constituents. Single values for properties such as log K_{OW} or BCF are not appropriate. Instead, there will be a wide range of values depending on the solubility and partitioning behaviour of individual congeners. Water solubility declines with increasing chain length and the log K_{OW} is high (around 7.5 for the shortest congeners but increasing to 10 or more as the number of carbon and chlorine atoms increase) (Section 3.3.4). Many congeners also have large molecular dimensions (Section 4.3.1.2).

The performance of modelling software to estimate an aquatic BCF for substances with log K_{OW} > 5 is frequently poor. The data presented for LCCPs in Section 4.3.1.2 should be treated with caution as they may not be reliable. One model predicts a high BCF (around 9 000 L/kg) for congeners with a log K_{OW} of around 7.5, but other models predict BCFs below 500 L/kg. Regulators in other jurisdictions (EC & HC, 2008) have suggested that liquid $C_{18\text{-}20}$ LCCPs have significant bioaccumulation potential based on predictions. In this instance, the EPIWIN model (v.3.11) was used to generate predictions for physicochemical properties including log K_{OW}. The Modified Gobas Bioaccumulation model was used to predict BAF from the log K_{OW} predictions generated by EPIWIN (Kowwin v.1.41) and assuming a Tier 2 mid trophic level prediction with no metabolism. The modified Gobas model predicts a log BAF of <0.01 to 4.96 for substances with a log k_{OW} in the range of 10.08-17.2. A log BAF of approximately 3.69, or greater, meets the bioaccumulation criteria of BAF ≥5 000 (Government of Canada, 2000).

While none of the $C_{>20}$ congeners were predicted to have a BAF ≥ 5 000; 12 out of 27 (44%) of the $C_{18\text{-}20}$ congeners were predicted to have a BAF ≥ 5 000. The model is considered applicable for LCCPs as they are simple hydrophobic and persistent chemicals. The very high molecular weight LCCPs are expected to not be bioaccumulative in the sense of the BAF exceeding the 5 000 threshold. For these chemicals aqueous uptake is insignificant, and the dietary intake rate is very low due to slow membrane transfer rates in the intestines (Personal communication, D Lee, Environment and Climate Change Canada, December 2021).

The available aquatic BCF data on LCCPs are not reliable as they were obtained using non-standard studies with exposure concentrations in excess of water solubility. Lipid normalisation was not considered, and analytical methods were generally not sophisticated enough to provide congener-specific information. It is also unclear if the duration of the studies was sufficient for steady state to be reached. Therefore, although these studies show that uptake does occur, it is not possible to obtain a reliable BCF value from them. Evidence for MCCPs indicate that CP congeners with 14 or 15 carbon atoms and around 45 to 50% Cl wt. have high fish and invertebrate BCFs (above 5 000 and 2 000 L/kg, respectively). The evidence suggests that metabolism is not sufficiently quick to prevent high levels of bioaccumulation for congeners at this level of chlorination. The trend for higher carbon numbers or differing chlorine contents is highly uncertain due to a lack of reliable data.

A recent study of bioaccumulation in the water flea (*D. magna*) was carried out below the water solubility limit (Castro *et al*., 2019). Uptake of LCCP congeners by passive diffusion was shown to occur over 48 hours. The results suggest very high BCF/BAFs, but there are major uncertainties in the numerical values which make them unreliable for regulatory decision making for LCCP congeners.

For substances with very low aqueous solubility and very high log K_{OW} like LCCPs, dietary exposure is a more relevant route for assessing aquatic bioaccumulation potential. Four non-standard studies using fish are available (one of these also investigated molluscs), but none were performed to modern standards. Two studies are unreliable, and the reliability of 2 others (Madeley and Birtley, 1980; Fisk *et al*., 2000) are unknown. The results show that LCCPs can be taken up via the diet, but in all cases the concentrations reached in the fish and mussels were less than those in the diet. This suggests that although uptake of the substance can occur via food, the levels should not increase through the food chain. Dietary BMF data for MCCPs suggest that the potential for uptake (as measured by assimilation efficiency) decreases with increasing carbon chain length and chlorine content. However, the Environment Agency has estimated depuration rate constants and half-lives from 2 studies that are of unknown reliability, and these are consistent with information from other substances that are known to have a fish BCF above 5 000 L/kg. LCCPs with chain lengths between C_{18} and C_{25} and chlorination levels of 42 to 49% may therefore have the capacity to bioaccumulate to a significant level in aquatic organisms, although a definitive conclusion is not possible given the limitations of the data available.

Chemical analysis is challenging and reported concentrations should be treated as qualitative or semi-quantitative depending on the methods used. This adds a layer of uncertainty to the findings of field monitoring studies. Nevertheless, LCCP congeners have been detected in a wide range of aquatic and terrestrial wildlife in Europe and China, including sensitive life stages (e.g. frog eggs) and several species at the top of the food chain, as well as humans (see Appendix G, Appendix H and Appendix I). This evidence demonstrates that they are bio-available and capable of crossing biological membranes. In general, levels of MCCP congeners (usually dominated by C_{14}) are higher than LCCPs in the same samples. This pattern could reflect lower use of/exposure to LCCPs, or a lower bioaccumulation potential in some species, or both. However, there are exceptions to this general pattern. For example, LCCP congeners up to C_{30} accounted for 55% of the total CP burden in Peregrine Falcon muscle (Yuan *et al*., 2019). In most species, LCCP congener group patterns are dominated by C_{18} CPs, followed by $C_{19\text{-}21}$ CPs. The concentrations of C_{18} (and sometimes even longer chain length) congeners can be similar to (and in some cases higher than) those of $C_{15\text{-}16}$ congeners, and in the case of Viviparous Eelpout muscle, around the same level as C_{14} congeners (Yuan *et al*., 2019). The evidence therefore indicates that some LCCP congener groups (in particular C_{18} and C_{19}) can accumulate to a similar level as MCCP congeners in some tissues.

The distribution of LCCPs in different tissues, and especially occurrence in muscle, suggests that accumulation may not always be driven by simple lipid partitioning. Non-lipid

dominated tissue distribution of substances with log K_{OW} > 5 is not uncommon and is discussed in Endo *et al*. (2013).

Two studies have compared lipid-normalised tissue concentrations in different wildlife species to estimate biomagnification potential (De Wit *et al*., 2020; Du *et al*., 2020). Predator-prey concentration ratios up to 3.3 for marine mammal/fish and bird/bird species pairs, and a maximum BMF of 4.5 for a simplistic frog-snake food chain, were reported. These estimates suggest that LCCPs undergoes trophic magnification. However, there are several reasons why these types of comparisons may be unreliable, including lack of information on LCCP levels in other dietary components, uncertainties around the relevance of lipid normalisation, use of single tissue concentrations to represent total body burdens, small sample numbers, mixing of samples from different areas and different times, and the statistical issues that arise when comparing complex analytical data. The Environment Agency therefore considers that whilst these studies flag a concern, they are not sufficient to show that biomagnification in specific food chains is occurring.

As hydrophobicity increases in a chemical series, the potential of a substance to accumulate in aquatic organisms eventually decreases as bioavailability reduces. However, terrestrial bioaccumulation may become increasingly important, and might become more significant than aquatic bioaccumulation for highly hydrophobic substances. The log K_{OA} of LCCPs is above 9 (see Section 4.2.3) and the log K_{OW} is above 7.5 (see Section 3.3). These exceed the screening thresholds of log K_{OA} > 5 and log K_{OW} > 4.5, suggesting some constituents of LCCPs may have a high bioaccumulation potential in air-breathing organism. However, as LCCPs contains constituents with much higher predicted log K_{OA} and log K_{OW} values, it is unlikely that the screening criteria are appropriate for the whole substance.

Nevertheless, the importance of terrestrial bioaccumulation appears to be borne out by the available monitoring evidence, which suggests that terrestrial species are more likely to accumulate longer, larger molecular weight CPs than aquatic species (although the amounts are often small). The highest concentrations reported to date are for muscle tissue from 2 terrestrial predators: Peregrine Falcon (10 000 ng/g lipid) and Short-tailed Mamushi (5 200 ng/g lipid) (although this was similar to that found in a semi-aquatic snake species) (Du *et al*., 2018). Differences between associated $\delta^{13}C$ measurements of the clusters and similarity in patterns of CP homologues and congeners within the clusters may be indicative that LCCPs can accumulate up the food chain.

Mammalian toxicokinetic data indicate that absorption via the oral route may be significant (about 50% of the administered dose). Excretion (between 60 and 95% of the dose, depending on the degree of chlorination) is mainly through the hepatobiliary pathway in faeces. The majority of excretion occurs in the first few days following exposure, but some of the dose remains within the body for more than 7 days, where it accumulates in liver and is then gradually distributed to fatty tissues and organs. Excretion via breast milk could therefore occur, and this is confirmed by biomonitoring (LCCP concentrations in human milk can be in the region of 10 to 500 ng/g lipid weight). It is possible that there will

be some metabolism of LCCPs, although this may become slower as carbon chain length and degree of chlorination increase, resulting in a lower elimination rate. Half-lives for a C_{18-30} CP, 42 to 52% Cl wt. product were estimated to be 4.5 days in rats and 0.6 years in humans, respectively.

In summary, a high level of bioaccumulation cannot be ruled out for LCCPs. The relevance of aquatic bioaccumulation appears to decline with increasing CP molecular weight, with accumulation in terrestrial predators becoming more important. LCCPs with chain lengths between C_{18} and C_{25} and chlorination levels in the range 40 to 50% appear to have the greatest capacity to bioaccumulate, although a definitive conclusion is not possible given the limitations of the data available.

5 Ecotoxicology

5.1 Aquatic compartment (including sediment)

Available aquatic ecotoxicity data for LCCPs have previously been reviewed in Environment Agency (2009a). Ecotoxicity data published since that review have been identified and evaluated as part of this assessment. Evaluation of available data were performed in conjunction with the relevant guidance text from ECHA R.11 and R.7.c (ECHA 2017 a and d).

5.1.1 Fish

The fish toxicity studies for LCCPs reviewed in Environment Agency (2009a) are summarised in Table 26. Two additional studies in the EU REACH registrations that were not reviewed in Environment Agency (2009a) are summarised in Table 27. Given their age, they have not been evaluated by the Environment Agency.

A single study on fish toxicity was identified during the literature search. Yang *et al*. (2019) investigated the toxicity of several CP products including CP-42 and CP-52a, supplied by a manufacturer in Jiangxi, China. Carbon skeleton chromatography was used to confirm the carbon chain length distribution of the products and deuterodechlorination combined with high resolution GC-MS was used to determine the degree of chlorination. The results for carbon chain length distribution are presented as a graph, but they show that CP-42 was found to be $C_{20\text{-}26}$ and that CP-52a was also mainly $C_{20\text{-}26}$ but also had around 1 to 5% of each of $C_{10\text{-}19}$. Degrees of chlorination were found to be consistent with their nominal values, i.e. CP-42 was 42% Cl wt. and CP-52a was 52% Cl wt. Stock solutions were prepared with DMSO before being serially diluted with test media.

Embryos of wild type Zebrafish (Tuebingen strain) were collected from the laboratory colony within 1 hour post fertilisation (hpf). Healthy embryos were selected and washed with Milli-Q water, before being placed into glass petri dishes in groups of 50. Exposure to nominal test concentrations of 10, 100 and 1 000 µg/L and a solvent control (0.1% v/v DMSO) began at 3 to 4 hpf. There was no analytical confirmation of the exposure concentrations. A semi-static exposure was used, with half of the test media replaced every day until the exposure ended at 5 days post fertilisation (dpf). At this point three different measures of larval behaviour were employed: a locomotion test, a path angle test and a two-fish interaction test.

Individual larvae were transferred into 96-well places. After an initial period of 10 minutes in the dark, the distance the larva travelled (the locomotion test) and the changes in direction relative to the current swimming direction (the path angle test) were quantified during three cycles of 10 minutes light followed by 10 minutes dark. In a separate test, two larvae were placed in each well of a 6-well plate. After an initial period of 10 minutes in the

dark, the average time the larvae were within 0.5 cm of each other (two-fish interaction test) was quantified during two cycles of 10 minutes light followed by 10 minutes dark.

No statistically significant effects were observed compared to the control in the locomotion test, path angle test or two-fish interaction test with CP-42.

A statistically significant reduction in total swimming distance was observed at 100 µg/L CP-52a, but there was no difference to the controls in either the 10 or 1 000 µg/L exposure. When results were analysed for each separate light and dark period, some significant reductions in swimming distance were found, but these only followed a dose response for the first light and first dark exposure period at 100 µg/L and above. For CP-52a there was a statistically significant increase at 10 and 100 µg/L and a significant decrease at 1 000 µg/L in the number of path angle changes in the range -90 to +90°. The authors speculate that this effect may be due to a disrupted sense of direction. A statistically significant reduction in the duration that the fish were in contact was also observed at 1 000 µg/L for CP-52a.

The lack of chemical analysis to confirm exposure concentrations is a drawback in the interpretation of this study, as although test volumes were small and replaced every day, LCCPs is highly hydrophobic and may therefore stick to vessel walls. This paper does not provide information on the acute toxicity of these two LCCP products as only healthy larvae without morphological deformities were selected for the behavioural experiments. No information was provided on the proportion of exposed larvae that had died or were malformed. For CP-42, the 5-d NOEC was ≥ 1 000 µg/L (nominal). Some statistically significant effects were observed for CP-52a, although the observed effects did not always follow a dose response or were only seen during certain cycles of the experiment. CP-52a has a higher degree of chlorination than CP-42, and its carbon number range is C_{10-26}, so it is uncertain which components were responsible for the observed sub-lethal effects. The Environment Agency considers this study to be Klimisch 2 (reliable with restrictions).

When considering all the available fish ecotoxicity data, LCCPs shows little or no toxicity at concentrations well in excess of water solubility in acute tests.

No effects were reported in 60-day studies with fish using both a C_{22-26}, 43% Cl wt. product and a $C_{>20}$, 70% Cl wt. product. However, the test method used is not equivalent to the fish early life stage test that is currently recommended to assess long-term toxicity. In particular, it did not include any of the potentially sensitive early life stages. There are no chronic studies for liquid C_{18-20} LCCPs either. However, aquatic invertebrates are the most sensitive trophic group for MCCPs or SCCPs (see Section 5.1.6), so the lack of definitive long-term toxicity data for fish is not a significant concern.

Table 26 Toxicity to fish (Environment Agency, 2009)

Species	Substance tested	Comments	Results	Reference	Val.[a]
Bleak (A*lburnus alburnus*)	C_{22-26}, 42% Cl wt.	Static test; acetone as cosolvent; 10 °C, brackish water (7‰), nominal concentrations. No effects seen at solubility.	96-h LC_{50} >5 000 mg/L	Lindén *et al*., 1979.	2
Bleak (A*lburnus alburnus*)	C_{18-26}, 49% Cl wt.	Semi-static bioaccumulation test, 10 °C, brackish water (7‰), nominal concentrations. No effects seen at solubility.	14-day NOEC ≥0.125 mg/L	Bengtsson *et al*., 1979	2
Bleak (A*lburnus alburnus*)	C_{18-26}, 49% Cl wt.	Observations as part of an accumulation study. No mortalities seen during 91 days exposure in food. No effects seen.	91-day LC_0 >3,400 mg/kg food	Bengtsson and Baumann Ofstad, 1982	2
Bluegill sunfish (*Lepomis macrochirus)*	Chlorowax LV	Static test, 20 °C, nominal concentrations. Test substance tentatively identified as $C_{>17}$, 39% Cl wt. No effects seen at solubility.	96-h LC_{50} >300 mg/L	Johnson and Finley, 1980	3
Bluegill sunfish (*Lepomis macrochirus)*	$C_{>20}$, 40–42% Cl wt.	Static test, 20 °C, nominal concentrations. No effects seen at solubility.	96-h LC_{50} >300 mg/L	Johnson and Finley, 1980	2
Bluegill sunfish (*Lepomis macrochirus)*	$C_{>20}$, 48–54% Cl wt.	Static test, 20 °C, nominal concentrations. No effects seen at solubility.	96-h LC_{50} >300 mg/L	Johnson and Finley, 1980	2
Bluegill sunfish (*Lepomis macrochirus)*	$C_{>20}$, 70% Cl wt.	Static test, 20 °C, nominal concentrations. No effects seen at solubility.	96-h LC_{50} >300 mg/L	Johnson and Finley, 1980	2
Golden orfe (*Leuciscus idus*)	C_{18-20}, 35% Cl wt.	Static test, substance added directly to test vessel. Effects seen at concentrations above solubility.	48-h toxic threshold = 400 mg/L	Hoechst AG, 1976	3
Golden orfe (*Leuciscus idus*)	C_{18-20}, 44% Cl wt.	Static test, substance added directly to test vessel. Effects seen at concentrations above solubility.	48-h toxic threshold = 500 mg/L	Hoechst AG, 1976	3

Golden orfe (*Leuciscus idus*)	C_{18-20}, 49% Cl wt.	Static test, substance added directly to test vessel. No effects seen at solubility.	48-h toxic threshold >500 mg/L	Hoechst AG, 1976	2
Golden orfe (*Leuciscus idus*)	C_{18-20}, 52% Cl wt.	Static test. No effects seen at solubility.	48-h toxic threshold >500 mg/L	Hoechst AG, 1977	2
Rainbow trout (*Oncorhynchus mykiss*)	Chlorowax LV	Static test; 10 °C, nominal concentration. Test substance tentatively identified as $C_{>17}$, 39% Cl wt. No effects seen at solubility.	96-h LC_{50} >300 mg/L	Johnson and Finley, 1980	3
Rainbow trout (*Oncorhynchus mykiss*)	$C_{>20}$, 40–42% Cl wt.	Static test; 10 °C, nominal concentration. No effects seen at solubility.	96-h LC_{50} >300 mg/L	Johnson and Finley, 1980	2
Rainbow trout (*Oncorhynchus mykiss*)	C_{20-30}, 42% Cl wt.	Substance tested as an emulsion. Semi-static test; 15 °C, measured emulsion concentrations. No effects seen at solubility.	96-h LC_{50} >770 mg/L	Madeley and Birtley, 1980	2
Rainbow trout (*Oncorhynchus mykiss*)	$C_{>20}$, 48–54% Cl wt.	Static test; 10 °C, nominal concentrations. No effects seen at solubility.	96-h LC_{50} >300 mg/L	Johnson and Finley, 1980	2
Rainbow trout (*Oncorhynchus mykiss*)	$C_{>20}$, 70% Cl wt.	Static test; 10 °C, nominal concentrations. No effects seen at solubility.	96-h LC_{50} >300 mg/L	Johnson and Finley, 1980	2
Rainbow trout (*Oncorhynchus mykiss*)	C_{22-26}, 43% Cl wt.	Flow-through test; acetone as cosolvent; measured concentrations. No effects seen at solubility.	60-day NOEC ≥4 mg/L	Madeley and Maddock, 1983a	2
Rainbow trout (*Oncorhynchus mykiss*)	$C_{>20}$, 70% Cl wt.	Flow-through test; acetone as cosolvent; measured concentrations. No effects seen at solubility.	60-day NOEC ≥3.8 mg/L	Madeley and Maddock, 1983b	2
Atlantic salmon (*Salmo salar*)	$C_{>20}$, 42% Cl wt.	Feeding study. A high level of mortality was seen in the control population. The results are not considered valid.	LT_{50} = 47 days at 10 mg/kg food LT_{50} = 80 days at 100 mg/kg food	Zitko, 1974	3

Atlantic salmon (*Salmo salar*)	$C_{>20}$, 70% Cl wt.	Feeding study. A high level of mortality was seen in the control population. The results are not considered valid.	LT_{50} = 71 days at 10 mg/kg food LT_{50} = 39 days at 100 mg/kg food	Zitko, 1974	3

Note: a - Validity markings: 1 – Valid without restriction; 2 – Use with care; 3 – Not valid; 4 – Not assignable.

Table 27 Additional studies on toxicity to fish included in EU REACH registrations (ECHA, 2020a)

Species	Substance tested	Comments	Results	Reference	Val.[a]
Rainbow trout (*Oncorhynchus mykiss*)	$C_{>20}$, 38-47% Cl	Static test; nominal concentrations. No effects seen at solubility.	>300 mg/L	Mayer 1986	4
Bluegill sunfish (*Lepomis macrochirus*)	$C_{>20}$, 38-47% Cl	Static test; nominal concentrations. No effects seen at solubility.	>300 mg/L	Mayer 1986	4

Note: a - Validity markings: 1 – Valid without restriction; 2 – Use with care; 3 – Not valid; 4 – Not assignable.

5.1.2 Aquatic invertebrates

The available invertebrate toxicity studies for LCCPs reviewed in Environment Agency (2009a) are summarised in Table 29. There are no additional studies in the EU REACH registration. There are no reproduction studies performed to the standard OECD test guidance OECD TG 211 (OECD, 2012b)

A single additional publication was identified during the literature search. Koh and Thiemann (2001) determined the toxicity of several CP products including three LCCP products to *D. magna* according to DIN 38412, part 11, which is equivalent to OECD TG 202. The products were CP 30 (C_{17-24}, 35% Cl wt.), CP 40 (C_{17-20}, 44% Cl wt.) and Hordaflex LC 50 (C_{17-20}, 52% Cl wt.) and were all supplied by Hoechst AG. The tests were carried out for 48 hours. The CPs were dissolved in acetone to prepare stock solutions which were then diluted with distilled water to give the maximum nominal concentrations of 200 µg/L CP 30 and CP 40 and 100 µg/L Hordaflex LC 50. The other exposure concentrations were not stated, and no measurements were carried out to verify the actual exposure concentration. A solvent control containing acetone at 0.1 mL/L was also tested. No further details on the test conditions are provided. The 48-hour EC_{50} values were 152.8 µg/L for CP 30, 126.1 µg/L for CP 40 and 48.5 µg/L for Hordaflex LC 50.

Only minimal details of the conditions of this study were provided in Koh and Thiemann (2001). This static test used a solvent to test concentrations above the water solubility and the exposure concentrations were not confirmed by analysis. Acute effects were observed for all three test compounds, but no information was provided on the control results. The validity of the test therefore cannot be independently assessed. As such, the reliability is unknown (Klimisch 4).

When considering all the available invertebrate ecotoxicity data, LCCPs generally show little or no toxicity at concentrations well in excess of their water solubility in acute tests. Effects have been seen on Daphnia at high concentrations, but these are likely to be physical effects rather than direct toxicity of the substance itself.

In long-term tests, effects have been seen in *Daphnia* reproduction studies. A 21-day NOEC of 29 to 32 µg/L was determined for a $C_{18–20}$, 52% Cl wt. product using water-soluble fractions from a loading rate of 10 g/L. As such, it is difficult to interpret as the toxicity seen could be due to impurities or additives present in the substance tested rather than the CP itself. It should be noted that this value is slightly above the expected water solubility for LCCPs of around 5 µg/L, but no experimental water solubility data for the liquid $C_{18–20}$ CPs are available. Another 21-day *Daphnia* reproduction study using a loading rate of 100 mg/L gave an apparent NOEC/LOEC of <1.2 µg/L, although Environment Agency (2009a) considers this result unreliable. A third 21-day *Daphnia* reproduction study with a $C_{18–20}$, 52% Cl wt. product, this time using a single concentration prepared by a column method, resulted in reduced reproduction compared with the control population at a concentration around 2 µg/L but the statistical significance of this result is debatable and the NOEC from this study can be taken as ≥2 µg/L. A 21-day *Daphnia* reproduction study

is also available for a $C_{>20}$, 43% Cl wt. substance. This showed no effects on reproduction at concentrations up to 55 µg/L.

For comparison, a *Daphnia* 21-d NOEC of 8.7 µg/L was reported for a C_{14-17}, 52% Cl wt. substance (see Section 5.1.6). It cannot be ruled out that the NOEC could lie in the range of 2 to 9 µg/L assuming solubilisation is feasible.

Table 28 Toxicity to invertebrates (Environment Agency, 2009)

Species	Substance tested	Comments	Results	Reference	Val.[a]
Water flea (*Daphnia magna*)	C_{18-20}, 52% Cl wt.	Tested as water-soluble fraction; measured results; variable results.	48-h EC_0 = 0.36 mg/L 48h EC_{15} = 0.4 to 0.5 mg/L	Frank, 1993; Frank and Steinhäuser, 1994	2
Water flea (*Daphnia magna*)	C_{18-20}, 52% Cl wt.	Tested as water-soluble fraction from a 10 g/L nominal solution; semi-static test; measured dissolved concentrations. Tested as water-soluble fraction from a 100 mg/L nominal solution; semi-static test; dissolved concentrations based on detection limit of analytical method Tested as water-soluble fraction from a 1 mg/L nominal solution; semi-static test; actual dissolved concentrations unknown	21-day NOEC = 0.029 to 0.032 mg/L Result unreliable due to inappropriate statistical analysis. No effects seen in 21-day study	Frank, 1993; Frank and Steinhäuser, 1994	2
Water flea (*Daphnia magna*)	$C_{18–20}$, 52% Cl wt.	Saturated test solution was generated using a column method. Substance tested contained a stabiliser. The mean number of young per adult was reduced compared to the control groups, but it is not clear if this was statistically significant or not.	Effects on reproduction may have occurred at around 2 µg/L	TNO, 1993	2
Water flea (*Daphnia magna*)	C_{18-27}, 60% Cl wt.	Static test; unstabilised product; emulsifier. Effects seen at concentrations above solubility.	24-h NOEC = 23 mg/L 24-h EC_{50} = 102 mg/L	BUA, 1992	3
Water flea (*Daphnia magna*)	C_{18-27}, 60% Cl wt.	Static test; stabilised product; emulsifier. Effects seen at concentrations above solubility.	24-h NOEC = 45 mg/L 24-h EC_{50} = 149 mg/L	BUA, 1992	3
Water flea (*Daphnia magna*)	C_{18-27}, 60% Cl wt.	Static test; unstabilised product; acetone as cosolvent. Effects seen at concentrations above solubility.	24-h NOEC = 100 mg/L 24-h EC_{50} = 553 mg/L	BUA, 1992	3
Water flea (*Daphnia magna*)	C_{18-27}, 60% Cl wt.	Static test; stabilised product; acetone as cosolvent. Effects seen at concentrations above solubility.	24-h NOEC = 100 mg/L 24-h EC_{50} = 1,024 mg/L	BUA, 1992	3
Water flea (*Daphnia magna*)	C_{18-27}, 60% Cl wt.	Emulsifier. Effects seen at concentrations above solubility.	21-day NOEC = 4.2 mg/L	BUA, 1992	3

			21-day EC_{50} = 40.8 mg/L		
Water flea (*Daphnia magna*)	$C_{>20}$, 43% Cl wt.	Water accommodated fraction tested. No effects seen at initial loadings of 0.21, 1.0 and 5.1 mg/L. It is not clear if the equilibration time was sufficient to allow a saturated solution to be prepared.	No adverse effects seen over 48 hours.	Thompson, 2005	2
Water flea (*Daphnia magna*)	$C_{>20}$, 43% Cl wt.	No effects were seen on reproduction. The adult survival in some of the exposures was lower than the control and solvent control populations but this was not statistically significant.	21-day NOEC for reproduction ≥55 µg/L	Sharpe and Penwell, 2007	2
Mussel (*Mytilus edulis*)	C_{22-26}, 43% Cl wt.	No mortality seen. Endpoint = decreased filtration activity. No effects seen at solubility.	60-day NOEC/LOEC = 2.18 mg/L	Madeley and Thompson, 1983a	2
Mussel (*Mytilus edulis*)	$C_{>20}$, 70% Cl wt.	No mortality seen. Endpoint = decreased filtration activity. No effects seen at solubility.	60-day NOEC/LOEC = 1.33 mg/L	Madeley and Thompson, 1983b	2
Marine crustacean (*Nitocra spinipes*)	C_{22-26}, 42% Cl wt.	No details available.	96-h LC_{50} >1 000 mg/L	Tarkpea *et al*., 1981	4
Marine crustacean (*Nitocra spinipes*)	C_{18-26}, 49% Cl wt.	No details available.	96-h LC_{50} >10 000 mg/L	Tarkpea *et al*., 1981	4

Note: a - Validity markings: 1 – Valid without restriction; 2 – Use with care; 3 – Not valid; 4 – Not assignable.

Table 29 Toxicity to algae (Environment Agency, 2009)

Species	Substance tested	Comments	Results	Reference	Val.[a]
Dunaliella tertiolecta,	$C_{>20}$, 50% Cl wt.	Static test, acetone solvent used to dose empty test vessel before addition of test media.	6-day NOE_bC >100 mg/L	Craigie and Hutzinger, 1975	3
Olisthodiscus sp.	$C_{>20}$, 50% Cl wt.	Static test, acetone solvent used to dose empty test vessel before addition of test media.	6-day NOE_bC >100 mg/L	Craigie and Hutzinger, 1975	3
Thalassiosira fluviatilis	$C_{>20}$, 50% Cl wt.	Static test, acetone solvent used to dose empty test vessel before addition of test media.	6-day NOE_bC >100 mg/L	Craigie and Hutzinger, 1975	3

Note: a - Validity markings: 1 – Valid without restriction; 2 – Use with care; 3 – Not valid; 4 – Not assignable.

5.1.3 Algae and aquatic plants

No data on the toxicity of LCCPs to freshwater algae or plants were identified in Environment Agency (2009a). A single study investigating the toxicity of LCCPs to marine algae was reviewed and is summarised. There are no additional studies on LCCPs in the EU REACH registrations.

A single additional publication was identified during the literature search. Koh and Thiemann (2001) determined the toxicity of several CP products including three LCCP products to *Scenedesmus subspicatus* according to DIN 38412, part 9. The products were CP 30 (C_{17-24}, 35% Cl wt.), CP 40 (C_{17-20}, 44% Cl wt.) and Hordaflex LC 50 (C_{17-20}, 52% Cl wt.) and were all supplied by Hoechst AG. The tests were carried out for 72 hours. The CPs were dissolved in acetone to prepare stock solutions which were then diluted with distilled water to give the final nominal concentrations of 200 µg/L CP 30 and CP 40, and 100 µg/L Hordaflex LC 50. The other exposure concentrations are not stated, and no measurements were carried out to verify the actual exposure concentration. A solvent control containing acetone at 0.1 ml/L was also tested. No further details on the test conditions are provided. The algal cell counts were determined by a particle counter device. No effects on biomass or growth rate were seen in any of the exposed populations, and the authors note that cell growth was higher than that of the control on occasion.

Only minimal details of the conditions of this study are provided in Koh and Thiemann (2001). This static test used a solvent to test concentrations above the water solubility and the exposure concentrations were not confirmed by analysis. No effects were observed for any of the three test compounds, but no information is provided on the growth of the controls to determine whether the test was valid. The reliability of the study therefore cannot be independently assessed. As such, the reliability is unknown (Klimisch 4).

There is no fully valid algal test available for LCCPs. However, aquatic invertebrates are the most sensitive trophic group for MCCPs or SCCPs (see Section 5.1.6), so the lack of definitive algal toxicity data is not a significant concern.

5.1.4 Sediment organisms

No measured data for this endpoint are presented in the EU REACH registrations (ECHA, 2021a). Instead, the EU REACH Registrants argue that due to the low water solubility of LCCPs and the lack of aquatic toxicity, LCCPs would not be expected to pose a significant risk to sediment dwelling organisms. No sediment organism toxicity data were identified in Environment Agency (2009a) or in the updated literature review.

5.1.5 Other aquatic organisms

No relevant information is available from standard studies.

Du *et al*. (2019) reported the relationship between CP burden in liver and physiological parameters, as part of a wildlife sampling study involving the Black-spotted Frog (*Pelophylax nigromaculatus*) (described in Section 4.3.1.4). In brief, the hepatosomatic index (HSI) was used to estimate energy status and as a biomarker for contaminant exposure. A negative correlation was found between HSI and total CP burden in the liver, where a higher CP load was observed in smaller livers. It was also noted that a negative correlation was observed between body size and CP load. The authors proposed that increased CP exposure may reduce energy storage in frog liver, since additional energy may be used by the organism to expel the contaminants. However, the Environment Agency considers that this is speculative since the presence and concentration of other substances in the frogs was not addressed. The relative concentration of LCCP congeners was also low, so this observation might have no relevance for LCCPs.

5.1.6 Data from structural analogues

Aquatic ecotoxicity data are available for both SCCPs (ECHA, 2008) and MCCPs (ECHA, 2019).

Chronic NOEC are available for fish, invertebrates and algae for SCCPs. The most sensitive chronic endpoint is a Daphnia 21-day NOEC of 0.005 mg/L [5 µg/L] obtained using a $C_{10\text{-}13}$ chlorinated n-alkane, 58% Cl wt. (ECHA, 2008).

For MCCPs, aquatic effects have almost exclusively been observed with *D. magna*. A 48-h EC_{50} of 0.0059 mg/L [5.9 µg/L] and 21-d NOEC of 0.0087 mg/L [8.7 µg/L] were reported for this species using a $C_{14\text{-}17}$, 52% Cl wt. substance. The similarity in acute and chronic endpoint values is highly unusual but is assumed to be related to differences in bioavailability (or elimination) caused by the presence of food in the chronic study. No toxicity has been observed in the available experiments with fish, other invertebrates, or algae (other than at concentrations significantly in excess of the solubility limit in pure water). No effects were seen with MCCPs in a 20-day embryo-larval fish test; although the method was deficient when compared to the current OECD TG 210, comparison with SCCPs suggest that fish are unlikely to be more sensitive than Daphnia in chronic studies (see EC, 2005 for further explanation). Nevertheless, effects have been observed on behaviour and liver histology in juvenile Rainbow Trout (*O. mykiss*) in a non-standard dietary study.

5.2 Terrestrial compartment

Evaluation of available data were performed in conjunction with the relevant guidance text from ECHA R.11 and R.7.c (ECHA 2017 a and d).

5.2.1 Experimental data

No measured data for this endpoint are presented in the EU REACH registrations (ECHA, 2021a). Instead, the EU REACH Registrants state that scientific studies to address these endpoints are scientifically not necessary or that there is other information available. No data were identified in Environment Agency (2009a) or in the updated literature review.

5.2.2 Data from structural analogues

No terrestrial toxicity data are available for SCCPs.

Long-term toxicity data are available for earthworms, plants and soil micro-organisms for MCCPs (ECHA, 2019). The most sensitive endpoint was a 56-day NOEC for earthworm reproduction of 280 mg/kg dw soil (around 248 mg/kg ww) using a radiolabelled $C_{14\text{-}17}$, 52% Cl wt. substance. Further data are presented in the POPs nomination for MCCPs, but these are not repeated here (UK Gov, 2021).

5.3 Assessment of endocrine disrupting (ED) properties

5.3.1 Experimental data

No tests investigating the effects of LCCPs on the endocrine system in aquatic organisms have been located.

Indications of non-monotonic dose responses and effects *in vitro* at environmental exposure concentrations were noted in Ren *et al*. (2019) discussed in Section 6.7. Some evidence of maternal transfer were also presented Section 4.3.

Sun *et al*. (2020) used a protein-affinity guided identification model to identify contaminants/components of commercial CP mixtures with affinity to transthyretin receptor (TTR) and thyroid receptor (TR) proteins. The cDNA which encodes for these proteins were prepared and amplified. The cDNA was then cloned into an expression vector with a histidine tag. Expression vectors were transformed into *Escherichia coli* (DH5α competent cells) expression plasmids, which were then transfected to a different E. coli strain (BL21 DE3) to generate recombinant proteins. These His-tagged proteins were then purified and incubated with 3 commercial CP products purchased from major manufacturers in China (CP-42, CP-52, and CP-70; 42, 52, and 70% Cl wt., respectively). Following incubation, His-tagged protein and compounds bound to it were removed from the mixture using His-select nickel magnetic beads. Contaminants were eluted from the beads in triplicate and analysis was carried out using UPLC-qTOF-MS. The experiment included both positive and negative controls and the Environment Agency considers the methodology scientifically robust.

Oxygen-containing CP-related compounds ("CP(O_2)s") were identified based on the protein based affinity purification and non-target analysis. Further analyses were carried out to elucidate chemical properties as well as structure (using Orbitrap mass spectrometry) of the isolated and hydrolysed fractions followed by Fourier transform infrared spectroscopy analysis to identify the functional groups of the CP(O_2)s. They were identified as novel chlorinated fatty acid methyl esters (CFAMES), and CFAMES with a carbon chain length of 17 to 19 and 3 to 11 chlorine atoms were detected at high percentages in CP-52 and CP-70. The Environment Agency notes that these compounds are not reported as impurities in CPs registered in the EU. The identified CFAMEs were reported by Sun *et al*. (2020) to be ubiquitous in environmental samples collected in Shenzhen, China. Detection frequencies for CFAMEs in human blood was ~67% with C_{17-19}-CFAMES predominant (the authors speculated that this may be the result of dietary intake of plant-based foods).

CFAMES were found to have a high affinity for TR and TTR proteins. They might therefore have the potential for thyroid toxicity. In addition, the affinity of CFAMES to TTR indicate potential for increased placental transfer during pregnancy, exposing the foetus during sensitive windows of development.

The Environment Agency considers this study to be Klimisch 4 (unknown reliability). It provides some *in vitro* evidence of thyroid disruption potential by CFAMES. The relevance of this information for LCCPs, produced in countries other than China are currently unknown.

5.3.2 Data on structural analogues

Three publications were identified during the literature search on the possible endocrine disrupting properties of SCCPs, 2 on fish and 1 on birds. None involved a standard test method (i.e. OECD GD 150 (OECD, 2018)) normally used to investigate endocrine disruption in fish or birds.

- Cooley *et al*. (2001) exposed juvenile Rainbow Trout (O. mykiss) to 6 different SCCPs via their diet. Three of the SCCPs were synthesised by chlorination of alkene starting materials and 3 were produced by free-radical chlorination of 14C labelled alkanes. The resulting test substances were C_{10}, 62.78% Cl wt., ^{14}C-C_{10}, 63.44% Cl wt., C_{11}, 57.12% Cl wt., ^{14}C-C_{12}, 58.37% Cl wt., C_{14}, 47.95% Cl wt. and ^{14}C-C_{14}, 55.30% Cl wt. (% Cl wt. calculated by Environment Agency rounded to two decimals). Fish food was spiked with a low, medium, and high dose of each substance (which varied between substances). The daily feeding rate was 1.5% of the mean fish weight, and food not consumed after 2 hours was removed from the tanks. Groups of 10 juvenile fish were exposed to each treatment, and 3 control groups were run in parallel. After 21 days, all fish in the medium and high treatments and 2 of the control groups were euthanised. The low treatment groups and the remaining control group were terminated on day 85. Concentrations of CPs in the food and fish tissue were determined by LSC for the radio-labelled test

compounds and by GC-ECD for the other test compounds. Concentrations detected in the whole fish samples ranged from 0.028 to 5.5 µg/g after 21 days exposure to the medium and high doses and 0.018 to 0.57 µg/g after 85 days exposure to the low dose.
Although the main focus of the paper was on acute toxicity and behavioural changes, the thyroid glands were also sampled and examined histologically. Cooley *et al*. (2001) noted that the thyroid glands were active in all fish, and that no lesions or anomalies were observed. No statistically significant differences were observed between the epithelial cell height (ECH) in the exposed fish and the controls at after 21 or 85 days exposure under these test conditions. Thyroid hormones levels were not investigated.

The Environment Agency considers this study to be Klimisch 4 (unknown reliability). It provides no evidence of thyroid disruption by several SCCP test substances in fish *in vivo*, although the extent of the investigation was limited.

- Liu *et al*. (2016) studied the toxicity and possible thyroid disrupting effects of SCCPs to Zebrafish (*Danio rerio*) embryos. Seven test substances were used: C_{10}, 50.2% Cl wt., C_{10}, 65.0% Cl wt., C_{12}, 45.3% Cl wt., C_{12}, 59.8% Cl wt., 1,2,5,6,9,10-C_{10}, 61.0% Cl wt., 1,1,1,3,10,12,12,12-C_{12}, 63.7% Cl wt. and the commercial product Cereclor 63L (63% Cl wt.). Exposure solutions were prepared using DMSO at 0.01%. Twenty 2-hour post fertilisation (hpf) embryos were placed in petri dishes and exposed until 96 hpf, with the test solutions fully replaced every 24 hours. Hatching rates, malformation rates and survival rates were monitored every 24 hours. Although a range of exposure concentrations were studied, effects on thyroid hormone levels and gene transcription were only investigated at 0.5 and 100 µg/L (nominal). These 2 concentrations resulted in no malformations, and survival and hatching success were not statistically different to those of the solvent control. Both exposure concentrations and a solvent control were tested in triplicate. Exposure concentrations were not confirmed using chemical analysis, so all results are based on nominal concentrations.
  The C_{10} CPs caused a statistically significant reduction in total triiodothyronine (TT3) concentrations compared to that of the controls, at both nominal concentrations in the case of the 2 higher chlorine content substances, but only at the highest dose for the lower chlorine content substance. The two higher chlorine content C_{10} CPs also caused a statistically significant reduction in total thyroxine (TT4) levels at 0.5 µg/L (nominal), with no effect seen at the high (100µg/L) dose. None of the other test compounds had a significant effect on TT3 or TT4 levels.
  For the majority of the test compounds no statistically significant changes were found in the expression of six genes related to the thyroid pathway. The lowest chlorine content C_{10} CP had the greatest effect, with significant down-regulation of tyr, ttr, dio2 and dio3 in a dose dependent manner, and significant up-regulation of thraa at 0.5 µg/L only. The lowest chlorine content C_{12} SCCP showed a significant down-regulation of ttr in a dose dependent manner.

The Environment Agency considers this study to be Klimisch 4 (unknown reliability). The results indicate that C_{10} CPs with higher chlorine content can cause a statistically significant reduction in TT3 and TT4 concentrations in Zebrafish embryos, and that exposure to C_{10} and C_{12} CPs with lower chlorine contents resulted in statistically significant changes in expression of genes related to the thyroid pathway, with the greatest changes at C_{10}. The authors suggest that the shorter chain length SCCPs may have the potential to disrupt the thyroid pathway.

- Fernie *et al*. (2020) injected American kestrel (*Falco sparverius*) eggs from captive breeding pairs with SCCPs (C_{10-13}, 55.5% Cl wt.) on embryonic day 5. The number of eggs in each treatment group ranged from 23 to 34. The test substance was dissolved in hexane and then added to 100% pure safflower oil which was out-gassed to remove the residual hexane. This stock solution was serially diluted to prepare the nominal SCCP exposure concentrations of 10, 50 and 100 ng/g egg ww which were injected into the air cell of the eggs. The concentrations in the dosing solutions were confirmed by GC-ECNI-MS and found to be equivalent to 10, 29 and 97 ng/g egg ww. A solvent control containing only safflower oil was also tested. When the eggs hatched on embryonic days 27 to 29 the chicks were euthanised and a number of endpoints measured related to hatching, hepatic oxidative stress, immune organs and thyroid status.
  After hatching, the yolk sac is still present in the chicks of this species and contains a small amount of yolk. This was sampled and analysed for SCCPs. SCCPs was detected at mean concentrations of 140, 170 and 360 ng/g lipid weight in the low, medium and high dose groups, respectively. However, SCCPs was also detected in the control yolk sacs at 76 ng/g lipid weight. Concentrations of SCCP in the chicks themselves were not determined.
  When data from male and female chicks were combined there were no statistically significant effects of SCCP exposure on hatching success, hatching rate, hatchling size, hepatic oxidative stress measures, immune organ measures or thyroid status measures. The only endpoint that was found to be statistically significantly different to the solvent controls was an increase in absolute liver weight of chicks in the lowest dose. No significant changes were observed in absolute liver weight of chicks in the higher two doses.
  When data from male and female chicks were considered separately, no statistically significant effects related to SCCP exposure were reported on hatching success, hatching rate, hatchling size, hepatic oxidative stress measures or immune organ measures. The majority of thyroid related endpoints were also not statistically different to those of the control, with no effects observed on TT3 or TT4 concentrations in blood, TT3 concentration in the thyroid gland, thyroid gland size or liver deiodinase enzymes. Although the TT4 concentration in the thyroid gland was not altered in females, in males it was statistically reduced in all exposures with the greatest reduction observed at the lowest dose. Thyroid gland structure was found to be statistically altered from the controls for the endpoints colloid area (CA), colloid diameter (CD), ECH and the ratio of ECH:CD which can be used as a

measured of thyroid activity. In females, effects on CA and CD were similar for all treatment groups, ECH did not follow a dose response and the ECH:CD ratio was only significantly reduced compared to the controls at the highest dose. In males, statistically significant effects were only seen in the low dose group, with lower CA and CD, higher ECH and reduced ECH:CD ratio.

This non-standard study indicates that exposure to SCCPs altered the histology of the thyroid gland in both male and female chicks and resulted in a statistically significantly reduced concentration of TT4 in male thyroid glands (with the greatest effect at the lowest exposure). However, the other measures of thyroid activity, including concentrations of TT3 and TT4 in the blood, together with a wide range of other apical endpoints, were unchanged from that of the controls. The contamination of the control cohort confounds the interpretation of the results overall. The authors suggest that the changes observed were likely compensatory mechanisms to maintain the correct functioning of the hypothalamus-pituitary-thyroid axis. As such, although this paper demonstrates that SCCPs has the potential to disrupt the thyroid pathway these changes did not lead to apical effects over this exposure period. The Environment Agency considers this study to be Klimisch 4 (unknown reliability). Egg injection studies do not use an environmentally relevant exposure route.

In summary, these non-standard tests suggest that SCCPs can alter the expression of thyroid-related genes in Zebrafish embryos (Liu *et al*., 2016), reduce concentrations of TT3 and TT4 in both fish and birds (Liu *et al*., 2016; Fernie *et al*., 2020), and alter the histology of the thyroid gland in birds exposed *in ovo* (Fernie *et al*., 2020). SCCPs may therefore have the potential to disrupt the thyroid pathway. However, adverse apical effects were not observed over the exposure periods studied. Given the significant differences in physico-chemical properties and bioaccumulation behaviour, the relevance of these observations for LCCPs is unknown.

6 Mammalian toxicology

The following information is taken from the ECHA public dissemination site (ECHA, 2021a). The reliability (Klimisch) scores are those of the EU REACH Registrants. The Environment Agency has not evaluated these studies for reliability or relevance, but has taken account of a recent regulatory review performed by EFSA (2020).

The focus is on those endpoints which are potentially relevant for the bioaccumulation assessment and the determination of the substance as Toxic ('T') according to the REACH Annex XIII criteria. Evaluation of available data were performed in conjunction with the relevant guidance text from ECHA R.11 and R.7.c (ECHA 2017 a and d).

6.1 Toxicokinetics

Toxicokinetic reviews are available in various regulatory reports (IPCS, 1996; Environment Agency, 2009; OECD, 2009a), with EFSA (2020) providing the most up to date summary.

The EU REACH registrations include 4 relevant studies, and a summary can be found in Appendix I. The EU REACH Registrants conclude that absorption via the oral and inhalation routes will be approximately 50% of the administered dose and that dermal absorption will be approximately 1%, with absorption decreasing with increasing carbon chain length and degree of chlorination. This is primarily based on 2 rat studies using $C_{22\text{-}26}$ CPs with 43% and 70% Cl wt. (IRDC, 1984 a & b), which were provided in full to EFSA for their review. Using the same studies, EFSA (2020) concluded that following oral administration, most of the elimination occurs through faecal excretion over the first 7 days (accounting for up to 95% of the administered radioactivity for the lower chlorine content substance, and between 61 and 88% for the higher chlorine content substance according to Environment Agency (2009a)). Little elimination occurs via urine or air (≤1% for both substances). Blood concentrations increased with dose for the higher chlorine content substance. The highest initial concentration was found in the liver in both studies, but this subsequently redistributed to adipose tissue. The concentration in adipose tissue increased up to 28 days and then declined only slightly by 90 days for the lower chlorinated substance. For the higher chlorinated substance, the adipose concentration increased slowly after dosing with only a small decline by 90 days. For the lower chlorinated substance, the concentration in ovaries was comparable with that in the adipose tissue at 28 days, whereas for the higher chlorinated substance, the concentration in ovaries was generally similar or lower than in other tissues. EFSA (2020) also cite a study by Yang *et al*. (1987) for a C_{18}, 50 to 53% Cl wt. product, which indicated that only around a quarter of the radioactivity in the faeces was present as the parent LCCP (transformation products were not identified).

The literature search performed by the Environment Agency identified 2 further studies that are not included in the EU REACH registrations and brief details are included below:

- Dong *et al*. (2020) established a physiologically based pharmacokinetic (PBPK) model in rats and humans for CPs. CP standards were purchased from Dr. Ehrenstorfer (Augsburg, Germany). SCCP standards contained C_{10-13} congeners with 51.0, 55.5 and 63% Cl wt., MCCP standards contained C_{14-17} congeners with 42, 52 and 57% Cl wt., and LCCP standards contained C_{18-30} congeners with 42 and 52% Cl wt. Rats were exposed to CPs *in vivo*, and rat and human liver microsomes *in vitro*. In addition, human biomonitoring was performed for internal and external exposures to a wide range of CPs over a 1-year period in Shenzen, China, and the results were used to calibrate the rat PBPK model to humans. Analysis was performed using reverse ultra-high pressure liquid chromatography coupled with chlorine enhanced electron spray ionisation quadrupole time-of-flight mass spectrometry (UHPLC-Cl-EI-qTOF-MS). The Environment Agency notes that the study followed rigorous scientific principles and applied the necessary controls and precautions.
  Half-lives in human and rat microsomes were long, suggesting limited potential for metabolism, which appears to contradict the observations of Yang *et al*. (1987) – although that study used a C_{18} substance only – and He *et al*. (2020) (see below). Following a single administration in rats, tissue concentrations in liver and adipose increased to a maximum by 72 hours and then decreased to a plateau by 14 days. Following calibration of the PBPK model parameters with internal and external exposures, concentrations of SCCPs, MCCPs, and LCCPs could be accurately predicted in blood. Mass balance calculations at the 14-day concentration plateau in rats showed that 78 to 95%, 84 to 99% and 87 to 98% of total SCCPs, MCCPs and LCCPs, respectively, were excreted through faeces. This is consistent with other *in vivo* study data (EFSA, 2020). The proportion of CPs excreted through urine and exhalation was very low. Half-lives in rats were estimated to be 4.5, 5.4 and 6.2 days for LCCPs, MCCPs and SCCPs, respectively. The extrapolated human half-lives were 0.6, 1.2 and 5.1 years for LCCPs, MCCPs and SCCPs, respectively. Clearance rates in rats were reported as 1.91, 0.75 and 0.65 L/kg/day for LCCPs, MCCPs and SCCPs, respectively. The equivalent clearance rates in humans were 0.065, 0.019 and 0.0041 L/kg/day. The model appears to be able to predict with reasonable accuracy concentrations in different body compartments at environmentally relevant exposure levels. The study concluded that lower maximum concentrations of LCCPs (and MCCPs) should be expected compared to SCCPs due to the higher biliary excretion rates.
  The Environment Agency considers this study to be Klimisch 4 (unknown reliability).
- He *et al*. (2020) used a two-tier *in vitro* approach to investigate the biotransformation of CPs in humans through liver microsome culture, under both viable and non-viable conditions. Direct injection analysis was performed using negative polarity DCM enhanced APCI-QTOF-MS. Procedural blanks were prepared in triplicate and incubated using the same protocol as the viable samples. Commercial CP mixtures were acquired from DR Ehrenstorfer (Augsburg, Germany), and these included SCCP 55.5% Cl wt., MCCP 52% Cl wt., and LCCP 49% Cl wt. Concentrations of LCCPs, MCCPs and SCCPs were measured as 0.12,

0.98 and 0.32 ng absolute in procedural blanks subjected to the same protocol as real samples. The nominal concentrations applied were 100nM of either SCCP, MCCP or LCCP in the 1mL reaction mixtures. Blank corrections were applied to all samples. A six-point isotope calibration in the concentration range 0.1 to 20 ng/µL for total CPs was prepared (R^2 = 0.99). Negative control samples were spiked with ^{13}C-BDE-209 (internal standard), which was used to calculate recoveries (87% to 109%) and accuracy (95 to 98%). The suitability of the brominated aromatic internal standard to assess recovery of the linear chlorinated paraffins is unknown. No interferences were observed amongst the target analytes.
Targeted instrumental monitoring was performed for CPs, including vSCCPs ($C_{<10}$), alcohols, ketones and carboxylic acids. Internal standard corrected peaks (ratio between peak area of a congener group and peak area of ^{13}C-BDE-209) were used for biotransformation product identification.
Total CP group concentrations decreased rapidly (~2 hours) by between 33 to 94%, depending on the group of enzymes used. Both Phase I and Phase II biotransformation were monitored. The authors reported that carbon chain shortening took place during biotransformation. Most LCCPs, MCCPs and SCCPs concentrations decreased during the experiment, with only a few LCCPs not conforming to this result. The results of this study appear to indicate that certain congeners are stable during biotransformation in all three CP classes. Furthermore, enzymatic transformation of LCCP and MCCPs was observed to lead to increased concentrations of MCCPs and SCCPs, respectively. The Environment Agency notes that these types of transformation are unexpected as LCCPs are expected to be less bioavailable than SCCPs due to their greater molecular size and hydrophobicity, however, it is possible that LCCPs due to their long chain and high variability in Cl atom number and location may fold and become stereochemically smaller and potentially resemble molecules for which active transport can occur. This hypothesis is supported by the detection of LCCPs in a wide range of biota. However, the mechanism has not been scientifically elucidated. The subsequent direct cleavage of the carbon chains is also unusual for hepatic enzymes. In addition, the authors state that all the major transformations products that they identified were also detected in the standards, albeit at lower concentrations, and other unknown transformation products were not accounted for.
The Environment Agency considers these data to be unreliable (Klimisch 3), because the results are contradictory and the suitability of decaBDE as a recovery standard is not understood.

In summary, limited toxicokinetic information is available for LCCPs. Based on the available information, absorption via the oral route may be significant (about half of the administered dose). Excretion is mainly through the hepatobiliary pathway in faeces. The majority of excretion occurs in the first few days following exposure, but some of the dose remains within the body for more than 7 days, where it accumulates in liver and is then gradually distributed to fatty tissues and other organs. Excretion via breast milk could therefore occur, and this is confirmed by biomonitoring (see Section 4.3.2.4). It is possible that there will be some metabolism of LCCPs, although this may be slower as carbon chain length and degree of chlorination increase, resulting in a lower elimination rate. Half-lives for a $C_{18\text{-}30}$ CP, 42 to

52% Cl wt. product were estimated to be 4.5 days in rats and 0.6 years in humans, respectively.

6.2 Acute toxicity

Three oral LD_{50} values are reported by EFSA (2020): >11.7 g/kg bodyweight (bw) (rat) and >23.7 g/kg bw (mouse) for a C_{23} CP, 43% Cl wt. product (Bucher *et al*., 1987); and >4 g/kg bw (rat) for Cereclor 42 (a $C_{20\text{-}30}$, 42% Cl wt. CP) (Birtley *et al*., 1980). These all indicate low acute toxicity via the oral route.

6.3 Repeated dose toxicity

Several repeated dose toxicity studies have been carried out in mice and rats and summarised in EFSA (2020). LCCPs appears to have little to no effects in mice, but some toxicity was seen in rats. The liver appears to be the target organ, with limited effects seen in male rat kidneys. This aligns with toxicokinetic data indicating higher concentrations in liver, adipose and ovarian tissues. Large differences in toxic effects were seen between dietary and oral gavage exposure studies.

The EU REACH Registrants do not classify LCCPs for repeat dose toxicity based on a "weight-of-evidence" evaluation, specifically:

- A 90-day repeated dose NOAEL of 900 mg/kg bw/day (oral dietary, male and female rat) has been established for solid grade LCCP, which does not require classification.
- NOAELs of 7 500 (90-day) and 5 000 (2 year) mg/kg bw/day were established for liquid grade LCCPs in mice during repeated dose toxicity studies. Classification not warranted.
- 90-day repeated dose NOAELs of 3 750 and 900 mg/kg bw/day were established for similar liquid grade LCCPs in separate studies of male rats, which do not require classification.
- Liquid LCCPs have been shown to produce liver inflammation in female rats following bolus gavage dosing for 90 days or 2 years and in male rats following bolus gavage dosing for 2 years. This effect occurred at the lowest doses tested (1 875 mg/kg bw/day for males: 100 mg/kg bw/day for females). The mechanism(s) by which this effect occurs are not known, nor are the reasons for the much greater sensitivity of the female rat to gavage doses and the remarkable species difference between rats and mice. The relevance of this finding to humans are not understood, although the dietary results are considered to be more relevant to the human exposure situation. Therefore, consideration of the full body of available evidence does not justify classification of LCCPs for repeated dose toxicity.

6.4 Mutagenicity

Twelve *in vitro* genetotoxicity studies have been performed (4 of which are considered unreliable (Klimisch 3) by the EU REACH Registrants), along with 2 *in vivo* genetic toxicity studies. Only 1 of the *in vitro* studies indicate possible mutagenicity, manifest as increased chromosomal aberrations following exposure to LCCPs. The substance is not classified for mutagenicity in the EU REACH registrations. The Environment Agency notes that there may have been some issues in terms of the delivery mechanism (oily droplets in the test media) in some cases.

6.5 Carcinogenicity

Two carcinogenicity studies are included in the EU REACH registrations and summarised in Appendix I. As with the repeated dose toxicity above, non-neoplastic, lymphohistiocytic inflammations in liver and in pancreatic and mesenteric lymph nodes were seen at the lowest dose tested, namely 100 mg/kg bw/day (female rats). According to EFSA (2020), there is evidence of carcinogenicity of LCCPs at very high doses (2 500 and 5 000 mg/kg bw/day) that exceed the limit dose. EFSA concluded that, since LCCPs do not appear to have mutagenic potential, carcinogenic activity is likely to be the result of a non-genotoxic mode of action and it can be assumed that the carcinogenicity will have a threshold exposure level.

The EU REACH Registrants do not classify LCCPs for carcinogenicity in the EU, but note that IARC assigned LCCPs as Class 3 based on malignant lymphomas reported in male mice at very high (5 000 mg/kg/day) doses. Furthermore, the registration dossier assigns a Carc. 2 classification H351 (Suspected of causing cancer) under classification and labelling.

6.6 Toxicity to reproduction (effects on fertility and developmental toxicity)

No specific reproductive toxicity studies are included in the EU REACH registrations. A short statement is provided, as follows:

Effects of LCCPs on fertility and reproductive performance have not been specifically investigated. No indications of changes in reproductive organs were noted in subchronic and chronic repeated dose toxicity studies. No effects on fertility were observed in 2 MCCP reproductive toxicity studies, a one-generation reproductive toxicity range-finding study and a definitive one-generation reproductive toxicity study. Haemorrhaging in dams and in pups were noted in the MCCP reproduction studies. A NOAEL of 100 mg/kg/day was identified for this effect. Available evidence suggests that MCCPs inhibit the absorption of vitamin K (ECHA, 2021). This effect occurs after the administration of high

doses of MCCP by gavage to female rats, a situation that would not arise under any reasonably foreseeable circumstances of exposure.

When this assessment was initiated, the LCCP REACH Registrants summarised their findings from other repeated dose toxicity studies and arrived at the conclusion that LCCPs should be self-classified as H362-lactation (may cause harm to breast-fed children). This applied to all chain lengths and chlorination levels. This classification is the same as that designated to Alkanes C_{14-17}, chloro (CAS 85535-85-9). The self-classification has since been withdrawn by the Registrants.

6.7 Other studies

The literature search performed by the Environment Agency has identified a recent study that focussed on *in vitro* endpoints. This is not included in the EU REACH registrations, and so brief details are included below:

- Ren *et al*. (2019) compared the effects of LCCPs, MCCPs and SCCPs on cell viability using a Hep G2 (human liver cell line). Cyclohexane stock solutions were prepared for the test substances (C_{18-20}, 49% Cl wt.; C_{14-17}, 52% Cl wt.; C_{10-13}, 51.5% Cl wt.) at concentrations of 1, 10, 100 and 1 000 µg/L for 24 hours (considered by the authors to be comparable to concentrations measured in human blood, milk, and foodstuffs). Though not clear from the text, the Environment Agency assumes that stock solutions made in cyclohexane were diluted into the culture medium, so that desired concentrations of the CPs were obtained while maintaining constant (and below toxicity) concentrations of cyclohexane, as per standard culture protocols.
  At all exposure concentrations cell viability was decreased, with the lowest cell viability observed at 100 µg/L for all CPs (indicative of a non-monotonic dose response). Similar toxicity was seen regardless of chain length.
  The group then determined the levels of adenosine triphosphate (ATP), reactive oxygen species (ROS), and malondialdehyde (MDA, a marker of oxidative stress) present in cells exposed to 100 µg/L. ATP levels were markedly decreased by all of the CPs with MCCPs causing the largest decrease (15.4% lower relative to control). All CPs resulted in increased ROS and MDA levels, indicative of increased oxidative stress. MCCPs caused the largest increase in ROS (46.9% increase relative to controls) and LCCPs caused the largest increase in MDA levels (103% increase relative to controls). The results suggest that MCCPs is the strongest inducer of oxidative stress and LCCPs is the strongest inducer of lipid peroxidation.
  The effects of CPs on 631 intracellular metabolites in a pseudo-targeted metabalomics approach were also investigated as part of the study. In a principal component analysis, the first principal component indicated a difference between CP treatments and controls. The second component separated the 3 CP treated groups, indicative of perturbed cell metabolism following exposure to environmentally relevant concentrations. All three CPs were shown to alter purine

metabolism with alternative mechanisms of action suspected for LCCPs versus SCCPs and MCCPs. LCCPs were also shown to reduce amino acid and choline levels and were suspected of altering cell membrane fluidity and trans-membrane transport.

This study may provide some mechanistic insights into the observation of inflammation in the mammalian liver (which may be induced by oxidative stress). The toxic effect of LCCPs is slightly different from those of SCCPs and MCCPs. The Environment Agency consider this study to be Klimisch 4 (unknown reliability).

6.8 Human biomonitoring

- Campbell and McConnell (1980) analysed post-mortem human tissues for the presence of CPs. Of the 24 subjects analysed, $C_{20–30}$ CPs were detected in fat tissues of 3 subjects (100 ng/g ww), the liver of one subject (80 ng/g ww) and the fat (3 500 ng/g ww) and liver (200 ng/g ww) of one further subject. The concentration of $C_{20–30}$ CPs in the remaining samples analysed was less than the limit of detection of the method used (i.e. <50 ng/g ww). In contrast, $C_{10–20}$ CPs were frequently detected in liver tissues (up to 1 500 ng/g ww), adipose tissues (up to ~500 to 600 ng/g ww) and kidney tissues (up to around 500 ng/g ww). No $C_{10–20}$ CPs were detected in brain tissues (the detection limit was 90 ng/g ww). Given the age of this study, the Environment Agency considers the data to provide qualitative evidence of detection only.
- Li *et al*. (2017) measured CPs in 6 g human blood samples (n = 50) from individuals living on the border between Shenzhen and Dongguan City, using a reversed ultra-high pressure liquid chromatography system coupled with chlorine enhanced electron spray ionisation quadrupole time of flight mass spectrometry. This allowed the simultaneous determination of 261 congener groups. Method detection limits for LCCPs, MCCPs and SCCPs were estimated at 0.4, 1 and 3.7 ng/g ww, respectively. Concentrations of LCCPs, MCCPs, and SCCPs in human blood samples were presented on a lipid weight basis. The sum of LCCPs, MCCPs and SCCPs were in the range 22 to 530, 130 to 3 200 and 370 to 35 000 ng/g lipid weight, respectively.
- Zhou *et al*. (2020) measured CPs in human milk from people living in urban areas of Sweden, China and Norway. The samples were collected following the World Health Organisations guidance (WHO, 2007). Samples were not pooled. A total of 19, 36, and 8 samples were collected from Sweden, China and Norway, respectively. The study used direct injection dichloromethane enhanced, atmospheric pressure chemical ionisation quadrupole time of flight high resolution mass spectrometry (APCI-QTOF-HRMS), with 5, 6 and 5 LCCP, MCCP and SCCP reference standards. The LOD was set at the average of the blank plus three times the standard deviation and the LOQ as the blank plus 10 times the standard deviation. The LOD was 1.1, 16 and 12 ng/g fat and the LOQ was 3.8, 32 and 25 ng/g fat for LCCPs, MCCPs and SCCPs, respectively. The study found that

concentrations of LCCPs, MCCPs and SCCPs were 3 times higher in first time mothers compared to second. LCCPs were detected in nearly all the analysed human milk samples (86%), although in most samples MCCPs were the most abundant CP group. CP concentrations varied in relation to sample origin. The highest concentration for LCCPs, MCCPs and SCCPs were 184 (Shaoxing), 1 260 (Shanghai) and 676 (Shanghai) ng/g fat, respectively. The mean LCCP, MCCP and SCCP concentrations were higher in samples from Chinese cities (8.8, 78.8 and 35 ng/g fat, respectively) than those for the Scandinavian cities (4.2, 29.6, and 14 ng/g fat, respectively). Further geographical differences were noted: for example, MCCP concentrations were higher in Norwegian samples (43.1 ng/g fat) than Swedish samples (27.4 ng/g).

- Van Mourik *et al*. (2020) investigated temporal trends of CPs from 200 pooled serum samples collected in Australia between 2004 and 2015. Samples were analysed with chlorine enhanced atmospheric pressure chemical ionisation time of flight mass spectrometry (APCI-QTOF-MS). LCCPs were below the limit of detection in all samples (0.16 ng/mL). For comparison, SCCPs were detected in 22% of samples and MCCPs in 94% of samples. C_9 CPs (vSCCP) were detected in 76% of samples, with peak sizes 4 to 19 times that of the blank and accounting for 2 to 7% of peak area (quantification was not possible since no reference standards exist for C_9 CPs).
- Dong *et al*. (2020) monitored human internal and external exposures to a range of CPs for a year in Shenzen, China. This study is discussed in more detail in Section 6.1.

6.9 Summary of mammalian toxicology

The Environment Agency notes that the available data do not necessarily cover all types of LCCP product. The wide range of physicochemical properties means that hazards may vary depending on chain length and degree of chlorination.

Low to very low acute or chronic toxicity were noted in toxicity studies presented by the Registrant. LCCPs do not appear to be mutagenic, although there is some evidence of carcinogenicity at high doses of LCCPs.

The main route of exposure for mammals is via their diet. LCCPs appear to accumulate in adipose tissue and in the liver and other organs.

One *in vitro* study has demonstrated a non-monotonic effect on viability of HepG2 cells, which may be a sign of potential hepatotoxicity (Ren *et al*., 2019). The study also indicates that exposure to CPs at ‘environmentally relevant’ concentrations increased markers of oxidative stress as well as perturbed cell metabolism. It showed that SCCPs, MCCPs, and LCCPs altered purine metabolism with alternative mechanisms of action suspected for LCCPs versus SCCPs and MCCPs. LCCPs were also shown to reduce amino acid and

choline levels and were suspected of altering cell membrane fluidity and trans-membrane transport.

The mammalian toxicity of LCCPs is therefore inconclusive at this stage and may require further study. The Environment Agency notes that determining the toxicity for such a broad range of chemicals captured under the name “LCCPs” will be difficult. Some congeners/degrees of chlorination may be more toxic than others and may be more prevalent in some mixtures than in others. Furthermore it needs to be established whether LCCPs produced in countries other than China also contain or can contain CFAMEs, which, as illustrated in Section 5.3, may affect thyroid function (ED).

The LCCP REACH Registrants do not currently self-classify the substance for any human health hazard endpoints.

7 Avian toxicity

Evaluation of available data were performed in conjunction with the relevant guidance text from ECHA R.11 and R.7.c (ECHA 2017 a and d).

7.1 Laboratory data

Environment Agency (2009a) presented a study that is not included in the EU registration dossier (ECHA, 2021).

Brunström (1983) studied the toxicity of a $C_{22\text{-}26}$, 42% Cl wt. CP to chicken embryos. The substance was injected into fertilized hens (*Gallus gallus domesticus*) eggs after 4 days of incubation in an emulsion of peanut oil, lecithin, and water at a dose of 100 or 200 mg/kg egg. No effects were seen on the incubation time, hatching rate, hatching weight, weight gain after hatch (the observations were made up to day 39 after the start of incubation) or liver weights of the chicks when compared with the control group.

In a further injection study, Brunström (1985) investigated the effects of a $C_{22\text{-}26}$, 42% Cl wt. CP on liver weight, microsomal enzyme activities and cytochrome P-450 concentration in chick embryos after 20 days of incubation. In this experiment the test substance concentration was 300 mg/kg egg. No effects were seen on the viability of the chick embryos, liver weights or AHH (aryl hydrocarbon (benzo[a]pyrene) hydroxylase) activity due to the treatment. A statistically significant ($p < 0.01$) increase in cytochrome P-450 concentration and decrease in APND (aminopyrine N-demethylase) and ECOD (7-ethoxycoumarin O-deethylase) activity was observed in the treated population when compared to the control population.

These egg injection studies provide some indication of the potential for adverse effects in birds, but not via an environmentally relevant exposure route. No significant effects were reported, but this was a non-standard study. The Environment Agency consider this study to be Klimisch 4 (unknown reliability).

7.2 Data on structural analogues

As discussed in Section 5.3, a non-standard study by Fernie *et al*. (2020) indicates that exposure to SCCPs altered the histology of the thyroid gland in both male and female American Kestrel chicks and resulted in a statistically significantly reduced concentration of TT4 in male thyroid glands (with the greatest effect at the lowest exposure). However, the other measures of thyroid activity, including concentrations of TT3 and TT4 in the blood, together with a wide range of other apical endpoints, were unchanged from that of the controls. The contamination of the control cohort confounds the interpretation of the results overall. The authors suggest that the changes observed were likely compensatory mechanisms to maintain the correct functioning of the hypothalamus-pituitary-thyroid axis.

As such, although this paper demonstrates that SCCPs has the potential to disrupt the thyroid pathway these changes did not lead to apical effects over this exposure period. The relevance of this finding for LCCPs is unknown. In addition, egg injection studies do not use an environmentally relevant exposure route. The Environment Agency consider this study to be Klimisch 4 (unknown reliability).

8 PBT and vPvB assessment

Conclusions from available data were drawn using relevant guidance text from ECHA R.11 (ECHA 2017a).

8.1 Persistence

No degradation studies are available for LCCPs that meet current regulatory standards. Key studies cited in the EU REACH registrations cannot be considered reliable. However, LCCPs are unlikely to undergo significant abiotic degradation based on structural considerations.

There are no simulation studies that would provide an unequivocal environmental half-life for LCCPs, but evidence for SCCPs and MCCPs indicates that the rate of biodegradation will vary according to chain length and chlorination level of the substance. Little degradation was observed for $C_{20\text{-}30}$, 42% Cl wt. and $C_{>20}$, 70% Cl wt. CP products in old biodegradation screening studies. Chain lengths found in LCCPs are expected to be less water soluble and more adsorptive than $C_{\leq 15}$ CP substances and so rates of degradation are likely to be lower. Aerobic sediment half-lives for a C_{14}, 50% Cl wt. CP substance exceed 120 days at 12 °C and are likely to exceed 180 days since chemical analysis showed no observable biotransformation over the duration of this study. In the absence of reliable measured data to the contrary, the assumption must be that a significant proportion of LCCP constituents will have long half-lives in freshwater sediments, most likely exceeding 180 days at 12 °C. This is supported indirectly by the detection of LCCPs in sediment cores; concentrations in locations relatively remote from industrial sources suggest that it can persist in sediments for many years (although this may also be related to redox conditions).

Based on similarity to MCCPs, it is possible that low chlorine content congeners (e.g. 30% Cl wt.) might not be persistent, but there are no definitive data available to confirm this. There is evidence that some adapted microorganisms may be capable of degrading LCCPs in the environment in acclimated or co-metabolic systems.

In the absence of reliable measured data to the contrary, the Environment Agency therefore concludes that LCCPs meet the persistent (P) and very persistent (vP) criteria in REACH Annex XIII based on likely sediment half-life. The EU REACH registrations do not provide a definitive conclusion for this endpoint but concede that LCCPs may meet the criteria for P or vP.

8.2 Bioaccumulation

LCCPs is a highly complex substance with a very large number of constituents. Single values for properties such as log K_{OW} are not appropriate. Instead, there will be a wide

range of values depending on the solubility and partitioning behaviour of individual congeners.

Water solubility declines with increasing chain length and the log K_{OW} is high (around 7.5 for the shortest congeners but rising to 10 or more as the number of carbon and chlorine atoms increase). Shorter chain length congeners therefore meet the screening criteria for both a bioaccumulative (B) (log K_{OW} > 4.5) and very bioaccumulative (vB) (log K_{OW} > 5) substance according to REACH Guidance Document R.11 (ECHA, 2017a). However, as the log K_{OW} increases, it becomes less reliable as a screening tool and the output of QSAR tools may also be misleading. In particular, the distribution of LCCPs in different wildlife tissues (especially occurrence in muscle) suggests that accumulation may not always be driven by simple lipid partitioning.

The log K_{OA} of LCCPs is above 9 and the log K_{OW} is above 7.5. These exceed the screening thresholds of log K_{OA} >5 and log K_{OW} > 4.5 in REACH Guidance Dcoument R.11 (ECHA, 2017a), suggesting some constituents of LCCPs may have a high bioaccumulation potential in air-breathing organisms. However, as LCCPs contain constituents with much higher predicted log K_{OA} and log K_{OW} values, it is unlikely that the screening criteria are appropriate for the whole substance.

Many congeners also have large molecular dimensions, although only highly chlorinated congeners (> 60% Cl wt.) with greater than 22 carbons are considered large enough to be screened out as not being potentially B.

The available fish and mollusc BCF data on LCCPs are not reliable as they were obtained using non-standard studies with exposure concentrations in excess of water solubility. Lipid normalisation was not performed and analytical methods were generally not sophisticated enough to provide congener-specific information. It is also unclear if the duration of the studies was sufficient for steady state to be reached. In contrast, a recent study of bioaccumulation in the water flea *Daphnia magna* was carried out below the water solubility limit. Uptake of LCCP congeners by passive diffusion was shown to occur over 48 hours. The results suggest very high BCF/BAFs, but there are major uncertainties in the numerical values, which make them unreliable for regulatory decision making for LCCP congeners. Therefore, although these studies show that uptake occurs, it is not possible to obtain a reliable BCF value from them. Information from MCCPs cannot be readily extrapolated. Consequently **there is no unequivocal evidence that LCCPs meet the definitive criteria in REACH Annex XIII for B (BCF > 2 000 L/kg) or vB (BCF > 5 000 L/kg).**

REACH Annex XIII includes additional aspects to consider as part of an overall assessment of bioaccumulation potential, but these lack definitive criteria. Therefore, the overall weight of evidence provided by such studies is very important.

- Dietary exposure is a relevant route for assessing aquatic bioaccumulation potential for highly hydrophobic substances like LCCPs. Four studies are available, but none were performed to modern standards and 2 are unreliable. The reliability of 2 others

is unknown due to information gaps. The results show that LCCPs can be taken up via the diet, but in all cases the concentrations reached in the organisms were less than those in the diet. This suggests that although uptake of the substance can occur via food, the levels should not increase through the food chain. Dietary BMF data for MCCPs suggest that the potential for uptake (as measured by assimilation efficiency) decreases with increasing carbon chain length and chlorine content. However, the Environment Agency has estimated depuration rate constants and half-lives from the 2 studies that are of unknown reliability, and these are consistent with information from other substances that are known to have a fish BCF above 5 000 L/kg. **LCCPs with chain lengths between C_{18} and C_{25} and chlorination levels of 42 to 49% may therefore have the capacity to bioaccumulate to a significant level in aquatic organisms, although a definitive conclusion is not possible given the limitations of the data available.**

- LCCP congeners have been detected in a wide range of aquatic and terrestrial wildlife, including sensitive life stages (e.g. frog eggs) and several species at the top of the food chain, as well as in human breast milk. Terrestrial species are more likely to accumulate longer, larger molecular weight CPs than aquatic species (although the amounts are often small). The highest concentrations reported to date are for muscle tissue from 2 terrestrial predators (10 000 ng/g lipid in Peregrine Falcon and 5 200 ng/g lipid in Short-tailed Mamushi). LCCP concentrations in human milk can be in the region of 10 to 500 ng/g lipid weight.
- Chemical analysis is challenging and reported concentrations should be treated as qualitative or semi-quantitative depending on the methods used, which adds a layer of uncertainty to the findings of field monitoring studies. This evidence demonstrates that various LCCP chain lengths are bio-available and that even C_{30} congeners can cross biological membranes. Levels are typically lower than MCCP congeners in the same samples, but there are exceptions to this general pattern. For example, LCCP congeners can account for just over half of the total CP burden in Peregrine Falcon muscle. In most species, LCCP congener group patterns in wildlife samples are dominated by C_{18} CPs, followed by $C_{19\text{-}21}$ CPs. The concentrations of C_{18} (and sometimes even longer chain length) congeners can be similar to (and in some cases higher than) those of $C_{15\text{-}16}$ congeners and in some samples can achieve a similar level as C_{14} congeners. **Therefore the evidence indicates that some LCCP congener groups (particularly C_{18} and C_{19}) can accumulate to a similar level as MCCP congeners in some tissues.**
- Two studies have compared lipid-normalised tissue concentrations in different wildlife species to estimate biomagnification potential and the reported values suggest that some LCCP constituents might undergo trophic magnification. However, there are several reasons why these types of comparisons may be unreliable, including lack of information on LCCP levels in other dietary components, uncertainties around the relevance of lipid normalisation, use of single tissue concentrations to represent total body burdens, small sample numbers, mixing of samples from different areas and different times and the statistical issues that arise when comparing complex analytical data. **The Environment Agency**

considers that whilst these studies flag a concern, they are not sufficient to show that biomagnification in specific food chains is actually occurring.

- There are no standard studies or assessment criteria for terrestrial bioaccumulation in the context of a PBT evaluation. Mammalian toxicokinetic data indicate that LCCPs will accumulate in fatty tissues and liver (as well as other organs). It is possible that there will be some metabolism of LCCPs, although this may become slower as carbon chain length and degree of chlorination increase, resulting in a lower elimination rate. In terms of the aims of protecting organisms from unpredictable adverse effects, a long depuration half-life is a key determinant of bioaccumulation potential. It is directly related to one of the protection aims of the PBT assessment, i.e. concentrations for a PBT substance may take a long time to decline once emissions cease. Therefore, the Environment Agency considers that using elimination half-lives to guide decision making is reasonable for LCCPs. Long elimination half-lives in mammals have been used in a weight of evidence analysis to identify some highly fluorinated chemicals as B or vB, although the values are typically 10 days or more in rodents and 1 year or more for humans (e.g. ECHA, 2017e). **Half-lives for a C_{18-30}, 42 to 52% Cl wt. CP product have been estimated in one study to be 4.5 days in rats and 0.6 years in humans. The half-lives for LCCPs appear to be below the benchmark provided by fluorinated substances.**

In summary, the relevance of aquatic bioaccumulation appears to decline with increasing CP molecular weight, with accumulation in terrestrial predators becoming more important. LCCPs with chain lengths between C_{18} and C_{25} and chlorination levels in the range 40 to 50% appear to have the greatest capacity to bioaccumulate. The available evidence provides a suitable, though incomplete, indication that a high level of bioaccumulation cannot be ruled out for some constituents of LCCPs. However, a definitive B/vB conclusion is not possible given the limitations of the data available. The EU REACH registration concludes that LCCPs are not B/vB (ECHA, 2021).

The Environment Agency considers that further work could help provide clearer information on bioaccumulation potential of specific congener groups, with a particular focus on C_{18-25} chain lengths, using modern analytical methods to provide more detailed analysis of variation with the degree of chlorination. Examples could include:

- Targeted investigation of bioaccumulation in *Daphnia*,
- One or more fish dietary bioaccumulation studies performed using OECD TG 305,
- Measurements of human half-lives using biomonitoring studies, and/or
- Field studies which derive total body burdens for LCCPs in defined food webs with samples collected a the same time of year at a single location.

Further work with *Daphnia* is likely to be the most straightforward approach for reasons of ethics and cost.

8.3 Toxicity

Aquatic invertebrates appear to be the most sensitive trophic group, with a 21-day NOEC for *Daphnia* reproduction of 29 to 32 µg/L (and ≥2 µg/L) for a $C_{18–20}$, 52% Cl wt. product and ≥55 µg/L for a $C_{>20}$, 43% Cl wt. CP substance. These are higher than the REACH Annex XIII toxicity (T) criterion of 0.01 mg/L [10 µg/L].

Read across from the structural analogue MCCPs indicate the potential for classification as H362 (may cause harm to breast-fed children), based on the effect of MCCPs on vitamin K absorption leading to haemorrhaging in dams and pups. However, LCCPs 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.

There is therefore insufficient evidence to indicate that LCCPs meet the T criterion based on mammalian effects.

No standardised avian toxicity data are available. There is limited evidence of potential effects on thyroid in birds and fish embryos from non-standard studies on SCCPs, but no conclusion can be drawn for LCCPs.

The EU REACH registration concludes that LCCPs are not T.

The Environment Agency notes that the available studies do not cover all LCCP product types. Additional toxicity testing for daphnids covering specific chain lengths and chlorination levels would provide more relevant information for individual congener groups, starting with $C_{18–20}$ substances as the most bioavailable congeners.

8.4 Overall conclusion

The Environment Agency considers that LCCPs are P/vP, but further work is needed to establish whether some constituents are B or vB and T.

9 Conclusion and recommendations

A large amount of information is available for LCCPs, although much of the data is of doubtful or unknown reliability. The evidence is not straightforward to interpret and there are significant analytical challenges.

Further work could be done to provide more representative physicochemical property information for the congener groups that are present in LCCPs at different chlorination levels. In particular, new measured water solubility and log K_{OW} values could be useful for exposure modelling purposes and to help interpret the environmental fate and behaviour data, as well as provide more reliable solubility limits for ecotoxicity studies.

The evidence evaluated in this report indicates that LCCPs are (very) persistent and some constituents have significant bioaccumulation potential in aquatic and terrestrial organisms. Further work is needed to confirm the level of bioaccumulation of different congener groups (particularly $C_{18\text{-}20}$ CPs), and further investigation of bioaccumulation in daphnids might be an appropriate first step for animal welfare reasons. This could be combined with additional toxicity testing for this species to provide more relevant information for individual congener groups and chlorination levels.

Additional biomonitoring of terrestrial predatory organisms and their food items – and measurement of a half-life in humans – could be useful provided this does not raise ethical issues. Further guidance is required to enable more reliable interpretation of such monitoring data based on limited sample numbers and tissue types. Monitoring in remote areas would also provide evidence about whether constituents of the substance can travel over long distances (e.g. adsorbed to particulates).

The potential relevance of CFAMEs in a UK context should also be investigated. If they are present in the commercial substance or are environmental transformation products, further investigation of their toxicity may be warranted. This could include further *in vitro* toxicity testing as a first step to test their potential for endocrine disruption.

Analytical standards are needed for future work. In general, LCCP standards would significantly improve analytical methods, since currently technical mixtures, with all their limitations, are often used.

Depending how it is worded, the final POP conclusion for MCCPs may also affect some types of LCCP products. For example, $C_{18\text{-}20}$ LCCP products can contain up to 20% C_{17} congeners and <1% C_{16} congeners. This would need to be considered as a risk management issue.

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11 List of abbreviations

%	Percentage (parts per 100)
‰	Per Mille – Parts per thousand
B	Bioaccumulative
BCF	Bioconcentration factor
BMF	Biomagnification factor
ca.	Approximately (circa)
CAS	Chemical Abstracts Service
Congener	The same carbon chain length with a varying number of chlorine atoms
Congener groups	A discrete range of carbon chain lengths, usually with an averaged degree of chlorination
CLP	Classification, labelling and packaging (of substances and mixtures)
cm	Centimetre
d	Day
DegT50	Degradation half-life or transformation half-life (days)
DT50	Dissipation half-life (days)
dw	Dry weight
EC10	10% effect concentration
EC50	50% effect concentration
ECHA	European Chemicals Agency
EPA	Environmental Protection Agency
EU	European Union
g	Gramme
GC	Gas chromatography
GC/MS	Gas chromatography – mass spectrometry

GLP	Good laboratory practice
h	Hours
HLC	Henry's Law constant
Homologue	Identical chemical formula but different smiles code, i.e. a different order of atoms along the carbon chain
HPLC	High performance liquid chromatography
IUPAC	International Union of Pure and Applied Chemistry
kg	Kilogram
kJ	Kilojoule
km	Kilometre
KOW	n-Octanol-water partition coefficient
kPa	Kilopascal
k	Rate constants (day-1)
L	Litre
LC50	50% lethal effect concentration
LOD	Limit of detection
Log	Logarithmic value
LOQ	Limit of quantification
M	Molar
m/z	Mass to charge ratio (Daltons)
mg	Milligram
min	Minute
mL	Millilitre
mol	Mole
MS	Mass spectrometry
m/z	mass to charge ratio

nm	Nanometre
NOAEL	No observed adverse effect level
LOAEL	Lowest observed adverse effect level
NOEC	No-observed effect concentration
NOEL	No observed effect level
OECD	Organisation for Economic Co-operation and Development
p	Statistical probability
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
ppb	Parts per billion (1 µg/L)
ppm	Parts per million (1 mg/L)
psi	pounds per square inch
QSAR	Quantitative structure-activity relationship
OPERA	OPEn structure–activity/property Relationship App
r2	Correlation coefficient
REACH	Registration, Evaluation, Authorisation and restriction of Chemicals (EU Regulation No. 1907/2006)
rpm	Revolutions per minute
SMILES	Simplified Molecular Input Line Entry System
t	Tonne
T.E.S.T	Toxicity Estimation Software Tool
TG	Test Guideline
US EPA	United Stated Environmental Protection Agency
UV	Ultraviolet
vB	Very bioaccumulative
vP	Very persistent

vPvB	Very persistent and very bioaccumulative
WAF	Water Accommodated Fraction
wt.	Weight
ww	Wet weight
µg	Microgram

12 Appendix A: Literature search

Literature searches were undertaken by the Environment Agency between 15 December 2019 and to date (latest 10 July 2021) to identify published information relevant to the PBT assessment of LCCPs. The keywords listed in Table A.1 were searched for in SCOPUS (https://www.scopus.com), PubMed (https://pubmed.ncbi.nlm.nih.gov/) and Science Direct (https://www.sciencedirect.com/) to maximise the number of records identified. Keywords were based on the substance name only. The Environment Agency tailored the publications to those from 2009 to current.

Table A.1 Literature search terms and number of hits

Search terms	Scopus	PubMed	Science Direct
Chlorinated paraffin (chlorinated AND paraffin)	568	442	2 648
Long chain chlorinated paraffin (long AND chain AND chlorinated AND paraffin)	110	82	3 402
LCCP	150	51	1 402

The identified records were screened manually for relevance to this assessment based on the title and abstract. Articles identified as of potential interest were obtained and reviewed for relevance. Those that were found to be relevant are discussed in the appropriate sections of this report. Further articles that were not identified as part of the literature search have been included. These were sourced from references within the literature search articles and contained information relevant to this assessment.

The full list of records that were identified as relevant to this assessment are available as an excel spread sheet on request. Those identified as relevant but not used in this text have been highlighted in Appendix B and an explanation given for their omission.

13 Appendix B: Publications (2009 to present) that have not been evaluated in full

Several publications were identified for CPs during the literature search for which a decision was made not to evaluate the full paper following a review of the abstract. The reasons are provided in the table below.

Table B.1 Unevaluated publications (2009 – present)

Publication	Comment
Aamir M (2019) Congener-Specific Mother–Fetus Distribution, Placental Retention, and Transport of C10–13 and C14–17 Chlorinated Paraffins in Pregnant Women. Environmental Science & Technology (2019**)** 53 (19), 11458-11466. DOI: 10.1021/acs.est.9b02116	No LCCP data
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	No LCCP data
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.	No LCCP data
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	No LCCP data
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	No LCCP data

of publication: 10.12.2020. Project no: 15312-02. Client (s): MAREANO program. Program: Marine processes and human impact	
Brandsma SH, Brits M, Groenewoud QR, van Velzen MJM, Leonards PEG, de Boer J. Chlorinated Paraffins in Car Tires Recycled to Rubber Granulates and Playground Tiles. Environ Sci Technol. 2019;53(13):7595-7603.	No relevant data
BS EN ISO 18219-1 Leather - Determination of chlorinated hydrocarbons in leather. Part 1. Chromatographic method for short chain chlorinated paraffins (SCCP). Standard number 19/30390880 DC. 02 April 2019. Draft	No LCCP data
BS EN ISO 18219-2 Leather - Determination of chlorinated hydrocarbons in leather. Part 2: Chromatographic method for medium chain chlorinated paraffins (MCCP). Standard number 19/30360635 DC. 08 July 2019. Pending	No LCCP data
Chibwe L, Myers AL, De Silva AO, Reiner EJ, Jobst K, Muir D, Yuan B. C_{12-30} α-Bromo-Chloro "Alkenes": Characterization of a Poorly Identified Flame Retardant and Potential Environmental Implications. Environ Sci Technol. 2019 Sep 17;53(18):10835-10844. DOI: 10.1021/acs.est.9b03760.	Not directly relevant to LCCPs
Conn KE, Liedtke TL, Takesue RK, Dinicola RS. Legacy and current-use toxic contaminants in Pacific sand lance (Ammodytes personatus) from Puget Sound, Washington, USA. Mar Pollut Bull. 2020 Sep;158:111287. DOI: 10.1016/j.marpolbul.2020.111287.	Data included in Appendix H. Not discussed in text
Cui, Q., Yitao Pan, Hongxia Zhang, Nan Sheng, Jianshe Wang, Yong Guo, and Jiayin Dai. 2018. Occurrence and Tissue Distribution of Novel Perfluoroether Carboxylic and Sulfonic Acids and Legacy Per/Polyfluoroalkyl Substances in Black-Spotted Frog (Pelophylax nigromaculatus). Environmental Science & Technology 2018 52 (3), 982-990. DOI: 10.1021/acs.est.7b03662	No new data
De Boer, J., ElSayed A, T., Fiedler, H.L., Muir, D.C., Nikiforev, V.A., Tomt, G.T., Tsunemi, K. 2010. Chlorinated Paraffins in De Boar, J. (Ed.), The Handbook of Environmental Chemistry, Chlorinated Paraffins. Springer-Verlag, Berlin, Berlin/Heidelberg.	-

Drouillard, K.G., Tomy G. T., Muir, D.C.G. and K.J. Friesen. 1998a. Volatility of chlorinated n-alkanes (C10-12): Vapour pressures and Henry's Law constants. Environmental Toxicology and Chemistry, 17, 1252-1260.	No LCCP data
Drouillard, K.G., Hiebert, T., Tran, P., Tomy, G.T., Muir, D.C.G. and K.J. Friesen. 1998b. Estimating the aqueous solubilities of individual chlorinated n-alkanes (C10-12) from measurements of chlorinated alkane mixtures. Environmental Toxicology and Chemistry, 17, 1261-1267	No LCCP data
Garcia, VOS, Ivy, C, Fu, J. Syntopic frogs reveal different patterns of interaction with the landscape: A comparative landscape genetic study of Pelophylax nigromaculatus and Fejervarya limnocharis from central China. Ecol Evol. 2017; 7: 9294– 9306. https://DOI.org/10.1002/ece3.3459	Background information only
Green W, 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	No LCCP data
Houghton K L, 1993 Chlorocarbons, -Hydrocarbons (paraffins). Kirk-Othmer Encyclopedia of Chemical Technology, 4th Edition, Volume 6. John Wiley and Sons, Inc.	Background information only
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.	No LCCP data
Hao Z, Xu H, Feng Z, Zhang C, Zhou X, Wang Z, Zheng J, Zou X. Spatial distribution, deposition flux, and environmental impact of typical persistent organic pollutants in surficial sediments in the Eastern China Marginal Seas (ECMSs). J Hazard Mater. 2021 Apr 5;407:124343.	Not yet reviewed for relevance
Huang D, Gao L, Qiao L, Cui L, Xu C, Wang K, Zheng M. Concentrations of and risks posed by short-chain and medium-chain chlorinated paraffins in soil at a chemical industrial park on the southeast coast of China. Environ Pollut. 2020 Mar;258:113704.	No LCCP data

Huang X, Cui Z, Ding C, Su Q, Lin X, Wang W, Yin Q, Wang X. Differential Accumulation of Short-, Medium-, and Long-Chain Chlorinated Paraffin in Free-Range Laying Hens from an E-Waste Recycling Area. J Agric Food Chem. 2021 Sep 8;69(35):10329-10337. DOI: 10.1021/acs.jafc.1c04546.	Not yet reviewed for relevance
Li T, Wan Y, Gao S, Wang B, Hu J. High-Throughput Determination and Characterization of Short-, Medium-, and Long-Chain Chlorinated Paraffins in Human Blood. Environ Sci Technol. 2017 Mar 21;51(6):3346-3354. DOI: 10.1021/acs.est.6b05149.	No relevant data, method development
Mézière M, Marchand P, Larvor F, Baéza E, Le Bizec B, Dervilly G, Cariou R. Accumulation of short-, medium-, and long- chain chlorinated paraffins in tissues of laying hens after dietary exposure. Food Chem. 2021 Jul 30;351:129289. DOI: 10.1016/j.foodchem.2021.129289.	-
Mézière M, Marchand P, Hutinet S, Larvor F, Baéza E, Le Bizec B, Dervilly G, Cariou R. Transfer of short-, medium-, and long-chain chlorinated paraffins to eggs of laying hens after dietary exposure. Food Chem. 2021 May 1;343:128491. DOI: 10.1016/j.foodchem.2020.128491.	-
Moeckel C, Breivik K, Nøst TH, Sankoh A, Jones KC, Sweetman A. Soil pollution at a major West African E-waste recycling site: Contamination pathways and implications for potential mitigation strategies. Environ Int. 2020 Apr;137:105563.	No LCCP data
Pan X, Zhen X, Tian C, Tang J. Distributions, transports and fates of short- and medium-chain chlorinated paraffins in a typical river-estuary system. Sci Total Environ. 2021 Jan 10;751:141769. DOI: 10.1016/j.scitotenv.2020.141769.	Not yet reviewed for relevance
Ribbenstedt, A.; Mustajärvi, L.; Breitholtz, M.; Gorokhova, E.; Mayer, P.; Sobek, A. Passive dosing of triclosan in multigeneration tests with copepods − stable exposure concentrations and effects at the low µg/L range. Environ. Toxicol. Chem. 2017, 36 (5), 1254−1260.	No LCCP data
Smith, K. E. C.; Dom, N.; Blust, R.; Mayer, P. Controlling and maintaining exposure of hydrophobic organic compounds in aquatic toxicity tests by passive dosing. Aquat. Toxicol. 2010, 98 (1), 15−24	Background information only

Sprengel J, Vetter W. Chlorinated paraffins in hinges of kitchen appliances. Environ Monit Assess. 2021 Apr 7;193(5):250. DOI: 10.1007/s10661-021-09023-z.	Use pattern
Tong Li, Yi Wan, Shixiong Gao, Beili Wang, and Jianying Hu. 2017. High-Throughput Determination and Characterization of Short-, Medium-, and Long-Chain Chlorinated Paraffins in Human Blood. Environmental Science & Technology 51 (6), 3346-3354. DOI: 10.1021/acs.est.6b05149	Method development
Washington Department of Ecology, 2012. PBTs Analyzed in Bottom Fish from Four Washington Rivers and Lakes: Hexabromocyclododecane, Tetrabromobisphenol A, Chlorinated paraffins, Polybrominated Diphenylethers, Polychlorinated Naphthalenes, Perfluorinated Organic Compounds, Lead, And Cadmium, Washington Department of Ecology Publication 12-03-042 http://refhub.elsevier.com/S0025-326X(20)30405-7/rf0330	Data included in Appendix H. Not discussed in text
Wei GL, Liang XL, Li DQ, Zhuo MN, Zhang SY, Huang QX, Liao YS, Xie ZY, Guo TL, Yuan ZJ. Occurrence, fate and ecological risk of chlorinated paraffins in Asia: A review. Environ Int. 2016 Jul-Aug;92-93:373-87	Review paper, no new data
Xia D, Vaye O, Yang Y, Zhang H, Sun Y. Spatial distributions, source apportionment and ecological risks of C_9-C_{17} chlorinated paraffins in mangrove sediments from Dongzhai Harbor, Hainan Island. Environ Pollut. 2021 Feb 1;270:116076.	No LCCP data
Yuan B, McLachlan MS, Roos AM, Simon M, Strid A, and de Wit CA. Long-Chain Chlorinated Paraffins Have Reached the Arctic. Environmental Science & Technology Letters 2021 8 (9), 753-759. DOI: 10.1021/acs.estlett.1c00470	Data included in Appendix H. Not discussed in text
Yuan B, Tay JH, Padilla-Sánchez JA, Papadopoulou E, Haug LS, de Wit CA. Human Exposure to Chlorinated Paraffins via Inhalation and Dust Ingestion in a Norwegian Cohort. Environ Sci Technol. 2021 Jan 19;55(2):1145-1154. DOI: 10.1021/acs.est.0c05891.	Human exposure - not relevant to PBT assessment
Yuan S, Wang M, Lv B, Wang J. Transformation pathways of chlorinated paraffins relevant for remediation: a mini review. Environ Sci Pollut Res Int. 2021 Feb;28(8):9020-9028. DOI: 10.1007/s11356-021-12469-w.	Remediation

14 Appendix C: Global LCCP inventory

This list has been provided by representatives of the EU REACH LCCPs Consortium (Personal Communication, 2019).

Table C.1 Global LCCP Inventory from the CAS registry

CAS No.	CAS name	Note	Regulatory Regions
61788-76-9[a]	Alkanes, chloro; alkanes, chlorinated	c	[1a], [1c], [2], [3], [4], [5a], [6a], [7], [8], [10], [11], [12]
63449-39-8[b]	Paraffin waxes and hydrocarbon waxes, chloro	b	[1a], [1b], [1c], [2], [3], [4], [5a], [6a], [6b], [7], [8], [9], [10], [11], [12]
68920-70-7	Alkanes, C_{6-18}, chloro	a	[1a], [1b], [1c], [2], [3], [4], [5a], [6a], [7], [8], [12]
71011-12-6	Alkanes, C_{12-13}, chloro	d	[2], [3], [5a]
84082-38-2	Alkanes, C_{10-21}, chloro	a	[1a], [1c], [3], [4], [5a], [7], [8], [9], [12]
84776-06-7	Alkanes, C_{10-32}, chloro	a	[1a], [1c], [3], [4], [5a], [7], [8], [9], [12]
84776-07-8	Alkanes, C_{16-27}, chloro	a	[1a]
85049-26-9	Alkanes, C_{16-35}, chloro	a	[1a], [4]
85422-92-0	Paraffin oils and hydrocarbon oils, chloro	c	[1a], [9]
85535-84-8	Alkanes, C_{10-13}, chloro	d	[1a], [1b][c], [1c], [3], [4], [5a], [6a], [7], [8], [12]
85535-85-9	Alkanes, C_{14-17}, chloro	b	[1a], [1b], [1c], [2], [3], [4], [5a], [5b], [7], [8], [9], [10], [12]
85535-86-0	Alkanes, C_{18-28}, chloro	a	[1a], [3], [4], [6a], [7], [9]
85536-22-7	Alkanes, C_{12-14}, chloro	a	[1a], [3], [4], [6a], [9], [12]
85681-73-8	Alkanes, C_{10-14}, chloro	a	[1a], [5a]
97553-43-0	Paraffins (petroleum), normal $C_{>10}$, chloro	a	[1a], [5a]
97659-46-6	Alkanes, C_{10-26}, chloro	a	[1a], [9]
106232-85-3	Alkanes, C_{18-20}, chloro	b	[2], [3], [4], [5a], [9], [10], [12]
106232-86-4	Alkanes, C_{22-40}, chloro	a	[1a], [4], [9]
108171-26-2	Alkanes, C_{10-12}, chloro	a	[1a], [7], [8], [9]
108171-27-3	Alkanes, C_{22-26}, chloro	a	[1a], [5a] [12]

288260-42-4	Alkanes, C_{22-30}, chloro	b	[2], [7]
198840-65-2	Tetradecane, chloro derivatives	b	[2]
1372804-76-6	Alkanes, C_{14-16}, chloro	b	[2]
2097144-48-2	Octadecane, chloro derivatives	b	[2]
2097144-45-9	Alkanes, C_{20-24}, chloro	b	[2]
2097144-43-7	Alkanes, C_{20-28}, chloro	b	[2]
2097144-44-8	Slackwax (petroleum), chloro	b	[2]
1417900-96-9	Alkanes, C_{21-34}-branched and linear, chloro	b	[2]
1401974-24-0	Alkanes, C_{22-30}-branched and linear, chloro	b	[2]
1402738-52-6	Alkanes, C_{24-28}, chloro	b	[2]
2097144-46-0	Hexacosane, chloro derivatives	b	[2]
2097144-47-1	Octacosane, chloro derivatives	b	[2]

[a]CAS 61788-76-9 replaces 11104-09-9, 12633-77-1, 51059-93-9, 53572-39-7 and 69430-53-1: [b]CAS 63449-39-8 replaces 8029-39-8, 11098-33-2, 37187-40-9, 39279-65-7, 39406-09-2, 39444-36-5, 50646-90-7, 51990-12-6, 52276-52-5, 52555-47-2, 52622-66-9, 52677-73-3, 52677-74-4, 52677-75-5, 53028-59-4, 53028-60-7, 53200-35-4, 54577-71-8, 55353-50-9, 56509-64-9, 56730-95-1, 58516-52-2, 60202-64-4, 66746-35-8 and 108688-63-7: [c]withdrawn

Note: a - Listed on at least one national inventory; b - Registered under legislation requiring dossier submission in 21st century; c - Broad scope with no carbon number definition (not favoured by some authorities); d - Subject to ban or restriction, substance of very high concern (EU) or Toxic Release Inventory requirement (USA).

Regulatory Regions: [1a] EU REACH pre-registered; [1b] EU REACH registered; [1c] EU CLP Inventory [2] USA TSCA (active list); [3] Canada DSL; [4] Australia (AICS); [5a] Korean Gazette No.; [5b] Korean REACH registered; [6a] Japan ENCS; [6b] Japan examined; [7] Philippines; [8] New Zealand; [9] Taiwan; [10] Turkey; [11] Switzerland; [12] China

15 Appendix D: Theoretical chlorine contents of LCCPs defined by carbon chain length

Table D.1 Molecular formula of chlorinated paraffins for chain lengths C_{18-30} with varying chlorination degrees

% Cl wt.	C_{18}	C_{19}	C_{20}	C_{21}	C_{22}	C_{23}	C_{24}	C_{25}	C_{26}	C_{27}	C_{28}	C_{29}	C_{30}	C_{31}	C_{32}
30-40	$C_{18}H_{34}Cl_4$	$C_{19}H_{36}Cl_4$	$C_{20}H_{38}Cl_4$ $C_{20}H_{37}Cl_5$	$C_{21}H_{40}Cl_4$ $C_{21}H_{39}Cl_5$	$C_{22}H_{42}Cl_4$ $C_{22}H_{41}Cl_5$	$C_{23}H_{44}Cl_4$ $C_{23}H_{43}Cl_5$	$C_{24}H_{45}Cl_5$ $C_{24}H_{44}Cl_6$	$C_{25}H_{47}Cl_5$ $C_{25}H_{46}Cl_6$	$C_{26}H_{49}Cl_5$ $C_{26}H_{48}Cl_6$	$C_{27}H_{51}Cl_5$ $C_{27}H_{50}Cl_6$ $C_{27}H_{49}Cl_7$	$C_{28}H_{53}Cl_5$ $C_{28}H_{52}Cl_6$ $C_{28}H_{51}Cl_7$	$C_{29}H_{55}Cl_5$ $C_{29}H_{54}Cl_6$ $C_{29}H_{53}Cl_7$	$C_{30}H_{56}Cl_6$ $C_{30}H_{55}Cl_7$	$C_{31}H_{58}Cl_6$ $C_{31}H_{57}Cl_7$ $C_{31}H_{56}Cl_8$	$C_{32}H_{60}Cl_6$ $C_{32}H_{59}Cl_7$ $C_{32}H_{58}Cl_8$
40-55	$C_{18}H_{33}Cl_5$ $C_{18}H_{32}Cl_6$ $C_{18}H_{31}Cl_7$ $C_{18}H_{30}Cl_8$	$C_{19}H_{35}Cl_5$ $C_{19}H_{34}Cl_6$ $C_{19}H_{33}Cl_7$ $C_{19}H_{32}Cl_8$	$C_{20}H_{36}Cl_6$ $C_{20}H_{35}Cl_7$ $C_{20}H_{34}Cl_8$ $C_{20}H_{33}Cl_9$	$C_{21}H_{38}Cl_6$ $C_{21}H_{37}Cl_7$ $C_{21}H_{36}Cl_8$ $C_{21}H_{35}Cl_9$	$C_{22}H_{40}Cl_6$ $C_{22}H_{39}Cl_7$ $C_{22}H_{38}Cl_8$ $C_{22}H_{37}Cl_9$ $C_{22}H_{36}Cl_{10}$	$C_{23}H_{42}Cl_6$ $C_{23}H_{41}Cl_7$ $C_{23}H_{40}Cl_8$ $C_{23}H_{39}Cl_9$ $C_{23}H_{38}Cl_{10}$	$C_{24}H_{43}Cl_7$ $C_{24}H_{42}Cl_8$ $C_{24}H_{41}Cl_9$ $C_{24}H_{40}Cl_{10}$ $C_{24}H_{39}Cl_{11}$	$C_{25}H_{45}Cl_7$ $C_{25}H_{44}Cl_8$ $C_{25}H_{43}Cl_9$ $C_{25}H_{42}Cl_{10}$ $C_{25}H_{41}Cl_{11}$	$C_{26}H_{47}Cl_7$ $C_{26}H_{46}Cl_8$ $C_{26}H_{45}Cl_9$ $C_{26}H_{44}Cl_{10}$ $C_{26}H_{43}Cl_{11}$ $C_{26}H_{42}Cl_{12}$	$C_{27}H_{48}Cl_8$ $C_{27}H_{47}Cl_9$ $C_{27}H_{46}Cl_{10}$ $C_{27}H_{45}Cl_{11}$ $C_{27}H_{44}Cl_{12}$	$C_{28}H_{50}Cl_8$ $C_{28}H_{49}Cl_9$ $C_{28}H_{48}Cl_{10}$ $C_{28}H_{47}Cl_{11}$ $C_{28}H_{46}Cl_{12}$ $C_{28}H_{45}Cl_{13}$	$C_{29}H_{52}Cl_8$ $C_{29}H_{51}Cl_9$ $C_{29}H_{50}Cl_{10}$ $C_{29}H_{49}Cl_{11}$ $C_{29}H_{48}Cl_{12}$ $C_{29}H_{47}Cl_{13}$	$C_{30}H_{54}Cl_8$ $C_{30}H_{53}Cl_9$ $C_{30}H_{52}Cl_{10}$ $C_{30}H_{51}Cl_{11}$ $C_{30}H_{50}Cl_{12}$ $C_{30}H_{49}Cl_{13}$ $C_{30}H_{48}Cl_{14}$	$C_{31}H_{55}Cl_9$ $C_{31}H_{54}Cl_{10}$ $C_{31}H_{53}Cl_{11}$ $C_{31}H_{52}Cl_{12}$ $C_{31}H_{51}Cl_{13}$ $C_{31}H_{50}Cl_{14}$	$C_{32}H_{57}Cl_9$ $C_{32}H_{56}Cl_{10}$ $C_{32}H_{55}Cl_{11}$ $C_{32}H_{54}Cl_{12}$ $C_{32}H_{53}Cl_{13}$ $C_{32}H_{52}Cl_{14}$ $C_{32}H_{51}Cl_{15}$
55-70	$C_{18}H_{29}Cl_9$ $C_{18}H_{28}Cl_{10}$ $C_{18}H_{27}Cl_{11}$ $C_{18}H_{26}Cl_{12}$ $C_{18}H_{25}Cl_{13}$ $C_{18}H_{24}Cl_{14}$ $C_{18}H_{23}Cl_{15}$	$C_{19}H_{31}Cl_9$ $C_{19}H_{30}Cl_{10}$ $C_{19}H_{29}Cl_{11}$ $C_{19}H_{28}Cl_{12}$ $C_{19}H_{27}Cl_{13}$ $C_{19}H_{26}Cl_{14}$ $C_{19}H_{25}Cl_{15}$ $C_{19}H_{24}Cl_{16}$	$C_{20}H_{32}Cl_{10}$ $C_{20}H_{31}Cl_{11}$ $C_{20}H_{30}Cl_{12}$ $C_{20}H_{29}Cl_{13}$ $C_{20}H_{28}Cl_{14}$ $C_{20}H_{27}Cl_{15}$ $C_{20}H_{26}Cl_{16}$ $C_{20}H_{25}Cl_{17}$	$C_{21}H_{34}Cl_{10}$ $C_{21}H_{33}Cl_{11}$ $C_{21}H_{32}Cl_{12}$ $C_{21}H_{31}Cl_{13}$ $C_{21}H_{30}Cl_{14}$ $C_{21}H_{29}Cl_{15}$ $C_{21}H_{28}Cl_{16}$ $C_{21}H_{27}Cl_{17}$ $C_{21}H_{26}Cl_{18}$	$C_{22}H_{35}Cl_{11}$ $C_{22}H_{34}Cl_{12}$ $C_{22}H_{33}Cl_{13}$ $C_{22}H_{32}Cl_{14}$ $C_{22}H_{31}Cl_{15}$ $C_{22}H_{30}Cl_{16}$ $C_{22}H_{29}Cl_{17}$ $C_{22}H_{28}Cl_{18}$ $C_{22}H_{27}Cl_{19}$	$C_{23}H_{37}Cl_{11}$ $C_{23}H_{36}Cl_{12}$ $C_{23}H_{35}Cl_{13}$ $C_{23}H_{34}Cl_{14}$ $C_{23}H_{33}Cl_{15}$ $C_{23}H_{32}Cl_{16}$ $C_{23}H_{31}Cl_{17}$ $C_{23}H_{30}Cl_{18}$ $C_{23}H_{29}Cl_{19}$ $C_{23}H_{28}Cl_{20}$	$C_{24}H_{38}Cl_{12}$ $C_{24}H_{37}Cl_{13}$ $C_{24}H_{36}Cl_{14}$ $C_{24}H_{35}Cl_{15}$ $C_{24}H_{34}Cl_{16}$ $C_{24}H_{33}Cl_{17}$ $C_{24}H_{32}Cl_{18}$ $C_{24}H_{31}Cl_{19}$ $C_{24}H_{30}Cl_{20}$	$C_{25}H_{40}Cl_{12}$ $C_{25}H_{39}Cl_{13}$ $C_{25}H_{38}Cl_{14}$ $C_{25}H_{37}Cl_{15}$ $C_{25}H_{36}Cl_{16}$ $C_{25}H_{35}Cl_{17}$ $C_{25}H_{34}Cl_{18}$ $C_{25}H_{33}Cl_{19}$ $C_{25}H_{32}Cl_{20}$ $C_{25}H_{31}Cl_{21}$	$C_{26}H_{41}Cl_{13}$ $C_{26}H_{40}Cl_{14}$ $C_{26}H_{39}Cl_{15}$ $C_{26}H_{38}Cl_{16}$ $C_{26}H_{37}Cl_{17}$ $C_{26}H_{36}Cl_{18}$ $C_{26}H_{35}Cl_{19}$ $C_{26}H_{34}Cl_{20}$ $C_{26}H_{33}Cl_{21}$ $C_{26}H_{32}Cl_{22}$	$C_{27}H_{43}Cl_{13}$ $C_{27}H_{42}Cl_{14}$ $C_{27}H_{41}Cl_{15}$ $C_{27}H_{40}Cl_{16}$ $C_{27}H_{39}Cl_{17}$ $C_{27}H_{38}Cl_{18}$ $C_{27}H_{37}Cl_{19}$ $C_{27}H_{36}Cl_{20}$ $C_{27}H_{35}Cl_{21}$ $C_{27}H_{34}Cl_{22}$ $C_{27}H_{33}Cl_{23}$	$C_{28}H_{44}Cl_{14}$ $C_{28}H_{43}Cl_{15}$ $C_{28}H_{42}Cl_{16}$ $C_{28}H_{41}Cl_{17}$ $C_{28}H_{40}Cl_{18}$ $C_{28}H_{39}Cl_{19}$ $C_{28}H_{38}Cl_{20}$ $C_{28}H_{37}Cl_{21}$ $C_{28}H_{36}Cl_{22}$ $C_{28}H_{35}Cl_{23}$ $C_{28}H_{34}Cl_{24}$	$C_{29}H_{46}Cl_{14}$ $C_{29}H_{45}Cl_{15}$ $C_{29}H_{44}Cl_{16}$ $C_{29}H_{43}Cl_{17}$ $C_{29}H_{42}Cl_{18}$ $C_{29}H_{41}Cl_{19}$ $C_{29}H_{40}Cl_{20}$ $C_{29}H_{39}Cl_{21}$ $C_{29}H_{38}Cl_{22}$ $C_{29}H_{37}Cl_{23}$ $C_{29}H_{36}Cl_{24}$ $C_{29}H_{35}Cl_{25}$	$C_{30}H_{47}Cl_{15}$ $C_{30}H_{46}Cl_{16}$ $C_{30}H_{45}Cl_{17}$ $C_{30}H_{44}Cl_{18}$ $C_{30}H_{43}Cl_{19}$ $C_{30}H_{42}Cl_{20}$ $C_{30}H_{41}Cl_{21}$ $C_{30}H_{40}Cl_{22}$ $C_{30}H_{39}Cl_{23}$ $C_{30}H_{38}Cl_{24}$ $C_{30}H_{37}Cl_{25}$ $C_{30}H_{36}Cl_{26}$	$C_{31}H_{49}Cl_{15}$ $C_{31}H_{48}Cl_{16}$ $C_{31}H_{47}Cl_{17}$ $C_{31}H_{46}Cl_{18}$ $C_{31}H_{45}Cl_{19}$ $C_{31}H_{44}Cl_{20}$ $C_{31}H_{43}Cl_{21}$ $C_{31}H_{42}Cl_{22}$ $C_{31}H_{41}Cl_{23}$ $C_{31}H_{40}Cl_{24}$ $C_{31}H_{39}Cl_{25}$ $C_{31}H_{38}Cl_{26}$	$C_{32}H_{50}Cl_{16}$ $C_{32}H_{49}Cl_{17}$ $C_{32}H_{48}Cl_{18}$ $C_{32}H_{47}Cl_{19}$ $C_{32}H_{46}Cl_{20}$ $C_{32}H_{45}Cl_{21}$ $C_{32}H_{44}Cl_{22}$ $C_{32}H_{43}Cl_{23}$ $C_{32}H_{42}Cl_{24}$ $C_{32}H_{41}Cl_{25}$ $C_{32}H_{40}Cl_{26}$ $C_{32}H_{39}Cl_{27}$
>70	$C_{18}H_{22}Cl_{16}$ and > Cl atoms	$C_{19}H_{23}Cl_{17}$ and > Cl atoms	$C_{20}H_{24}Cl_{18}$ and > Cl atoms	$C_{21}H_{25}Cl_{19}$ and > Cl atoms	$C_{22}H_{26}Cl_{20}$ and > Cl atoms	$C_{23}H_{27}Cl_{21}$ and > Cl atoms	$C_{24}H_{29}Cl_{21}$ and > Cl atoms	$C_{25}H_{30}Cl_{22}$ and > Cl atoms	$C_{26}H_{31}Cl_{23}$ and > Cl atoms	$C_{27}H_{32}Cl_{24}$ and > Cl atoms	$C_{28}H_{33}Cl_{25}$ and > Cl atoms	$C_{29}H_{34}Cl_{26}$ and > Cl atoms	$C_{30}H_{35}Cl_{27}$ and > Cl atoms	$C_{31}H_{37}Cl_{27}$ and > Cl atoms	$C_{32}H_{38}Cl_{28}$ and > Cl atoms

Table D.2 Molecular weights of LCCPs (determined from carbon chain length and number of associated chlorine atoms)

No. Cl atoms	C_{18}	C_{19}	C_{20}	C_{21}	C_{22}	C_{23}	C_{24}	C_{25}	C_{26}	C_{27}	C_{28}	C_{29}	C_{30}	C_{31}	C_{32}
4	392	406	420	434	448	462	476	490	504	518	532	546	560	574	588
5	426	440	454	468	482	496	510	524	538	552	566	580	594	608	622
6	461	475	489	503	517	531	545	559	573	587	601	615	629	643	657
7	495	509	523	537	551	565	579	593	607	621	635	649	663	677	691
8	530	544	558	572	586	600	614	628	642	656	670	684	698	712	726
9	564	578	592	606	620	634	648	662	676	690	704	718	732	746	760
10	599	613	627	641	655	669	683	697	711	725	739	753	767	781	795
11	633	647	661	675	689	703	717	731	745	759	773	787	801	815	829
12	667	681	695	709	723	737	751	765	779	793	807	821	835	849	863
13	702	716	730	744	758	772	786	800	814	828	842	856	870	884	898
14	736	750	764	778	792	806	820	834	848	862	876	890	904	918	932
15	771	785	799	813	827	841	855	869	883	897	911	925	939	953	967
16	805	819	833	847	861	875	889	903	917	931	945	959	973	987	1001
17	840	854	868	882	896	910	924	938	952	966	980	994	1008	1022	1036
18		888	902	916	930	944	958	972	986	1000	1014	1028	1042	1056	1070
19			937	951	965	979	993	1007	1021	1035	1049	1063	1077	1091	1105
20				985	999	1013	1027	1041	1055	1069	1083	1097	1111	1125	1139
21					1033	1047	1061	1075	1089	1103	1117	1131	1145	1159	1173
22						1082	1096	1110	1124	1138	1152	1166	1180	1194	1208
23							1130	1144	1158	1172	1186	1200	1214	1228	1242
24								1179	1193	1207	1221	1235	1249	1263	1277
25									1227	1241	1255	1269	1283	1297	1311
26										1276	1290	1304	1318	1332	1346
27											1324	1338	1352	1366	1380
28												1373	1387	1401	1415

Note: Greyed out cells indicate molecular weights that exceed 1 100 g/mol

Table D.3 Percentage chlorine by weight of LCCPs (Carbon Chain Length/ % Cl wt)

No. Cl atoms	C_{18}	C_{19}	C_{20}	C_{21}	C_{22}	C_{23}	C_{24}	C_{25}	C_{26}	C_{27}	C_{28}	C_{29}	C_{30}	C_{31}	C_{32}
4	36	35	34	33	32	31	30	29	28	27	27	26	25	25	24
5	42	40	39	38	37	36	35	34	33	32	31	31	30	29	28
6	46	45	44	42	41	40	39	38	37	36	35	35	34	33	32
7	50	49	47	46	45	44	43	42	41	40	39	38	37	37	36
8	54	52	51	50	48	47	46	45	44	43	42	41	41	40	39
9	57	55	54	53	51	50	49	48	47	46	45	44	44	43	42
10	59	58	57	55	54	53	52	51	50	49	48	47	46	45	45
11	62	60	59	58	57	55	54	53	52	51	50	50	49	48	47
12	64	62	61	60	59	58	57	56	55	54	53	52	51	50	49
13	66	64	63	62	61	60	59	58	57	56	55	54	53	52	51
14	67	66	65	64	63	62	61	59	59	58	57	56	55	54	53
15	69	68	67	65	64	63	62	61	60	59	58	58	57	56	55
16	70	69	68	67	66	65	64	63	62	61	60	59	58	57	57
17	72	71	69	68	67	66	65	64	63	62	62	61	60	59	58
18		72	71	70	69	68	67	66	65	64	63	62	61	60	60
19			72	71	70	69	68	67	66	65	64	63	63	62	61
20				72	71	70	69	68	67	66	65	65	64	63	62
21					72	71	70	69	68	67	67	66	65	64	63
22						72	71	70	69	69	68	67	66	65	65
23							72	71	70	70	69	68	67	66	66
24								72	71	71	70	69	68	67	67
25									72	71	71	70	69	68	68
26										72	71	71	70	69	68
27											72	72	71	70	69

Note: Greyed out cells indicate molecular weights that exceed 1 100 g/mol

16 Appendix E: Estimated physico-chemical properties of selected LCCP congeners

The Environment Agency used the US EPA EPI Suite™ programme (US EPA, 2012) to estimate vapour pressure, water solubility and log K_{ow} values for a selected distribution of LCCP congeners with even chlorination.

Table E.1 Estimated vapour pressure, water solubility and log K_{OW} of a selected distribution of evenly chlorinated LCCPs

Formula	% Cl. wt.	Molecular weight	Vapour pressure[1] (Pa at 25 °C)	Water solubility[2] (mg/L at 25 °C)	Log K_{ow}[3]
$C_{18}H_{33}Cl_5$	41.6	426.73	2.48×10^{-4}	1.45×10^{-5}	10.23
$C_{18}H_{30}Cl_8$	53.6	530.06	2.54×10^{-5}	3.04×10^{-6}	10.7
$C_{20}H_{36}Cl_6$	43.6	489.23	5.14×10^{-5}	9.53×10^{-7}	11.32
$C_{20}H_{33}Cl_9$	53.9	592.56	2.36×10^{-6}	1.65×10^{-7}	11.86
$C_{25}H_{45}Cl_7$	41.9	593.81	6.31×10^{-7}	1.60×10^{-9}	13.96
$C_{25}H_{42}Cl_{10}$	50.9	697.14	2.68×10^{-8}	2.69×10^{-10}	14.5
$C_{25}H_{29}Cl_{23}$	71.3	1 144.93	3.35×10^{-15}	1.98×10^{-14}	16.84
$C_{30}H_{53}Cl_9$	43.6	732.83	2.38×10^{-9}	1.43×10^{-12}	16.77
$C_{30}H_{49}Cl_{13}$	53.0	870.61	1.37×10^{-11}	1.08×10^{-13}	17.57
$C_{30}H_{35}Cl_{27}$	70.8	1 352.84	3.69×10^{-19}	3.94×10^{-18}	20.09

Note: [1], [2] WSKOW v 1.41; [3]KOWWIN v 1.67

Table E.2 **Estimated vapour pressure, Henry's law constant, log K_{AW}, log K_{OA}, Water solubility, log K_{OW}, Boiling point, Second order rate constant for air degradation with OH radicals, and log K_{OC}, determined using COSMOtherm modelling software (Personal communication, 2021, Juliane Glüge).**

Formula	Homogenous or preferential terminal chlorination	% Cl. wt.	Molecular weight	Vapour pressure (Pa at 25 °C)	Henry's Law Constant in water ($Pa.m^3/mol$)	Log K_{AW}	Henry's Law Constant in octanol	Log K_{OA}	Water solubility[2] (mg/L at 25 °C)	Log k_{ow} (wet octanol)	Log k_{ow} (dry octanol)	Boiling point (°C)	Second order rate constant for air degradation with OH radicals (cm^3/s)	Log K_{oc}
$C_{14}H_{24}Cl_6$	Homogenous	53	405	$7.05x10^{-6}$	$2.86x10^{-2}$	-4.93	$1.15x10^{-8}$	11.33	$9.99x10^{-2}$	6.274	6.397	449	$2.24x10^{-12}$	5.2656
$C_{14}H_{24}Cl_6$	Terminal	53	405	$8.20x10^{-6}$	$6.78x10^{-2}$	-4.56	$1.16x10^{-8}$	11.33	$4.90x10^{-2}$	6.602	6.766	453	$2.62x10^{-12}$	5.538
$C_{14}H_{24}Cl_6$	Terminal	53	405	$7.24x10^{-7}$	$5.41x10^{-3}$	-5.65	$1.83x10^{-9}$	12.13	$5.41x10^{-2}$	6.33	6.47	489	$3.18x10^{-12}$	5.249
$C_{17}H_{29}Cl_7$	Homogenous	52	481	$2.63x10^{-8}$	$4.56x10^{-3}$	-5.73	$3.73x10^{-12}$	13.67	$2.77x10^{-3}$	7.74	7.93	519	$2.47x10^{-12}$	6.193
$C_{18}H_{33}Cl_5$	Homogenous	42	426	$3.72x10^{-8}$	$9.51x10^{-3}$	-5.41	$1.52x10^{-10}$	13.21	$1.67x10^{-3}$	7.636	7.797	515	$4.33x10^{-12}$	5.327
$C_{18}H_{33}Cl_5$	Terminal	42	426	$2.22x10^{-8}$	$3.94x10^{-2}$	-4.79	$4.85x10^{-11}$	13.71	$2.40x10^{-4}$	8.672	8.911	519	$6.54x10^{-12}$	5.815
$C_{18}H_{22}Cl_{16}$	Terminal	70	805	$3.28x10^{-13}$	$3.77x10^{-5}$	-7.81	$1.42x10^{-16}$	19.24	$4.90x10^{-6}$	11.172	11.425	639	$8.90x10^{-13}$	9.687
$C_{18}H_{22}Cl_{16}$	Terminal	70	805	$2.94x10^{-13}$	$3.83x10^{-5}$	-7.8	$2.01x10^{-16}$	19.09	$6.19x10^{-6}$	11.012	11.281	657	$1.18x10^{-12}$	9.497
$C_{20}H_{36}Cl_6$	Homogenous	44	489	$9.68x10^{-10}$	$3.7x10^{-3}$	-5.82	$3.73x10^{-12}$	14.82	$1.28x10^{-4}$	8.78	9.00	555	$4.52x10^{-12}$	6.076
$C_{20}H_{36}Cl_6$	Terminal	44	489	$9.39x10^{-9}$	$2.54x10^{-3}$	-5.98	$6.87x10^{-13}$	15.56	$3.81x10^{-5}$	9.317	9.568	572	$6.11x10^{-12}$	6.277
$C_{20}H_{36}Cl_6$	Terminal	44	489	$9.39x10^{-9}$	$7.02x10^{-1}$	-3.54	$8.72x10^{-12}$	14.45	$6.54x10^{-6}$	10.567	10.907	514	$8.88x10^{-12}$	7.443
$C_{20}H_{24}Cl_{18}$	Homogenous	70	902	$6.89x10^{-14}$	$4.88x10^{-5}$	-7.70	$4.34x10^{-17}$	19.76	$5.28x10^{-7}$	11.82	12.05	637	$882x10^{-13}$	9.432
$C_{20}H_{24}Cl_{18}$	Terminal	70	902	$9.23x10^{-16}$	$1.35x10^{-6}$	-9.26	$8.83x10^{-19}$	21.45	$3.6x10^{-7}$	11.922	12.185	694	$1.16x10^{-12}$	9.973
$C_{25}H_{45}Cl_7$	Homogenous	42	594	$1.14x10^{-13}$	$1.76x10^{-4}$	-7.14	$6.17x10^{-16}$	18.6	$3.84x10^{-7}$	11.14	11.46	641	$5.75x10^{-12}$	7.345
$C_{25}H_{29}Cl_{23}$	Homogenous	71	1145	$3.05x10^{-19}$	$4.61x10^{-7}$	-9.72	$3.09x10^{-22}$	24.9	$1.40x10^{-10}$	14.93	15.17	760	$1.17x10^{-12}$	12.374

Table E.3 Estimated BCF values of selected LCCPs using EPISuite™ v4.1 software (US EPA, 2012) for BCFBAF (V3.01) (L/kg wet-wt) and VEGA v1.2.8 software (IRCCS, 2021) for Arnot-Gobas v1.0.0 (L/Kg), CAESAR V2.1.14 (L/Kg) and Meylan V1.0.2 (L/kg)

Chemical formula	SMILES	% Cl. wt.	Molecular weight	BCFBAF (v3.01) (L/kg wet-wt)	Arnot-Gobas v1.0.0 (L/kg)	CAESAR v2.1.14 (L/kg)	Meylan v1.0.3 (L/kg)
$C_{18}H_{30}Cl_8$	CC(CC(CC(CCCC(CC(CC(C(CCCCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	53.6	530.06	51.9	10	1	205
$C_{18}H_{33}Cl_5$	C(CCC(CCCCC(CCCCC(CCCl)Cl)Cl)Cl)CCCl	41.6	426.73	87.99	17	4	348
$C_{20}H_{33}Cl_9$	CC(C(CCC(CCC(C(CCCC(C(CCC(CCCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	53.9	592.56	13.98	2	4	55
$C_{20}H_{36}Cl_6$	CC(CCC(CCC(CCCC(CCCC(CCCCCl)Cl)Cl)Cl)Cl)Cl	43.6	489.23	25.75	3	13	102
$C_{25}H_{29}Cl_{23}$	CC(C(C(C(C(C(C(C(C(C(C(CC(C(C(C(C(C(C(C(C(C(CCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	71.3	1144.93	3.16	0.93	1	3
$C_{25}H_{42}Cl_{10}$	CC(C(CCC(CCCC(C(CCC(CCCC(CCC(C(CCCCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	50.9	697.14	3.16	0.94	3	3
$C_{25}H_{45}Cl_7$	CC(CCCC(CCCC(CCCC(CCCC(CCCC(CCCCl)Cl)Cl)Cl)Cl)Cl)Cl	41.9	593.81	5.2	0.94	5	5
$C_{30}H_{35}Cl_{27}$	C(C(C(C(CC(C(C(C(C(C(C(CCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)C(C(C(C(C(C(C(CC(C(C(C(C(C(C(CCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	70.8	1352.84	3.16	0.93	0.77	3
$C_{30}H_{49}Cl_{13}$	C(CCCl)CC(C(CC(C(CCCC(C(CCC(CCCC(CCC(C(CCCC(CCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	53	870.61	3.16	0.93	1	3
$C_{30}H_{53}Cl_9$	CC(CCCC(CCCC(CCCC(CCC(C(CCCC(CCCC(CCCCCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	43.6	732.83	3.16	0.93	3	3

Table E.4 Physicochemical indicators to identify substances with limited bioaccumulation potential/hindered uptake due to their molecular size have been developed as part of the PBT assessment. Table is adapted from Environment Agency (2009b).

Chlorinated paraffin	SMILES	MW (Da)	$D_{max\ ave}$[a] (Å[b])
$C_{18}H_{30}Cl_8$	CC(CC(CC(CCCC(CC(CC(C(CCCCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	530.06	51.9
$C_{18}H_{33}Cl_5$	C(CCC(CCCCC(CCCCC(CCCl)Cl)Cl)Cl)CCCl	426.73	87.99
$C_{20}H_{33}Cl_9$	CC(C(CCC(CCC(C(CCCC(C(CCC(CCCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	592.56	13.98
$C_{20}H_{36}Cl_6$	CC(CCC(CCC(CCCC(CCCC(CCCCCl)Cl)Cl)Cl)Cl)Cl	489.23	25.75
$C_{25}H_{29}Cl_{23}$	CC(C(C(C(C(C(C(C(C(C(C(CC(C(C(C(C(C(C(C(C(C(C(CCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	1144.93	3.16
$C_{25}H_{42}Cl_{10}$	CC(C(CCC(CCCC(C(CCC(CCCC(CCC(C(CCCCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	697.14	3.16
$C_{25}H_{45}Cl_7$	CC(CCCC(CCCC(CCCC(CCCC(CCCC(CCCCl)Cl)Cl)Cl)Cl)Cl)Cl	593.81	5.2
$C_{30}H_{35}Cl_{27}$	C(C(C(C(CC(C(C(C(C(C(C(CCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)C(C(C(C(C(C(C(CC(C(C(C(C(C(C(C(CCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	1352.84	3.16
$C_{30}H_{49}Cl_{13}$	C(CCCl)CC(C(CC(C(CCCC(C(CCC(CCCC(CCC(C(CCCC(CCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	870.61	3.16
$C_{30}H_{53}Cl_9$	CC(CCCC(CCCC(CCCC(CCC(C(CCCC(CCCC(CCCCCl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	732.83	3.16

[a] $D_{max\ aver}$ - average maximum diameter

[b] 1 Å = 1 nm (10^{-9} m)

17 Appendix F: LCCP concentrations in biota from Environment Agency (2009a)

Table F.1 Aquatic organisms (Campbell and McConnell, 1980) CP concentration (µg/kg ww)

Species	No. of specimens	C_{10-20} Mean	C_{10-20} Range	C_{20-30} Mean	C_{20-30} Range
Mussel (*Mytilus edulis*)	9	3,250	100–12,000	10	ND–100
Plaice (*Pleuronectes platessa*)	6	30	ND–200	30	ND–200
Pouting (*Trisopterus luscus*)	4	100	ND–200	ND	ND
Pike (*Esox lucius*)	2	25	ND–50	25	ND–50
Grey Seal (*Halichoerus grypus*) - liver and blubber	4	75	40–100	ND	ND

Note: ND = not detected (detection limit = 50 µg/kg ww)

Table F.2 Birds (Campbell and McConnell, 1980) CP concentration (µg/kg ww)

Species	Tissue	C_{10-20}	C_{20-30}
Grey Heron (*Ardea cinerea*)	Liver	100–1 200	ND–1 500
Guillemot (*Uria aalge*)	Liver	100–1 100	ND
Herring Gull (*Larus argentatus*)	Liver	200–900	100–500

Note: ND = not detected (detection limit = 100 µg/kg ww).

Table F.3 Number of seabirds[a] eggs containing CPs (Campbell and McConnell, 1980)

CP concentration (µg/kg)	C_{10-20}	C_{20-30}
Not detected (<50 µg/kg)	7	17
50	3	3
100	3	3
200	5	0
300	1	0
400	2	0
600	1	0
>600 (=2 000 µg/kg)	1	0

Note: [a] Species included were: Cormorant (*Phalocrocorax carbo*); Gannet (*Morus bassanus*); Great Skua (*Catharacta skua*); Guillemot (*Uria aalge*); Black-legged Kittiwake (*Rissa tridactyla*); Atlantic Puffin (*Fratercula arctica*); Manx Shearwater (*Puffinus puffinus*); Razorbill (*Alca torda*) and European Shag (*Phalacrocorax aristotelis*).

Table F.4 Human foodstuffs (Campbell and McConnell, 1980) CP concentration (µg/kg ww)

Foodstuff class	No. of samples analysed	C_{10-20}[a]	C_{20-30}[b]
Dairy products	13	300	190
Vegetable oils and derivatives	6	150	ND
Fruit and vegetables	16	5	25
Beverages	6	ND	ND

Notes: ND - not detected (detection limit = 50 µg/kg).

[a] - C10–20 CPs detected in approximately 70% of samples; average concentration given.

[b] - C20–30 CPs found in only one sample of cheese (190 µg/kg ww), one sample of potato crisps (25 µg/kg ww) and one sample of peach fruit (25 µg/kg ww).

18 Appendix G: Reported LCCP Concentrations - Environmental Field Monitoring

Table G.1 LCCP concentrations reported in environmental field samples

KEY: NM[1]= Not measured/reported TS[2]= Total solids S:N[3]= Signal to noise ratio TOC[4]= Total Organic Carbon

Location	Year/Comment	Units	Concentration **measured SCCP**	Concentration **measured MCCP**	Concentration **measured LCCP**	**LOD/LOQ SCCP**	**LOD/LOQ MCCP**	**LOD/LOQ LCCP**	**Analysis**	**Reference**
Norway	2017 Storm water (n=4 **2 dissolved** and 2 particulate fractions)	µg/L	**0.06** NM[1]	**0.0685** NM[1]	Not measured	LOD (3δ blank)	LOD (3δ blank)	Not measured	GC-HRMS	Ruus *et al.* (2018)
Norway, Bekkelaget	2017 **Effluent water** and sludge n=2	µg/L	**0.07** NM[1]	**0.08** NM[1]	Not measured	LOD (3δ blank)	LOD (3δ blank)	Not measured	GC-HRMS	Ruus *et al.* (2018)
Norway, Ildjernet, Inner Oslofjord	2017 Sediment (<63µm=73% dw; TOC=33.8µg/mg dw) n=1	mg/kg dw	0.39	0.14	Not measured	LOD (3δ blank)	LOD (3δ blank)	Not measured	GC-HRMS	Ruus *et al.* (2018)
Norway, Ildjernet, Inner Oslofjord (P. crassa, Lumbrineridae, Terbellidae, *Aphrodita aculeata*, miscellaneous)	Polychaetes, same location as sediment, n=3 pooled samples	µg/L			Not measured	LOD (3δ blank)	LOD (3δ blank)	Not measured	GC-HRMS	Ruus *et al.* (2018)
Norway	2018 Sediment (<63µm=55% dw; TOC=89µg/mg dw) n=1	mg/kg dw	0.64	0.98	Not measured	LOD (3δ blank)	LOD (3δ blank)	Not measured	GC-HRMS	Ruus *et al.* (2019)
Norway	2018 Storm water	µg/L	0.05 NM[1]	0.13 NM[1]	Not measured	LOD (3δ blank)	LOD (3δ blank)	Not measured	GC-HRMS	Ruus *et al.* (2019)

Location	Year/Comment	Units	Concentration **measured** SCCP	Concentration **measured** MCCP	Concentration **measured** LCCP	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
	(n=4 **2 dissolved** and 2 particulate fractions)									
Norway, Bekkelaget	2018 **Effluent water** (suspended solids 3.3, and 4.3mg/L) and sludge (TOC 245, and 150 µg/mg dw) n=2 each	µg/L	0.07 NM[1]	0.09 NM[1]	Not measured	LOD (3δ blank)	LOD (3δ blank)	Not measured	GC-HRMS	Ruus *et al*. (2019)
Norway	Sludge n=70 from 18 STPs average (median; min-max)	µg/kg TS[2]	517 (285; <50-2500)	4 031 (2200; 120 - 17 000)	Not measured	50 (n=68 >LOD) LOD= 3xS:N[3]	LOD= 3xS:N[3]	Not measured	GC-NCI-MS	Norsk Vann (2018)
Norway	Sludge Average (median; min-max)	µg/kg TS[2]	1151 (416; 74-12258)	699 (385; 14-7000)	Not measured	No data available	No data available	Not measured	No data available	Thomas *et al*. (2011)
Jiaojiang River, China	Soil samples (5 km of the e-waste centres) n=9 sampling sites, 5 samples per site (min - max)	ng/g dw	68.5 – 2.2x10^5	507 - 4.40×10^6	Not measured	Mean of blank+ 3SD	Mean of blank+ 3SD	Not measured	GCx GC-ECNI-MS	Xu *et al*. (2019)
Jiaojiang River, China	Sediment samples (5 km of the e-waste centres) n=21 (min - max)	ng/g dw	32.5 – 1.29x10^4	271 – 2.72×10^4	Not measured	Mean of blank+ 3SD	Mean of blank+ 3SD	Not measured	GCx GC-ECNI-MS	Xu *et al*. (2019)
Pearl River Delta, China	2012/2013 surface sediment n=16 mean (min - max)	ng/g dw	334 (46.3-1540)	1720 (102-6650)	Not measured	LOD 0.6 ng/g dw (3δ blank)	LOD 1.0 ng/g dw (3δ blank)	Not measured	GC-ECNI-LRMS	Zeng *et al*. (2017)
Shenzhen, China	2012/2013 surface sediment n=8 mean (min - max)	ng/g dw	317 (14.7-574)	960 (10.9-2 500)	Not measured	LOD 0.6 ng/g dw (3δ blank)	LOD 1.0 ng/g dw (3δ blank)	Not measured	GC-ECNI-LRMS	Zeng *et al*. (2017)
Hong Kong, China	2012/2013 surface sediment n=35 mean (min - max)	ng/g dw	22.0 (<LOD-75.9)	58.7 (<LOD-286)	Not measured	LOD 0.6 ng/g dw (3δ blank)	LOD 1.0 ng/g dw (3δ blank)	Not measured	GC-ECNI-LRMS	Zeng *et al*. (2017)
Tokyo Bay. Japan	2012/2013 surface sediment n=8 mean (min - max)	ng/g dw	10.3 (1.3-27.4)	19.2 (3.2-56.8)	Not measured	LOD 0.6 ng/g dw (3δ blank)	LOD 1.0 ng/g dw (3δ blank)	Not measured	GC-ECNI-LRMS	Zeng *et al*. (2017)

Location	Year/Comment	Units	Concentration **measured SCCP**	Concentration **measured MCCP**	Concentration **measured LCCP**	**LOD/LOQ SCCP**	**LOD/LOQ MCCP**	**LOD/LOQ LCCP**	**Analysis**	**Reference**
Hong Kong, China	2004 sediment core n=1 0-80cm depth (2004-1951) Minimum-maximum	ng/g dw	0.9-29.0	< LOD - 20.3	Not measured	LOD 0.6 ng/g dw (3δ blank)	LOD 1.0 ng/g dw (3δ blank)	Not measured	GC-ECNI-LRMS	Zeng *et al.* (2017)
Tokyo Bay. Japan N35º35'39.12" E139°54'24.48"	2012 sediment core n=1 2-80cm depth (2010-1959) Minimum-maximum	ng/g dw	1.3-26.4	2.7-61.3	Not measured	LOD 0.6 ng/g dw (3δ blank)	LOD 1.0 ng/g dw (3δ blank)	Not measured	GC-ECNI-LRMS	Zeng *et al.* (2017)
Tokyo Bay. Japan N35°28'14.52" E139°45'23.04"	2012 sediment core n=1 0-76cm depth (2012-1940) Minimum-maximum	ng/g dw	5.1-57.9	7.9-180	Not measured	LOD 0.6 ng/g dw (3δ blank)	LOD 1.0 ng/g dw (3δ blank)	Not measured	GC-ECNI-LRMS	Zeng *et al.* (2017)
Lake Bosten, China	2014 surface sediment n=3 mean (min - max)	ng/g dw	59.7 (46-74)	87 (35-150)	103.3 (71-160)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al.* (2019)
Lake Qinghai, China	2014 surface sediment n=1	ng/g dw	59	120	160	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al.* (2019)
Lake Hongfeng, China	2018 surface sediment n=2 mean (n_1;n_2)	ng/g dw	640 (600; 680)	425 (420;430)	450 (350; 550)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al.* (2019)
Lake Chaohu, China	**2011** & 2014 surface sediment	ng/g dw	**68** 59	**12** 30	**76** 190	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al.* (2019)
Lake Taihu, China	2014 surface sediment n=4 mean (min - max)	ng/g dw	192.5 (140-260)	385 (260-690)	108 (80-170)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al.* (2019)
Lake Dianchi, China	2014 surface sediment n=2 mean (n_1;n_2)	ng/g dw	335 (430;240)	405 (360;450)	475 (220;730)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al.* (2019)
Lake Erhai, China	2014 surface sediment n=2 mean (n_1;n_2)	ng/g dw	93 (100; 86)	865 (1500; 230)	230 (330; 130)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al.* (2019)

Location	Year/Comment	Units	Concentration **measured SCCP**	Concentration **measured MCCP**	Concentration **measured LCCP**	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Lake Bosten, China	2006 (107 years) sediment core 0-30cm depth 2006-1899 First detected (conc) **Min (year)** Max (year)	ng/g dw	1920 (8.9) **<MDL (1899-1913; 1920-1935)** 28 (1999-2006)	1942 (20) **<MDL (1899-1935)** 40 (2006)	1949 (20) **<MDL (1899-1942)** 43 (1999)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Qinghai, China	2006 (164 years) sediment core 0-24cm depth 2006-1842 First detected (conc) **Min (year)** Max (year)	ng/g dw	1869 (18) **<MDL (1842-1855)** 53 (1992-2006)	1883 (20) **<MDL (1842-1869; 1896-1979)** 86 (1992-2006)	1979 (19) **<MDL (1842-1965)** 130 (1992-2006)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Hongfeng, China	2006 (37 years) sediment core 0-30cm depth 2006-1969 First detected (conc) **Min (year)** Max (year)	ng/g dw	1973 (8.4) **8.4 (1969-1973)** 400 (2002-2006)	1973 (38) **18 (1976-1980)** 430 (2002-2006)	1984 (23) **<MDL (1969-1980; 1984-1988)** 300 (1991-1995; 2002-2006)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Hongfeng, China	2019 (25 years) sediment core 0-20cm depth 2019-1994 **Min (year)** Max (year)	ng/g dw	**210 (1994-2000)** 650 (2013-2019)	**280 (1994-2000)** 430 (2007-2019)	**310 (1994-2000)** 590 (2013-2019)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Sihailongwan, China	2006 (241 years) sediment core 0-38cm depth 1765-2006 First detected (conc) **Min (year)** Max (year)	ng/g dw	1791 (25) **<MDL (1892-1917)** 320 (1993-2006)	1867 (53) **<MDL (1765-1841; 1892-1917)** 270 (1993-2006)	1955 (22) **<MDL (1765-1943; 1955-1968; 1981-1993)** 240 (1993-2006)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Chaohu, China	2006 (100 years) sediment core 0-19cm depth 1936-2006 First detected (conc) **Min (year)** Max (year)	ng/g dw	1936 (9.6) **<MDL (1939-1943)** 73 (1991-1995)	1969 (16) **<MDL (1936-1965)** 31 (1991-1995)	1954 (23) **<MDL (1936-1951; 1958-1962)** 81 (1991-1995)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Chaohu, China	2011 (70 years) sediment core 0-15cm depth 1955-2011 First detected (conc) **Min (year)** Max (year)	ng/g dw	1989 (15) **<MDL (1955-1985)** 92 (2004-2007)	1985 (11) **<MDL (1955-1978)** 44 (2000-2004)	1985 (13) **<MDL (1955-1978)** 170 (2004-2007)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)

Location	Year/Comment	Units	Concentration **measured SCCP**	Concentration **measured MCCP**	Concentration **measured LCCP**	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Lake Taihu, China	2006 (56 years) sediment core 0-26cm depth 1942-2006 First detected (conc) **Min (year)** Max (year)	ng/g dw	1957 (12) **<MDL (1942-1952; 1957-1977; 1982-1991)** 160 (2001-2006)	1977 (15) **<MDL (1942-1972)** 230 (1986-1991)	1996 (26) **<MDL (1942-1991)** 51 (2001-2006)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Taihu, China	2017 sediment core 0-24cm depth 1958-2017 First detected (conc) **Min (year)** Max (year)	ng/g dw	1985 (52) **<MDL (1958-1980)** 500 (2015-2017)	1985 (110) **<MDL (1958-1980)** 850 (2015-2017)	1990 (9.8) **<MDL (1958-1985)** 240 (2015-2017)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Chengai, China	2006 sediment core 0-28cm depth 1970-2006 First detected (conc) **Min (year)** Max (year)	ng/g dw	1973 (16) **16 (1970-1973)** 370 (2005-2006)	1973 (23) **<MDL (1998-2000)** 2700 (2005-2006)	1986 (27) **<MDL (1970-1983; 1986-1988; 1989-1993; 1994-1996)** 320 (2005-2006)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Dianchi, China	2006 sediment core 0-24cm depth 1920-2006 First detected (conc) **Min (year)** Max (year)	ng/g dw	1935 (15) **<MDL (1920-1927)** 170 (1999-2006)	1935 (30) **<MDL (1920-1927; 1949-1956)** 280 (1999-2006)	1992 (51) **<MDL (1920-1985)** 650 (1999-2006)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Dianchi. China	2018 sediment core 0-20cm depth 1947-2018 First detected (conc) **Min (year)** Max (year)	ng/g dw	1968 (39) **<MDL (1947-1961)** 210 (2004-2011)	1968 (12) **<MDL (1947-1961)** 350 (2011-2018)	1982 (33) **<MDL (1947-1975)** 290 (2004-2011)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)
Lake Erhai, China	2006 sediment core 0-30cm depth 1863-2006) First detected (conc) **Min (year)** Max (year)	ng/g dw	1877 (8.2) **<MDL (1877-1892; 1920-1935)** 63 (1992-2006)	1877 (30) **<MDL (1920-1935)** 470 (1992-2006)	2006 (110) **<MDL (1863-1992)** 110 (1992-2006)	MDL (estimated) 6.2	MDL (estimated) 5.0	MDL (estimated) 4.1	UPLC-QTOFMS	Zhang *et al*. (2019)

Location	Year/Comment	Units	Concentration **measured SCCP**	Concentration **measured MCCP**	Concentration **measured LCCP**	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Himmerfjärden, Sweden Near sewage treatment plant	05/09/2016 sediment core 1881-2015 First detected (conc) **Min (year)** Max (year)	ng/g dw	1960 (1.7) **<LOQ (1881-1951)** 54 (1991)	1960 (8.0) **<LOQ (1881-1951)** 15 (1985-1991)	1960 (0.69) **ND (1881-1951)** 30 (1985)	LOQ blank + 10SD =1.4	LOQ blank + 10SD =6.5	S:N 10:1 =0.067	APCI-QTOF-MS	Yuan *et al*. (2017b)
Umeå, Sweden Near wood related industry	09/09/2016 sediment core 1954-2015 First detected (conc) **Min (year)** Max (year)	ng/g dw	1954 (2.8) **<LOQ (1959)** 14 (1993)	1954 (14) **<LOQ (1959)** 93 (2015)	1954 (12) **1.8 (1959)** 110 (1993)	LOQ blank + 10SD =1.4	LOQ blank + 10SD =6.5	S:N 10:1 =0.067	APCI-QTOF-MS	Yuan *et al*. (2017b)
Nyköping , Sweden Near steel factory	13/09/2016 sediment core 1882-2008 First detected (conc) **Min (year)** Max (year)	ng/g dw	1882 (2.9) **2.0 (1893)** 140 (1942)	1930 (23) **<LOQ (1882-1917)** 1200 (2008)	1882 (0.93) **0.93 (1882)** 200 (1955 & 2008)	LOQ blank + 10SD =1.4	LOQ blank + 10SD =6.5	S:N 10:1 =0.067	APCI-QTOF-MS	Yuan *et al*. (2017b)
Xiaoqing River, China	2014 (n=22) (16, others lost?) surface sediment mean (min-max)	ng/g dw	1300 (48-16000)	6 020 (130-27000)	Not measured	MDL (estimated) 1.3	MDL (estimated) 0.87	Not measured	GC-ECNI-LRMS	Pan *et al*. (2021)
Laizhou Bay, China	2014 (n=5) surface sediment mean (min-max)	ng/g dw	13 (9.1-20)	(2.4 - 9.0)	Not measured	MDL (estimated) 1.3	MDL (estimated) 0.87	Not measured	GC-ECNI-LRMS	Pan *et al*. (2021)
Xiaoqing River/ Laizhou Bay, China	2014 (n=30?) water column **Sum of dissolved and particulate phases** Dissolved phase mean (min-max)	ng/L	**43 (<MDL-470)** 23 (<MDL-230)	**28 (<MDL–120)** 5.9 (<MDL-47)	Not measured	MDL (estimated) 1.4 filters 1.2 dissolved phase	MDL (estimated) 0.93 filters 1.0 dissolved phase	Not measured	GC-ECNI-LRMS	Pan *et al*. (2021)
Shanghai river system, China	2016 (n=74) water median (min-max)	ng/L	278 (40.3-3870)	939 (40.3-3870)	Not measured	MDL (estimated) 2.50	MDL (estimated) 2.05	Not measured	GC-ECNI-LRMS	Wang *et al*. (2019)
Shanghai river system, China	2016 (n=74) sediment mean (min-max)	ng/g	89.3 (<MDL-2020)	947 (10.1-10800)	Not measured	MDL (estimated) 1.70	MDL (estimated) 1.92	Not measured	GC-ECNI-LRMS	Wang *et al*. (2019)
Yangkou Chemical Industrial Park,	2018 (n=20) Total soil	ng/g dw	37.5-995.7	15.1-739.6	Not measured	MDL (blank + 3δ) 23	MDL (blank + 3δ) 4	Not measured	GCx GC-ECNI/MS	Huang *et al*. 2020

Location	Year/Comment	Units	Concentration measured SCCP	Concentration measured MCCP	Concentration measured LCCP	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Jiangsu Province, China	(min-max)									
Yangkou Chemical Industrial Park, Jiangsu Province, China	2018 (n=4) STP soil mean (min-max)	ng/g dw	353 (210-706)	282 (83.1-591)	Not measured	MDL (blank + 3δ) 23	MDL (blank + 3δ) 4	Not measured	GCx GC-ECNI/MS	Huang *et al*. 2020
Yangkou Chemical Industrial Park, Jiangsu Province, China	2018 (n=3) Canal soil Mean (min-max)	ng/g dw	455.7 (137-996)	327.3 (100-740)	Not measured	MDL (blank + 3δ) 23	MDL (blank + 3δ) 4	Not measured	GCx GC-ECNI/MS	Huang *et al*. 2020
Yangkou Chemical Industrial Park, Jiangsu Province, China	2018 (n=13) Road soil mean (min-max)	ng/g dw	133 (37.5-321)	109 (15.1-295)	Not measured	MDL (blank + 3δ) 23	MDL (blank + 3δ) 4	Not measured	GCx GC-ECNI/MS	Huang *et al*. 2020
Mid-lower reach of the Yellow River and tributaries, China	2014 (May, August, December; normal/wet/dry) (n = 69) surface sediment mean ± sd (min-max)	ng/g dw	262±478 (11.8-2792)	97.1±227 (1.56-1558)	Not measured	MDL (blank + 3δ) 4.70	MDL (blank + 3δ) 1.18	Not measured	GC-ECNI/LRMS	Li *et al*. 2018
Mid-lower reach of the Yellow River and tributaries, China	2014 (n = 68) suspended particulate matter mean ± sd (min-max)	ng/g dw	17055± 28456 (213-170038)	2573±3250 (28.6-14428)	Not measured	MDL (blank + 3δ) 6.63	MDL (blank + 3δ) 2.22	Not measured	GC-ECNI/LRMS	Li *et al*. 2018
Dongguan City, Pearl River Delta, China	2011 (n=49) surface soil samples industrial zones mean (min-max)	ng/g dw	172 (6.75-993)	369 (23.9-2427)	Not measured	MDL (blank + 3δ) 8.90	MDL (blank + 3δ) 12.8	Not measured	LC-ESI-uHRMS	Wu *et al*. 2020b
Dongguan City, Pearl River Delta	2011 (n=7) reservoir sediment samples industrial zones mean (min-max)	ng/g dw	59.8 (4.00-223)	206 (29.1 - 601)	Not measured	MDL (blank + 3δ) 8.90	MDL (blank + 3δ) 12.8	Not measured	LC-ESI-uHRMS	Wu *et al*. 2020b

Location	Year/Comment	Units	Concentration measured SCCP	Concentration measured MCCP	Concentration measured LCCP	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Dongguan City, Pearl River Delta	2011 (n=10) river sediment samples industrial zones mean (min-max)	ng/g dw	219 (6.01-613)	694 (14.0-1581)	Not measured	MDL (blank + 3δ) 8.90	MDL (blank + 3δ) 12.8	Not measured	LC-ESI-HRMS	Wu *et al.* 2020b
Dongguan City, Pearl River Delta	2011 (n=17) Sediment (Total) River+Reservoir Mean (min-max)	ng/g dw	153 (4.0-613)	493 (14.0-1581)	Not measured	MDL (blank + 3δ) 8.90	MDL (blank + 3δ) 12.8	Not measured	LC-ESI-HRMS	Wu *et al.* 2020b
Tibetan Plateau **All areas**	2011-2015 Soil (n=78) Minimum-maximum	µg/g TOC[4]	1.0-4.3	0.8-3.3	Not measured	MDL (blank + 3δ) 2.66 ng/g	MDL (blank + 3δ) 1.65 ng/g	Not measured	GC-NCO-QTOF-HRMS	Wu *et al.* 2020c
Tibetan Plateau, Ngari	2012 Soil (n=31) Mean (median; min-max)	µg/g TOC	2.7 (2.7; 1.0-4.3)	2.1 (2.1; 0.8-3.3)	Not measured	MDL (blank + 3δ) 2.66 ng/g	MDL (blank + 3δ) 1.65 ng/g	Not measured	GC-NCO-QTOF-HRMS	Wu *et al.* 2020c
Tibetan Plateau, Nyingchi	2011 Soil (n=17)	µg/g TOC	1.9 (1.4; 1.1-2.6)	1.6 (1.2; 1.0-2.2)	Not measured	MDL (blank + 3δ) 2.66 ng/g	MDL (blank + 3δ) 1.65 ng/g	Not measured	GC-NCO-QTOF-HRMS	Wu *et al.* 2020c
Tibetan Plateau, Namco	2011 Soil (n=4)	µg/g TOC	3.2 (2.8; 2.1-4.3)	2.5 (2.1; 1.7-3.2)	Not measured	MDL (blank + 3δ) 2.66 ng/g	MDL (blank + 3δ) 1.65 ng/g	Not measured	GC-NCO-QTOF-HRMS	Wu *et al.* 2020c
Tibetan Plateau, Sergyla Mountain	2014-2015 Soil (n=26)	µg/g TOC	2.4 (2.5; 1.3-3.6)	1.5 (1.7; 0.9-2.1)	Not measured	MDL (blank + 3δ) 2.66 ng/g	MDL (blank + 3δ) 1.65 ng/g	Not measured	GC-NCO-QTOF-HRMS	Wu *et al.* 2020c
Suburban soils, Shanghai	2011 (n=101) total soil samples mean (median; min-max) TOC Mean (median; min-max) 4.44 (4.28; 1.36-12.0)	ng/g	18.8 (3.52; <MDL-697)	42.3 (15.3; <MDL-666)	Not measured	MDL (blank + 3δ) 1.70	MDL (blank + 3δ) 1.92	Not measured	GC-ECNI/LRMS	Wang *et al.* 2017
Suburban soils, Shanghai	2011 (n=42) farmland soil median TOC Mean (median; min-max) 4.44 (4.28; 1.36-12.0)	ng/g	3.24	15.0	Not measured	MDL (blank + 3δ) 1.70	MDL (blank + 3δ) 1.92	Not measured	GC-ECNI/LRMS	Wang *et al.* 2017

Location	Year/Comment	Units	Concentration measured SCCP	Concentration measured MCCP	Concentration measured LCCP	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Suburban soils, Shanghai	2011 (n=16) wasteland soil median TOC Mean (median; min-max) 4.44 (4.28; 1.36-12.0)	ng/g	3.43	13.8	Not measured	MDL (blank + 3δ) 1.70	MDL (blank + 3δ) 1.92	Not measured	GC-ECNI/LRMS	Wang *et al*. 2017
Suburban soils, Shanghai	2011 (n=27) greenland soil median TOC Mean (median; min-max) 4.44 (4.28; 1.36-12.0)	ng/g	5.76	20.4	Not measured	MDL (blank + 3δ) 1.70	MDL (blank + 3δ) 1.92	Not measured	GC-ECNI/LRMS	Wang *et al*. 2017
Suburban soils, Shanghai	2011 (n=16) woodland soil median TOC Mean (median; min-max) 4.44 (4.28; 1.36-12.0)	ng/g	3.38	15.5	Not measured	MDL (blank + 3δ) 1.70	MDL (blank + 3δ) 1.92	Not measured	GC-ECNI/LRMS	Wang *et al*. 2017
Oceanic marine sediments MAREANO programme	2017 (n=5) 1 of 5 samples contained MCCPs > LOD	mg/kg		2.8			not stated		ECNI-HRMS	Boitsov and Klungsøyr, 2018
Oceanic marine sediments **MAREANO programme**	2018 (n=8) 1 site contained SCCP >LOD 2 of 8 samples contained MCCP > LOD	ng/g	1. 105 Kongsfjorden 2. <MDL Rijpfjorden	1. 410 Kongsfjorden 2. 536 Rijpfjorden 3. 1376 Svalbard (2017 samples) 4. 655 Svalbard (2017 samples)	Not measured	Not stated	not stated	Not measured	ECNI-HRMS	Boitsov *et al*. 2019
Oceanic marine sediments **MAREANO programme**	2019 (n=10)	ng/g		< LOD in all sediments			not stated		ECNI-HRMS	Boitsov and Sanden, 2020
Yangtze River, China	Sediments from the middle reaches of the Yangtze River	ng/g dw		504			MDL (blank + 3δ) 1.98 ng/g		GC x GC TOF-HRMS	Qiao *et al*. 2016

Location	Year/Comment	Units	Concentration measured SCCP	Concentration measured MCCP	Concentration measured LCCP	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Swedish sewage treatment plants (median of 9)	n=9 Sewage treatment plants, 3 composite samples per plant median 2004-2010 Dewatered digested (anaerobic) sludge Stabilised (aerobic) sludge	µg/kg d.w (ng/g dw)	1100	3800	31000	LOQ= 3x LOD	LOQ= 3x LOD	LOQ= 3x LOD	GC-MS (Reth *et al*. 2005)	Olofsson *et al*. (2012)
15 Sewage treatment plants across Australia	2014 n=15 STPs, 8 samples each	ng/g dw	<57-1421	542-3645	116-960	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 1, South-East Queensland, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.65 R^2: MCCP=0.89 R^2: LCCP=0.42 Cl_2: SCCP=60.9 Cl_2: MCCP=56.7 Cl_2: LCCP=44.1	ng/g dw	<156	561	116	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3xblank (all MCCPs >10x blank)	LOD= 3xblank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 2, South-East Queensland, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.84 R^2: MCCP=0.86 R^2: LCCP=0.64 Cl_2: SCCP=57.9 Cl_2: MCCP=53.5 Cl_2: LCCP=42.3	ng/g dw	820	3150	446	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 3, North Queensland, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.16 R^2: MCCP=0.61 R^2: LCCP=0.47 Cl_2: SCCP=61.6 Cl_2: MCCP=55.6 Cl_2: LCCP=44.9	ng/g dw	<130	710	156	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)

Location	Year/Comment	Units	Concentration measured SCCP	Concentration measured MCCP	Concentration measured LCCP	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Sewage treatment plant 4, Northern Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.76 R^2: MCCP=0.95 R^2: LCCP=0.05 Cl_2: SCCP=59.5 Cl_2: MCCP=54.0 Cl_2: LCCP=39.9	ng/g dw	1421	3645	814	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 5, South-East Queensland, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.72 R^2: MCCP=0.85 R^2: LCCP=0.29 Cl_2: SCCP=62.2 Cl_2: MCCP=56.5 Cl_2: LCCP=45.0	ng/g dw	296	1162	364	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 6, South-East Queensland, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.70 R^2: MCCP=0.82 R^2: LCCP=0.71 Cl_2: SCCP=61.2 Cl_2: MCCP=55.3 Cl_2: LCCP=45.1	ng/g dw	315	1772	349	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 7, Central New South Wales, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.75 R^2: MCCP=0.78 R^2: LCCP=0.50 Cl_2: SCCP=62.4 Cl_2: MCCP=56.5 Cl_2: LCCP=48.3	ng/g dw	<85	716	154	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)

Location	Year/Comment	Units	Concentration measured SCCP	Concentration measured MCCP	Concentration measured LCCP	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Sewage treatment plant 9, Southern Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.64 R^2: MCCP=0.89 R^2: LCCP=0.32 Cl_2: SCCP=58.6 Cl_2: MCCP=54.3 Cl_2: LCCP=42.7	ng/g dw	685	3192	960	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 10, South-East Queensland Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.60 R^2: MCCP=0.81 R^2: LCCP=0.57 Cl_2: SCCP=58.9 Cl_2: MCCP=54.9 Cl_2: LCCP=43.9	ng/g dw	<147	813	305	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 11, Central New South Wales, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.24 R^2: MCCP=0.56 R^2: LCCP=0.53 Cl_2: SCCP=60.8 Cl_2: MCCP=56.0 Cl_2: LCCP=47.1	ng/g dw	<57	790	250	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 12(1), Southern Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.59 R^2: MCCP=0.71 R^2: LCCP=0.11 Cl_2: SCCP=60.7 Cl_2: MCCP=55.9 Cl_2: LCCP=42.5	ng/g dw	<86	995	625	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)

Location	Year/Comment	Units	Concentration measured SCCP	Concentration measured MCCP	Concentration measured LCCP	LOD/LOQ SCCP	LOD/LOQ MCCP	LOD/LOQ LCCP	Analysis	Reference
Sewage treatment plant 12(2), Southern Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.58 R^2: MCCP=0.60 R^2: LCCP=0.09 Cl_2: SCCP=61.0 Cl_2: MCCP=55.2 Cl_2: LCCP=43.2	ng/g dw	<60	1016	527	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 13, Western Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.55 R^2: MCCP=0.81 R^2: LCCP=0.67 Cl_2: SCCP=57.8 Cl_2: MCCP=54.6 Cl_2: LCCP=46.0	ng/g dw	435	3449	683	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 14, North Queensland, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.69 R^2: MCCP=0.68 R^2: LCCP=0.33 Cl_2: SCCP=62.4 Cl_2: MCCP=56.3 Cl_2: LCCP=47.2	ng/g dw	<83	542	137	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3xblank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant 15, North Queensland. Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.68 R^2: MCCP=0.84 R^2: LCCP=0.40 Cl_2: SCCP=61.6 Cl_2: MCCP=57.5 Cl_2: LCCP=46.5	ng/g dw	325	974	398	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)

Location	Year/Comment	Units	Concentration **measured SCCP**	Concentration **measured MCCP**	Concentration **measured LCCP**	**LOD/LOQ SCCP**	**LOD/LOQ MCCP**	**LOD/LOQ LCCP**	**Analysis**	**Reference**
Sewage treatment plant 16, North Queensland, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.65 R^2: MCCP=0.86 R^2: LCCP=0.51 Cl_2: SCCP=63.0 Cl_2: MCCP=56.0 Cl_2: LCCP=46.4	ng/g dw	406	1474	270	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant blank 1, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.002 R^2: MCCP=0.93 R^2: LCCP=0.00 Cl_2: SCCP=66.2 Cl_2: MCCP=49.5 Cl_2: LCCP=33.2	ng absolute	9	24	0.4	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)
Sewage treatment plant blank 2, Australia	2014 1 Pooled sample (n=8 subsamples) R^2: SCCP=0.001 R^2: MCCP=0.90 R^2: LCCP=0.00 Cl_2: SCCP=64.0 Cl_2: MCCP=49.0 Cl_2: LCCP=33.4	ng absolute	16	22	0.5	LOD= 3x blank (SCCPs <3x blank reported as <LOQ)	LOD= 3x blank (all MCCPs >10x blank)	LOD= 3x blank (all LCCPs >10x blank)	APCI-qTOF-HRMS	Brandsma *et al*. (2017)

19 Appendix H: Reported LCCP Concentrations- Biota Monitoring

Table H.1 Reported concentrations of LCCPs detected in biota

KEY: $Conc^{m}$ – measured concentration LOD/Q - limit of detection/quantification; MDL - method detection limit; MQL - method quantification limit; dw - dry weight; ww - wet weight; lw - lipid weight; med. - median; min- minimum; max- maximum; n=number of individuals; specified where pooled. Composite Aquatic foods sample[1]= **mixture of freshwater fish** (*Cyprinus carpio, Piceus, Ctenopharyn odon idellus, Carassius cuvieri, Monopterus albus Silurus asotus, Hypophthalmichthys molitrix,* and *Megalobrama terminalis*), **marine fish** (*Trichiurus lepturus, Scomber japonicas, Pampus argenteus*, and *Pseudosciaena polyactis*), **shrimp and oysters.**

Location	Species	Year /Comment	Units	$Conc^{m}$ SCCP	$Conc^{m}$ MCCP	$Conc^{m}$ LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Landsort, Sweden	Herring (*Clupea harengus*)	2011, 2014, 2017 (n=12, 12 & 13) 3 Pooled Muscle samples; female	ng/g lw	40 34 40	44 30 51	15 26 17	LOQ: 26	LOQ: 28	LOQ: 4.2	APCI-QTOF-MS	Yuan *et al.* (2019b)
Byxelkrok, Sweden	Herring (*Clupea harengus*)	2014 (Liver, n= 38 pooled) (**Muscle**, n = 40 pooled); male and female	ng/g lw	48 54	140 **120**	44 24	LOQ: 26	LOQ: 28	LOQ: 4.2	APCI-QTOF-MS	Yuan *et al.* (2019b)
Byxelkrok, Sweden	Herring (*Clupea harengus*)	2016 (Liver, n= 38 pooled) (**Muscle**, n = 40 pooled); male and female	ng/g lw	39 97	170 140	14 27	LOQ: 26	LOQ: 28	LOQ: 4.2	APCI-QTOF-MS	Yuan *et al.* (2019b)
Christiansø, Denmark	Common Eider (*Somateria mollissima*)	2015 (Liver, n=5 pooled) (Liver, n=5 pooled) Female	ng/g lw	200 150	440 **290**	120 34	LOQ: 33	LOQ: 37	LOQ: 5.4	APCI-QTOF-MS	Yuan *et al.* (2019b)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Christiansø, Denmark	Common Eider (*Somateria mollissima*)	2015 (Egg, n=5 pooled) (**Egg**, n=5 pooled)	ng/g lw	110 82	140 200	18 52	LOQ: 33	LOQ: 37	LOQ: 5.4	APCI-QTOF-MS	Yuan *et al.* (2019b)
Western Gotland Basin, Baltic Sea	Guillemot (*Uria aalge*)	2016 (Egg, n=4 pooled) (**Egg**, n=5 pooled)	ng/g lw	88 48	67 58	36 18	LOQ: 9.3	LOQ: 10	LOQ: 1.5	APCI-QTOF-MS	Yuan *et al.* (2019b)
Stockholm/ Uppsala Counties, Sweden	White-tailed Sea-eagle (*Haliaeetus albicila*)	2015 (Egg, n=4 pooled)	ng/g lw	220	250	34	LOQ: 37	LOQ: 41	LOQ: 6.1	APCI-QTOF-MS	Yuan *et al.* (2019b)
Kalmar/ Blekinge Counties, Sweden	White-tailed Sea-eagle (*Haliaeetus albicila*)	2015 (Egg, n=5 pooled)	ng/g lw	130	140	76	LOQ: 37	LOQ: 41	LOQ: 6.1	APCI-QTOF-MS	Yuan *et al.* (2019b)
Åland Sea/ Northern Baltic Proper	Grey Seal (*Halichoerus grypus*)	2006-2008 Juvenile (male) (Liver, n=4 pooled) (**Blubber**, n=3 pooled)	ng/g lw	140 45	210 83	86 20	LOQ: 29	LOQ: 32	LOQ: 4.9	APCI-QTOF-MS	Yuan *et al.* (2019b)
Western Gotland Basin	Grey Seal (*Halichoerus grypus*)	2009-2010 Adult (male) (Liver, n=5 pooled) (Blubber, n=4 pooled)	ng/g lw	140 37	230 32	71 6	LOQ: 29	LOQ: 32	LOQ: 4.9	APCI-QTOF-MS	Yuan *et al.* (2019b)
Western Gotland Basin/ Southern Baltic Proper	Harbour Seal (*Phoca vitulina*)	2014-2015 Juveniles (Liver, n=5 pooled) (**Blubber**, n=5 pooled)	ng/g lw	180 26	540 100	120 14	LOQ: 25	LOQ: 28	LOQ: 4.1	APCI-QTOF-MS	Yuan *et al.* (2019b)
Western Gotland Basin/ Southern	Harbour Seal (*Phoca vitulina*)	2012-2016 Adult (Liver, n=4 pooled)	ng/g lw	150 34	230 64	53 14	LOQ: 25	LOQ: 28	LOQ: 4.1	APCI-QTOF-MS	Yuan *et al.* (2019b)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Baltic Proper		(Blubber, n=4 pooled)									
Southern Baltic Proper	Harbour Porpoise (*Phocoena phocoena*)	2006-2012 Adult (3 females and 1 male) (Liver, n=4 pooled) (**Blubber**, n=4 pooled)	ng/g lw	110 300	140 36	63 48	LOQ: 22	LOQ: 24	LOQ: 3.6	APCI-QTOF-MS	Yuan *et al*. (2019b)
Southern Baltic Proper	Harbour porpoise (*Phocoena phocoena*)	2008 Adult (1 female and 1 male) (Liver, n=2 pooled) (Blubber, n=2 pooled)	ng/g lw	330 120	440 59	130 25	LOQ: 22	LOQ: 24	LOQ: 3.6	APCI-QTOF-MS	Yuan *et al*. (2019b)
Våstmanland, Sweden	Moose (*Alces alces*)	2012 – 2015 Adult (both sexes) Muscle (n=10 pooled)	ng/g lw	1500	1600	180	LOQ: 70	LOQ: 78	LOQ: 12	APCI-QTOF-MS	Yuan *et al*. (2019b)
Värmland, Sweden	Bank vole (*Myodes glareolus*)	2014 Both sexes Muscle (n=10 pooled)	ng/g lw	400	370	36	LOQ: 12	LOQ: 13	LOQ: 2.0	APCI-QTOF-MS	Yuan *et al*. (2019b)
Västmanland, Sweden	Lynx (*Lynx pardinus*)	2012-2016 Adult (both sexes) Muscle (n=10 pooled)	ng/g lw	800	750	92	LOQ: 34	LOQ: 38	LOQ: 5.6	APCI-QTOF-MS	Yuan *et al*. (2019b)
Västmanland, Sweden	Wolf (*Canis lupis*)	2012-2016 Adult (both sexes) Muscle (n=10 pooled)	ng/g lw	1100	830	100	LOQ: 30	LOQ: 34	LOQ: 5.0	APCI-QTOF-MS	Yuan *et al*. (2019b)
South-middle Sweden	Starling (Sturnus vulgaris)	2012-2015 Fledglings (both sexes) Muscle (n=10 pooled)	ng/g lw	350	310	25	LOQ: 13	LOQ: 14	LOQ: 2.1	APCI-QTOF-MS	Yuan *et al*. (2019b)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Västerbotten, Sweden	Common kestrel (*Falco tinnunculus*)	2014 Egg (n=3 pooled)	ng/g lw	88	85	51	LOQ: 4.3	LOQ: 4.8	LOQ: 0.7	APCI-QTOF-MS	Yuan *et al*. (2019b)
South-middle Sweden	Tawny owl (*Strix aluco*)	2014 Egg (n=4 pooled)	ng/g lw	85	87	49	LOQ: 2.7	LOQ: 3.0	LOQ: 0.4	APCI-QTOF-MS	Yuan *et al*. (2019b)
South-middle Sweden	Eagle owl (*Bubo bubo*)	2013-2017 Adults (both sexes) Muscle (n=10 pooled)	ng/g lw	730	720	380	LOQ: 26	LOQ: 29	LOQ: 4.3	APCI-QTOF-MS	Yuan *et al*. (2019b)
South-middle Sweden	Marsh harrier (*Circus aeruginosus*)	2012-2015 Adults (both sexes) Muscle (n=10 pooled)	ng/g lw	220	180	100	LOQ: 8.9	LOQ: 9.9	LOQ: 1.5	APCI-QTOF-MS	Yuan *et al*. (2019b)
South-middle Sweden	Golden eagle (*Aquila chrysaetos*)	2012-2016 Adults (both sexes) Muscle (n=10 pooled)	ng/g lw	550	360	210	LOQ: 9.0	LOQ: 10	LOQ: 1.5	APCI-QTOF-MS	Yuan *et al*. (2019b)
South-middle Sweden	Peregrine falcon (*Falco peregrinus*)	2012-2016 Adults (both sexes) Muscle (n=10 pooled)	ng/g lw	540	410	1200	LOQ: 12	LOQ: 13	LOQ: 1.9	APCI-QTOF-MS	Yuan *et al*. (2019b)
Paddy fields, Yangtze River Delta	Pond Loach (*Misgurnus anguillicaudatus*)	n=20 4 pooled muscle samples δ13C -27.8±0.7‰ Lipid 2.4±0.38% mean (min-max)	ng/g lw	2300 (1100-3600)	2500 (1400-2600)	610 (480-1300)	LOQ <52 ng/g dw	LOQ <24 ng/g dw	LOQ <1.3 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)
Paddy fields, Yangtze River Delta	Rice Field Eel (*Monopterus albus*)	n=30 6 pooled muscle samples δ^{13}C -26.5±1.0‰ Lipid 1.21±0.24% mean (min-max)	ng/g lw	1800 (1100-2600)	2600 (820-3700)	1600 (730-2900)	LOQ <25 ng/g dw	LOQ <12 ng/g dw	LOQ <0.7 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)
Paddy fields, Yangtze River Delta	Red-backed Rat Snake	n=6 δ^{13}C -24.9±1.0‰ Lipid 0.78±0.15	ng/g lw	3400 (2300-6300)	3800 (2100-7900)	1100)930-1800)	LOQ <41 ng/g dw	LOQ <19 ng/g dw	LOQ <1.1 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
	(*Elaphe rufodorsata*)	mean (min-max)									
Paddy fields, Yangtze River Delta	Red-banded Snake (*Dinodon rufozonatum*)	n=1 $\delta^{13}C$ -23.8‰ Lipid 0.92%	ng/g lw	6200	13000	4200	LOQ <26 ng/g dw	LOQ <12 ng/g dw	LOQ <0.7 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)
Paddy fields, Yangtze River Delta	Short-tailed Mamushi (*Gloydius brevicaudus*)	n=6 $\delta^{13}C$ -23.4±0.3‰ Lipid 1.19±0.12% mean (min-max)	ng/g lw	16000 (9500-22000)	17000 (7400-19000)	1700 (980-5100)	LOQ <59 ng/g dw	LOQ <28 ng/g dw	LOQ <1.5 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)
Paddy fields, Yangtze River Delta	Yellow Weasel (*Mustela sibirica*)	n=5 $\delta^{13}C$ -22.6±0.9‰ Lipid 1.79±0.36% mean (min-max)	ng/g lw	8900 (7400-43000)	12000 (6700-33000)	740 (450-2100)	LOQ <40 ng/g dw	LOQ <19 ng/g dw	LOQ <1.0 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)
Paddy fields, Yangtze River Delta	Peregrine Falcon (*Falco peregrinus*)	n=6 $\delta^{13}C$ -24.5±1.0‰ Lipid 3.49±1.01% mean (min-max)	ng/g lw	1300 (840-14000)	2100 (1300-29000)	690 (530-10000)	LOQ <38 ng/g dw	LOQ <18 ng/g dw	LOQ <1.0 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)
Paddy fields, Yangtze River Delta	Collared Scops-owl (*Otus lettia*)	n=7 $\delta^{13}C$ -26.1±0.3‰ Lipid 7.65±2.26% mean (min-max)	ng/g lw	200 (<91-450)	270 (96-440)	84 (18-340)	LOQ <38 ng/g dw	LOQ <18 ng/g dw	LOQ <1.0 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)
Paddy fields, Yangtze River Delta	Common Cuckoo (*Cuculus canorus*)	n=5 $\delta^{13}C$ -26.8±0.5‰ Lipid 2.76±0.73% mean (min-max)	ng/g lw	270 (<140-3100)	200 (<170-1400)	60 (14-1800)	LOQ <27 ng/g dw	LOQ <13 ng/g dw	LOQ <0.7 ng/g dw	APCI-QTOF-MS	Du *et al*. (2018)/ Zhou *et al*. (2019)
Paddy fields,	Black-spotted Frog	(n=12) liver (female)	ng/g lw[7]	1418.44 ± 945.63	271.87 ± 185.19	33.49 ± 27.19	LOQ: <181.25	LOQ: <23.64	LOQ: <6.70	APCI-QTOF-MS	Du *et al*. (2019)

[7] The Environment Agency used the average % lipid from samples to convert concentrations from ng/g ww to ng/g lw.

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Yangtze River Delta	(*Pelophylax nigromaculatus*)	Lipid content: 25.38 ±6.40 % mean ± sd (min-max)		(748.62-3585.50)	(122.14 – 748.62)	(<LOQ – 102.44)					
Paddy fields, Yangtze River Delta	Black-spotted Frog (*Pelophylax nigromaculatus*)	(n=12) liver (male) Lipid content: 18.77±8.46% mean ± sd (min-max)	ng/g lw	1704.85 ± 1598.30 (149.17 – 4848.16)	362.28 ± 314.33 (29.30 – 958.98)	149.17 ± 181.14 (ND – 586.04)	LOQ: <229.09	LOQ: < 29.83	LOQ: < 8.52	APCI-QTOF-MS	Du *et al*. (2019)
Paddy fields, Yangtze River Delta	Black-spotted Frog (*Pelophylax nigromaculatus*)	(n=12) egg (paired with female liver samples) Lipid content: 9.87±2.26% mean ± sd (min-max)	ng/g lw	628.17 ± 648.43 (ND-2228.98)	162.11 ± 141.84 (<LOQ – 526.85)	29.38 ± 57.75 (ND – 202.63)	LOQ: <162.11	LOQ: <21.28	LOQ: < 6.08	APCI-QTOF-MS	Du *et al*. (2019)
Paddy fields, Yangtze River Delta	Black-spotted Frog (*Pelophylax nigromaculatus*)	(n=45; male and female) 3 (female) Pooled muscle samples Lipid content: 0.53±0.03% (mean±SD)	ng/g lw	1301.89 ± 528.30	943.40 ± 566.04	490.57 ± 396.23	LOQ: <924.53	LOQ: <120.75	LOQ: <33.96	APCI-QTOF-MS	Du *et al*. (2019)
Paddy fields, Yangtze River Delta	Black-spotted Frog (*Pelophylax nigromaculatus*)	(n=45; male and female) 2 (male) Pooled muscle samples Lipid content: 0.57-0.66% (0.615%avg) (low-high)	ng/g lw	2276.42-5040.65	4065.04-8130.08	1235.77-2601.63	LOQ: <796.75	LOQ: <104.07	LOQ: <29.27	APCI-QTOF-MS	Du *et al*. (2019)
Paddy fields, Yangtze River Delta	Short-tailed Mamushi snake	Oct 2011 (n=7) Liver Lipid 2.32±1.45%	ng/g lw	5200±4300 (1900-13000)	1800±1800 (<LOQ-5100)	730±860 (95-2300)	LOQ: <1300	LOQ: <610	LOQ: <34	APCI-QTOF-MS	Du *et al*. (2020)

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
	(*Gloydius brevicaudus*)	mean ± sd (min-max)									
Paddy fields, Yangtze River Delta	Short-tailed Mamushi snake (Gloydius *brevicaudus*)	Oct 2011 (n=7) muscle Lipid 1.13±0.15% mean ± sd (min-max)	ng/g lw	16000±5900 (8900-22000)	14000±5700 (7400-22000)	2200±1600 (980-5100)	LOQ: <970	LOQ: <450	LOQ: <25	APCI-QTOF-MS	Du *et al*. (2020)
Paddy fields, Yangtze River Delta	Short-tailed Mamushi snake (Gloydius *brevicaudus*)	Oct 2011 (n=7) adipose Lipid 68.6±12.4% mean ± sd (min-max)	ng/g lw	73±41 (<LOQ-160)	170±110 (44-290)	130±100 (44-270)	LOQ: <41	LOQ: <19	LOQ: <1.1	APCI-QTOF-MS	Du *et al*. (2020)
Paddy fields, Yangtze River Delta	Red-backed Rat Snake (*Elaphe rufodorsata*)	Oct 2011 (n=9) Liver Lipid 1.28±0.53% mean ± sd (min-max)	ng/g lw	9000±5600 (3800-19000)	1500±970 (<LOQ-3500)	500±600 (57-1800)	LOQ: <1400	LOQ: <660	LOQ: <37	APCI-QTOF-MS	Du *et al*. (2020)
Paddy fields, Yangtze River Delta	Red-backed Rat Snake (*Elaphe rufodorsata*)	Oct 2011 (n=9) Muscle Lipid 0.76±0.12% mean ± sd (min-max)	ng/g lw	4400±2200 (1900-7700)	5500±3500 (2100-11000)	1800±1600 (810-5900)	LOQ: <1000	LOQ: <470	LOQ: <26	APCI-QTOF-MS	Du *et al*. (2020)
Paddy fields, Yangtze River Delta	Red-backed Rat Snake (*Elaphe rufodorsata*)	Oct 2011 (n=9) Adipose Lipid 78.5±12.5% mean ± sd (min-max)	ng/g lw	52±52 (<LOQ-155)	230±420 (<LOQ-5100)	110±120 (12-380)	LOQ: <12	LOQ: <5.8	LOQ: <0.32	APCI-QTOF-MS	Du *et al*. (2020)
Dianshan Lake, Freshwater ecosystem, Yangtze River Delta	Grass carp (Ctenopharyn-*godon idella*)	(n=1) Whole muscle Mean lipid 6.6%	ng/g lw	2200	340	2.5	LOQ: <18 ng/g dw	LOQ: <12 ng/g dw	LOQ: <0.5 ng/g dw	APCI-QTOF-MS	Zhou *et al*. (2019)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Dianshan Lake, Freshwater ecosystem, Yangtze River Delta	Predatory carp (*Erythroculter ilishaeformis*)	(n=2) Whole muscle Mean lipid 0.53% mean (min-max)	ng/g lw	8800 (2200-15000)	1900 (610-3100)	<LOQ	LOQ: <57 ng/g dw	LOQ: <39 ng/g dw	LOQ: <1.7 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Dianshan Lake, Freshwater ecosystem, Yangtze River Delta	Bigmouth Grenadier Anchovy (*Coilia ectenes*)	(n=40, 2 pooled whole muscle samples) Mean lipid 3.3% mean (min-max)	ng/g lw	1100 (690-1600)	360 (270-440)	15 (13-17)	LOQ: <20 ng/g dw	LOQ: <14 ng/g dw	LOQ: <0.6 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Dianshan Lake, Freshwater ecosystem, Yangtze River Delta	Snake-head fish (*Channa argus*)	(n=1) Whole muscle Mean lipid 0.6%	ng/g lw	3200	500	<LOQ	LOQ: <24 ng/g dw	LOQ: <16 ng/g dw	LOQ: <0.7 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Dianshan Lake, Freshwater ecosystem, Yangtze River Delta	Yellow Catfish (*Pelteobagrus fulvidraco*)	(n=2) Whole muscle Mean lipid 1.6% mean (x1;x2)	ng/g lw	10000 (4200-16000)	1800 (760-2800)	25 (17-33)	LOQ: <21 ng/g dw	LOQ: <14 ng/g dw	LOQ: <06 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Dianshan Lake, Freshwater ecosystem, Yangtze River Delta	Crucian Carp (*Carassius auratus*)	(n=1) Whole muscle Mean lipid 1.2%	ng/g lw	4400	1200	55	LOQ: <23 ng/g dw	LOQ: <15 ng/g dw	LOQ: <0.7 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Dianshan Lake, Freshwater ecosystem,	Common Carp (*Cyprinius carpio*)	(n=1) Whole muscle Mean lipid 0.63%	ng/g lw	15000	2000	<LOQ	LOQ: <33 ng/g dw	LOQ: <22 ng/g dw	LOQ: <1.0 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Yangtze River Delta											
Dianshan Lake, Freshwater ecosystem, Yangtze River Delta	Freshwater mussel/clam (*Corbicula aurea Heude*)	(n=100, 2 pooled whole soft tissue samples) Mean lipid 3.2% mean (min-max)	ng/g lw	9800 (5100-14000)	1500 (770-2200)	88 (46-130)	LOQ: <40 ng/g dw	LOQ: <27 ng/g dw	LOQ: <1.2 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Dianshan Lake, Freshwater ecosystem, Yangtze River Delta	Freshwater snail (*Bellamya aeruginosa*)	(n=150, 3 pooled whole intestine samples) Mean lipid 1.6% mean (min-max)	ng/g lw	9900 (1900-19000)	3000 (210-5500)	220 (67-380)	LOQ: <170 ng/g dw	LOQ: <110 ng/g dw	LOQ: <2.8 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Paddy fields, Wetland ecosystem, Yangtze River Delta	Chicken egg (*Gallus gallus domesticus*)	(n=1) Mean lipid 9.6%	ng/g lw	290	370	360	LOQ: <8.4 ng/g dw	LOQ: <5.6 ng/g dw	LOQ: <0.2 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Paddy fields, Wetland ecosystem, Yangtze River Delta	Duck egg (*Anas platyrhynchos*)	(n=1) Mean lipid 1.6%	ng/g lw	120	120	5	LOQ: <6.5 ng/g dw	LOQ: <4.4 ng/g dw	LOQ: <0.2 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)
Paddy fields, Wetland ecosystem, Yangtze River Delta	Chinese Pond Heron (*Ardeola bacchus*)	(n=5) Pectoral muscle Mean lipid 4.1% mean (min-max)	ng/g lw	630 (280-1300)	1500 (290-4600)	520 (88-1700)	LOQ: <24 ng/g dw	LOQ: <16 ng/g dw	LOQ: <0.7 ng/g dw	APCI-QTOF-MS	Zhou *et al.* (2019)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Longtang Town, Guangdong Province	Grasshopper larvae (*Oxya chinensis*)	April - May 2016 (n=95, 3 pooled whole body samples) $\delta^{13}C$ -17.4 ± 2.94‰ $\delta^{15}N$ 3.1 ± 0.57‰ Lipid 7.0 ± 1.5% mean (min-max)	ng/g lw	5400 (3700-5700)	6000 (4000-6600)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL[8] (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Grasshopper (*Oxya chinensis*)	Spring and Summer 2015 – 2016 (n=78, 3 pooled whole body samples) $\delta^{13}C$ -14.0 ± 0.10‰ $\delta^{15}N$ 3.8 ± 0.08‰ Lipid 5.8 ± 0.9% mean (min-max)	ng/g lw	5100 (4500-6300)	6500 (6000-8400)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Beetle (*Anomala corpulenta*)	Spring and Summer 2015 – 2016 (n=45, 6 pooled whole body samples) $\delta^{13}C$ -24.3 ± 0.99‰ $\delta^{15}N$ 3.3 ± 0.50‰ Lipid 6.6 ± 1.3% mean (min-max)	ng/g lw	2200 (1200-7100)	990 (110-1100)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020

[8] The Environment agency notes that the authors determined the MQL as the Σconcentrations of SCCP congeners in the blank +3δ, this would normally be the MDL with the MQL blank+10δ

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Longtang Town, Guangdong Province	Cricket (*Gryllulus chinensis*)	Spring and Summer 2015 – 2016 (n=55, 5 pooled whole body samples) $\delta^{13}C$ -23.3 ± 3.24‰ $\delta^{15}N$ 4.2 ± 0.33‰ Lipid 18.0 ± 2.6% mean (min-max)	ng/g lw	5000 (2300-8800)	3600 (1600-4600)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Mole cricket (*Gryllotalpa orientalis*)	Spring and Summer 2015 – 2016 (n=63, 8 pooled whole body samples) $\delta^{13}C$ -21.4 ± 1.23‰ $\delta^{15}N$ 5.3 ± 0.59‰ Lipid 17.0 ± 3.9% mean (min-max)	ng/g lw	3800 (3000-6600)	3200 (2600-5400)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Mantis (*Tenodera sinensis*)	Spring and Summer 2015 – 2016 (n=28, 4 pooled whole body samples) $\delta^{13}C$ -20.3 ± 1.16‰ $\delta^{15}N$ 6.8 ± 0.48‰ Lipid 8.5 ± 2.1% mean (min-max)	ng/g lw	9000 (8000-14000)	5100 (1500-7700)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Dragonfly larvae (*Anisoptera sp.*)	April - May 2016 (n=80, 3 pooled whole body samples) $\delta^{13}C$ -22.7 ± 0.64‰ $\delta^{15}N$ 4.4 ± 0.21‰ Lipid 8.7 ± 0.7% mean (min-max)	ng/g lw	2500 (1400-4100)	1100 (950-3200)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Longtang Town, Guangdong Province	Dragonfly larvae (*Anisoptera sp.*)	April - May 2016 (n=250, 6 pooled whole body samples) $\delta^{13}C$ -29.4 ± 0.55‰ $\delta^{15}N$ 8.2 ± 0.50‰ Lipid 8.2 ± 0.5% mean (min-max)	ng/g lw	12000 (4700-24000)	7500 (2000-19000)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Dragonfly (*Aeshnidae rambur*)	Spring and Summer 2015 – 2016 (n=65, 3 pooled whole body samples) $\delta^{13}C$ -23.0 ± 0.68‰ $\delta^{15}N$ 8.4 ± 0.11‰ Lipid 7.0 ± 0.2% mean (min-max)	ng/g lw	8700 (6400-10000)	5500 (3600-8800)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Dragonfly (*Libellulidae rambur*)	Spring and Summer 2015 – 2016 (n=100, 3 pooled whole body samples) $\delta^{13}C$ -24.3 ± 0.30‰ $\delta^{15}N$ 7.4 ± 0.11‰ Lipid 11 ± 1.0% mean (min-max)	ng/g lw	7400 (3700-10000)	19000 (14000-27000)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Tadpole (frog and toad)	April - May 2016 (n=60, 3, pooled whole body samples) $\delta^{13}C$ -not measured $\delta^{15}N$ -not measured Lipid 3.1 ± 0.2%	ng/g lw	13000 (11000-14000)	20000 (19000-22000)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
		mean (min-max)									
Longtang Town, Guangdong Province	Asian Painted Frog (*Kaloula pulchra*)	Autumn 2016 (n=9, 5 pooled muscle samples) $\delta^{13}C$ -22.6 ± 1.54‰ $\delta^{15}N$ 6.6 ± 1.78‰ Lipid 8.7 ± 3.2% mean (min-max)	ng/g lw	17000 (11000-24000)	9300 (4600-17000)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Black Spectacled Toad (*Duttaphrynus melanostictus*)	Autumn 2016 (n=6) Muscle $\delta^{13}C$ -25.0 ± 0.47‰ $\delta^{15}N$ 8.9 ± 0.61‰ Lipid 12.6 ± 0.9% mean (min-max)	ng/g lw	12000 (8100-16000)	7200 (5300-11000)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Oriental Garden Lizard (*Calotes versicolor*)	Autumn 2016 (n=9) Muscle $\delta^{13}C$ -25.2 ± 0.96‰ $\delta^{15}N$ 6.4 ± 0.96‰ Lipid 5.9 ± 2.3% mean (min-max)	ng/g lw	14000 (8900-32000)	9100 (5400-21000)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Oriental Magpie Robin (*Copsychus saularis*)	Autumn 2016 (n=3) Muscle $\delta^{13}C$ -25.7 ± 0.29‰ $\delta^{15}N$ 2.5 ± 0.09‰ Lipid 3.6 ± 0.1% mean (min-max)	ng/g lw	34000 (19000-48000)	18000 (10000-33000)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Long-tailed Shrike (*Lanius schach*)	Autumn 2016 (n=2) Muscle $\delta^{13}C$ -25.2‰ and -23.2‰ $\delta^{15}N$ 3.9‰ and 9.4‰ Lipid 5.2% and 4.1%	ng/g lw	6100; 9200	2000; 3300	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Longtang Town, Guangdong Province	Eurasian Blackbird (*Turdus merula*)	Autumn 2016 (n=1) Muscle $\delta^{13}C$ -24.8‰ $\delta^{15}N$ 5.9‰ Lipid 4.7%	ng/g lw	27000	13000	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Grass leaves (*Gramineae*)	Autumn 2015 (n=3) $\delta^{13}C$ -13.3 ± 0.17‰ $\delta^{15}N$ 3.1 ± 0.13‰ mean (min-max)	ng/g dw	390 (350-510)	450 (430-600)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Guava leaves (*Psidium guajava*)	Autumn 2015 (n=3) $\delta^{13}C$ -30.5 ± 1.18‰ $\delta^{15}N$ 4.2 ± 0.77‰ mean (min-max)	ng/g dw	470 (440-730)	420 (380-650)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Longtang Town, Guangdong Province	Soil (corn field and paddy fields)	Autumn 2015 (n=6) mean (min-max)	ng/g dw	160 (27-330)	220 (57-390)	-	MQL (blanks + 3δ) 71 ng/g lw	MQL (blanks + 3δ) 67 ng/g lw		GC-ECNI-MS	Liu *et al*. 2020
Constructed wetland eco-system,	Common Reed (*Phragmites australis*)	2017 mean ± sd min-max	ng/g dw	127±116[9] (71-340)	289±148[1] (235-435)	188±116[1] (88-377)	MDL plant material 10-20[10]	MDL plant material 10-20[2] MDL	MDL plant material 10-20[2]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021

[9] Note: The authors presented data for all 11 plant species together, and also presented data for the predominant plant species *Phragmites australis*.

[10] Overall MDL for plant material for SCCPs, MCCPs, and LCCPs

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Beijing Olympic Forest Park							MDL (blank + 3δ) 1.88 - 7.62[11]	(blank + 3δ) 1.67 - 10.65[3]	MDL (blank + 3δ) 1.74 – 2.15[3]		
Constructed wetland eco-system, Beijing Olympic Forest Park	Manchurian wild rice (*Zizania latifola*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Constructed wetland eco-system, Beijing Olympic Forest Park	Plant (*Acorus calamus*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Constructed wetland eco-system, Beijing Olympic Forest Park	Soft-stem Bulrush (Scirpus *validus*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ)	MDL plant material 10-20[2] MDL (blank + 3δ)	MDL plant material 10-20[2] MDL (blank + 3δ)	UPLC-ESI-QTOF-MS	Wang *et al*. 2021

[11] MDL specific to chain length based on SD +3δ

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
							1.88 - 7.62[3]	1.67 - 10.65[3]	1.74 – 2.15[3]		
Constructed wetland eco-system, Beijing Olympic Forest Park	Plant (*Lythrum salicaria*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Constructed wetland eco-system, Beijing Olympic Forest Park	Pygmy Water Lily (*Nymphaea tetragona*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Constructed wetland eco-system, Beijing Olympic Forest Park	Common Duckweed (*Lemna minor*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Constructed wetland eco-system, Beijing Olympic Forest Park	Green algae (*Enteromorpha prolifera*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Constructed wetland eco-system, Beijing Olympic Forest Park	Water-shield (*Brasenia schreberi*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Constructed wetland eco-system, Beijing Olympic Forest Park	Water Thyme (*Hydrilla verticillata*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Constructed wetland eco-system, Beijing Olympic Forest Park	Plant (*Vallisneria natans*)	2017 mean ± sd (min-max)	ng/g dw	127±116[1] (13-593)	289 ± 148[1] (21-785)	188±116[1] (27-561)	MDL plant material 10-20[2] MDL (blank + 3δ) 1.88 - 7.62[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.67 - 10.65[3]	MDL plant material 10-20[2] MDL (blank + 3δ) 1.74 – 2.15[3]	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Constructed wetland eco-system, Beijing Olympic Forest Park	Reclaimed water	2017 Dissolved phase mean ± sd	ng/L	C_{10} – 2.0±1.5 C_{11} – 5.3±3.6 C_{12} – 7.9±6.6 C_{13} - 17±15	C_{14} - 124±81 C_{15} - 106±44 C_{16} - 111±59 C_{17} - 114±52	C_{18} - 15±6.0 C_{19} - 17±4.1 C_{20} - 12±1.9 C_{21} – 3.9±0.6 C_{22+} - ND	MDL (blank + 3δ) 0.81 – 8.64	MDL (blank + 3δ) 2.03 - 8.76	MDL (blank + 3δ) 1.06 – 5.64	UPLC-ESI-QTOF-MS	Wang *et al*. 2021

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Constructed wetland eco-system, Beijing Olympic Forest Park	Reclaimed water	2017 Particulate phase (adsorbed) mean ± sd	ng/g dw	C_{10} – 15±13 C_{11} – 47±21 C_{12} – 66±39 C_{13} - 270±125	C_{14} - 1324±611 C_{15} - 572±193 C_{16} - 505±285 C_{17} - 580±166	C_{18} - 995±581 C_{19} - 706±434 C_{20} - 599±148 C_{21} – 430±159 C_{22} - 307±204 C_{23} – 267±156 C_{24} – 212±181 C_{25} – 162±52 C_{26} – 84±23 C_{27} - 73±46	MDL (blank + 3δ) 0.81 – 8.64 ng/L	MDL (blanks + 3δ) 2.03 - 8.76 ng/L	MDL (blank + 3δ) 1.06 – 5.64 ng/L	UPLC-ESI-QTOF-MS	Wang *et al*. 2021
Western and Eastern Australian Coast	Southern Hemisphere Humpback Whale (*Megaptera novaeangliae*)	2007 - 2015 n=9 Blubber samples (2 g)	ng/g lw	<MDL–46	<MDL - >33	Not measured	MDL ∑MCCPs 33 ng (absolute mass)	MDL ∑MCCPs 33 ng (absolute mass)	n/a	Cl--APCI-QTOF-MS	Casa *et al*. 2019
South China Sea; Pearl river estuary	Indo-Pacific Humpback Dolphin (*Sousa chinensis*)	2004-2014 (n=25) Blubber samples Lipid mean: 49±19% Mean ± SD (min - max)	ng/g dw	2500 ± 2300 (430-9100	6200 ± 6500 (530-23000)	Not measured	MDL (3 x back-ground) 40	MDL (3 x back-ground) 60	Not measured	GC-ECNI-MS	Zeng *et al*. 2015
South China Sea	Finless Porpoise (*Neophocaena phocaenoides*)	2004-2014 (n=50) Blubber samples Lipid mean: 65±23%	ng/g dw	1800 ± 1000 (280-3900	3200 ± 2200	Not measured	MDL (3 x back-ground) 40	MDL (3 x back-ground) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2015

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
		Mean ± SD (min - max)			(320-8600)						
South China Sea	Broad-banded Cardinalfish (*Apogon fasciatus*)	August - November 2012 1 Pool (n=3-10) Lipid: 4.6%	ng/g lw	1010	3800	Not measured	MDL (3 x SD back-ground) 40	MDL (3 x SD back-ground) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Chinese Gizzard Shad (*Clupanodon thrissa*)	August - November 2012 n=13 Lipid (average ± sd): 41.1±10.3% mean ± sd	ng/g lw	720±175	1960±677	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Large-scale Tonguesole (*Cynoglossus arel*)	August - November 2012 1 Pool (n=3-10) Lipid: 7.9%	ng/g lw	598	810	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Goatee Croaker (*Dendrophysa russelii*)	August - November 2012 1 Pool (n=3-10) Lipid: 7.0%	ng/g lw	1050	2090	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Crimson sea-bream (*Evynnis cardinalis*)	August - November 2012 1 Pool (n=3-10) Lipid: 13.0%	ng/g lw	812	1000	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Japanese Flathead (*Inegocia japonica*)	August - November 2012 1 Pool (n=3-10) Lipid: 1.6%	ng/g lw	955	2590	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Large-scale croaker	August - November 2012 n=4	ng/g lw	886±106	1660±561	Not measured	MDL (3 x SD	MDL (3 x SD	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
	(*Johnius heterolepis*)	Lipid (mean ± sd): 7.4±3.8% mean ± sd					background) 40	background) 60			
South China Sea	Shortnose Ponyfish (*Leiognathus brevirostris*)	August - November 2012 n=6 Lipid (mean ± sd): 10.0±0.8%mean ± sd	ng/g lw	693±59.2	1540±630	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Red Big-eye (*Priacanthus macracanthus*)	August - November 2012 1 Pool (n=3-10) Lipid: 5.4%	ng/g lw	622	1230	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Silver Croaker (*Pennahia argentata*)	August - November 2012 1 Pool (n=3-10) Lipid: 6.0%	ng/g lw	903	1260	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Black-spotted Threadfin (*Polydactylus sextarius*)	August - November 2012 1 Pool (n=3-10) Lipid: 8.7%	ng/g lw	1000	1470	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Bartail Flathead (*Platycephalus indicus*)	August - November 2012 1 Pool (n=3-10) Lipid: 4.5%	ng/g lw	1220	2370	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Richard's Dragonet (*Repomucenus richardsonii*)	August - November 2012 1 Pool (n=3-10) Lipid: 4.0%	ng/g lw	781	1320	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
South China Sea	White-spotted Spinefoot (Signatus *canaliculatus*)	August - November 2012 n=7 Lipid (mean ± sd): 13.8±7.2% mean ± sd	ng/g lw	739±373	2040±1320	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Ovate Sole (*Solea ovata*)	August - November 2012 1 Pool (n=3-10) Lipid: 7.7%	ng/g lw	739	1320	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Redy Goby (*Trypaucehn vagina*)	August - November 2012 1 Pool (n=3-10) Lipid: 3.9%	ng/g lw	761	1480	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Squillid mantis shrimp (*Harpiosquilla harpax*)	August - November 2012 n=4 Lipid (mean ± sd): 8.9±1.7% mean ± sd	ng/g lw	586±94.3	975±330	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Jinga shrimp (*Metapenaeus affinis*)	August - November 2012 n=5 Lipid (mean ± sd): 5.1±0.7% mean ± sd	ng/g lw	464±177	503±272	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Small-eyed squillid mantis shrimp (*Miyakea nepa*)	August - November 2012 1 Pool (n=3-10) Lipid: 4.0%	ng/g lw	278	471	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Greasyback shrimp	August - November 2012	ng/g lw	413	525	Not measured	MDL (3 x SD	MDL (3 x SD	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
	(*Meapenaeus ensis)*	1 Pool (n=3-10) Lipid: 4.3%					background) 40	background) 60			
South China Sea	Three-spotted crab (*Portunus sanguinolentus*)	August - November 2012 n=5 Lipid (mean ± sd): 5.8±1.2% mean ± sd	ng/g lw	368±186	496±151	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Blue swimmer crab (*Portunus pelagicus*)	August - November 2012 1 Pool (n=3-10) Lipid: 4.4%	ng/g lw	474	855	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Swimming crab (*Portunus trituberculatus*)	August - November 2012 1 Pool (n=3-10) Lipid: 10.5%	ng/g lw	261	392	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Rusty Ark (mollusc) (*Anadara ferruginea*)	August - November 2012 1 Pool (n=3-10) Lipid: 10.7%	ng/g lw	363	596	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Common Frog Shell (mollusc) (*Bufonaria rana*)	August - November 2012 1 Pool (n=3-10) Lipid: 10.9%	ng/g lw	408	754	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
South China Sea	Rare-spined Murex (*Murex trapa*)	August - November 2012 1 Pool (n=3-10) Lipid: 7.7%	ng/g lw	280	563	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
South China Sea	Turreted sea snail (*Turritella bacillum*)	August - November 2012 1 Pool (n=3-10) Lipid: 6.3%	ng/g lw	302	515	Not measured	MDL (3 x SD background) 40	MDL (3 x SD background) 60	Not measured	HRGC ECNI-LRMS	Zeng *et al*. 2017
Yangtze River basin, 7 crab farms Anhui province, China	Chinese Mitten Crab (*Eriocheir* sinensis)	September – October 2019 Pooled crab meat sample (farm 1) Lipid % = 16.0	ng/g ww	28	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled crab feed sample (farm 1) Lipid % = 7.7	ng/g ww	85	18	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled frozen fresh fish (feed) sample (farm 1) Lipid % = 8.3	ng/g ww	191	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled sediment sample (farm 1)	ng/g dw	52	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 2) Lipid % = 17.7	ng/g ww	59	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled crab feed sample (farm 2) Lipid % = 9.2	ng/g ww	201	4.1	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled sediment sample (farm 2)	ng/g dw	90	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 3) Lipid % = 17.3	ng/g ww	14	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled crab feed sample (farm 3) Lipid % = 6.7	ng/g ww	346	11	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled frozen fresh fish (feed) sample (farm 3) Lipid % = 5.4	ng/g ww	155	24	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui	-	September – October 2019 Pooled sediment sample (farm 3)	ng/g dw	89	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
province, China											
Yangtze River basin, 7 crab farms Anhui province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 4) Lipid % = 17.9	ng/g ww	26	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled crab feed sample (farm 4) Lipid % = 3.3	ng/g ww	57	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled sediment sample (farm 4)	ng/g dw	60	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	Chinese Mitten Crab (*Eriocheir sinensis)*	September – October 2019 Pooled crab meat sample (farm 5) Lipid % = 20.3	ng/g ww	68	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled crab feed sample (farm 5) Lipid % = 7.8	ng/g ww	87	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms	-	September – October 2019	ng/g ww	123	3.4	Not measured	MDL (3 x SD	MDL (3 x SD	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Anhui province, China		Pooled frozen fresh fish (feed) sample (farm 5) Lipid % = 7.0					background) 7.9	background) 2.6			
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled sediment sample (farm 5)	ng/g dw	62	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 6) Lipid % = 16.9	ng/g ww	77	1.8	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled crab feed sample (farm 6) Lipid % = 12.4	ng/g ww	448	16	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled sediment sample (farm 6)	ng/g dw	79	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 7) Lipid % = 17.8	ng/g ww	25	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled crab feed sample (farm 7) Lipid % = 6.1	ng/g ww	241	11	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled frozen fresh fish (feed) sample (farm 7) Lipid % = 5.1	ng/g ww	88	4.4	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 7 crab farms Anhui province, China	-	September – October 2019 Pooled sediment sample (farm 7)	ng/g dw	59	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021
Yangtze River basin, 3 crab farms Jiangxi province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 1) Lipid % = 19.5	ng/g ww	90	2.0	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi province, China	-	September – October 2019 Pooled crab feed sample (farm 1) Lipid % = 6.8	ng/g ww	675	5.6	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi	-	September – October 2019 Pooled frozen fresh fish (feed) sample (farm 1)	ng/g ww	38	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
province, China		Lipid % = 5.1									
Yangtze River basin, 3 crab farms Jiangxi province, China		September – October 2019 Pooled aquatic plant sample (farm 1)	ng/g ww	6.5	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi province, China	-	September – October 2019 Pooled sediment sample (farm 1)	ng/g dw	76	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 2) Lipid % = 13.5	ng/g ww	60	2.5	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi province, China	-	September – October 2019 Pooled crab feed sample (farm 2) Lipid % = 7.2	ng/g ww	64	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi province, China	-	September – October 2019 Pooled sediment sample (farm 2)	ng/g dw	92	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms	Chinese Mitten Crab	September – October 2019	ng/g ww	42	Not detected	Not measured	MDL (3 x SD	MDL (3 x SD	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Jiangxi province, China	(*Eriocheir sinensis*)	Pooled crab meat sample (farm 3) Lipid % = 18.9					background d) 7.9	background d) 2.6			
Yangtze River basin, 3 crab farms Jiangxi province, China	-	September – October 2019 Pooled crab feed sample (farm 3) Lipid % = 6.2	ng/g ww	275	86	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi province, China	-	September – October 2019 Pooled frozen fresh fish (feed) sample (farm 3) Lipid % = 4.6	ng/g ww	18	Not detected	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi province, China	-	September – October 2019 Pooled aquatic plant sample (farm 3)	ng/g ww	23	Not detected	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 3 crab farms Jiangxi province, China	-	September – October 2019 Pooled sediment sample (farm 3)	ng/g dw	52	Not detected	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 1) Lipid % = 19.8	ng/g ww	246	54	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled crab feed sample (farm 1) Lipid % = 8.6	ng/g ww	157	12	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al.* (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled sediment sample (farm 1)	ng/g dw	93	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al.* (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 2) Lipid % = 14.6	ng/g ww	61	3.4	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al.* (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled crab feed sample (farm 2) Lipid % = 7.4	ng/g ww	747	94	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al.* (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled sediment sample (farm 2)	ng/g dw	113	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al.* (2021)
Yangtze River basin, 7 crab farms Shanghai	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 3) Lipid % = 23.2	ng/g ww	86	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al.* (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
province, China											
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled crab feed sample (farm 3) Lipid % = 10.2	ng/g ww	68	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled sediment sample (farm 3)	ng/g dw	164	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 4) Lipid % = 16.0	ng/g ww	127	109	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled crab feed sample (farm 4) Lipid % = 7.2	ng/g ww	256	359	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled sediment sample (farm 4)	ng/g dw	111	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms	Chinese Mitten Crab	September – October 2019	ng/g ww	291	14	Not measured	MDL (3 x SD	MDL (3 x SD	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Shanghai province, China	(*Eriocheir sinensis*)	Pooled crab meat sample (farm 5) Lipid % = 16.6					background d) 7.9	background d) 2.6			
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled corn (feed) sample (farm 5)	ng/g ww	Not detected	Not detected	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled sediment sample (farm 5)	ng/g dw	75	Not detected	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 6) Lipid % = 14.8	ng/g ww	163	4.2	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled corn (feed) sample (farm 6)	ng/g ww	Not detected	Not detected	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled sediment sample (farm 6)	ng/g dw	48	Not detected	Not measured	MDL (3 x SD background d) 7.9	MDL (3 x SD background d) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Yangtze River basin, 7 crab farms Shanghai province, China	Chinese Mitten Crab (*Eriocheir sinensis*)	September – October 2019 Pooled crab meat sample (farm 7) Lipid % = 16.0	ng/g ww	68	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled frozen fresh fish (feed) sample (farm 7) Lipid % = 5.7	ng/g ww	42	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Yangtze River basin, 7 crab farms Shanghai province, China	-	September – October 2019 Pooled sediment sample (farm 7)	ng/g dw	76	Not detected	Not measured	MDL (3 x SD background) 7.9	MDL (3 x SD background) 2.6	Not measured	Tandem 2D GCxGC-MS/MS NCI	Dong *et al*. (2021)
Shanghai, China	Domestic chicken eggs (*Gallus Gallus domesticus*)	Composite samples (n=90)	ng/g ww	28	23	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Shanghai, China	Cow's milk	Composite samples (n=90)	ng/g ww	13	5.4	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Shanghai, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	39	13	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Shanghai, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	40	12	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Fujian, China	Domestic chicken eggs (*Gallus Gallus domesticus*)	Composite samples (n=90)	ng/g ww	69	48	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Fujian, China	Cow's milk	Composite samples (n=90)	ng/g ww	34	13	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Fujian, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	81	53	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Fujian, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	75	47	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Jiangxi, China	Domestic chicken eggs (*Gallus Gallus domesticus*)	Composite samples (n=90)	ng/g ww	53	53	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Jiangxi, China	Cow's milk	Composite samples (n=90)	ng/g ww	46	15	Not Measured	MDL (3 x SD background)	MDL (3 x SD background)	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
							3.2	2.0			
Jiangxi, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	32	37	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Jiangxi, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	42	36	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Jiangsu, China	Domestic chicken eggs (*Gallus Gallus domesticus*)	Composite samples (n=90)	ng/g ww	65	87	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Jiangsu, China	Cow's milk	Composite samples (n=90)	ng/g ww	22	5.5	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Jiangsu, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	120	100	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Jiangsu, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	56	17	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Zhejiang, China	Domestic chicken eggs (*Gallus* Gallus *domesticus*)	Composite samples (n=90)	ng/g ww	70	23	Not Measured	MDL (3 x SD background)	MDL (3 x SD background)	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
							3.2	2.0			
Zhejiang, China	Cow's milk	Composite samples (n=90)	ng/g ww	43	17	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Zhejiang, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	98	57	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Zhejiang, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	71	30	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Hubei, China	Domestic chicken eggs (*Gallus Gallus domesticus*)	Composite samples (n=90)	ng/g ww	61	51	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Hubei, China	Cow's milk	Composite samples (n=90)	ng/g ww	64	23	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Hubei, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	80	95	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Hubei, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	87	72	Not Measured	MDL (3 x SD background)	MDL (3 x SD background)	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
							3.2	2.0			
Guangxi, China	Domestic chicken eggs (*Gallus* Gallus *domesticus*)	Composite samples (n=90)	ng/g ww	74	40	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Guangxi, China	Cow's milk	Composite samples (n=90)	ng/g ww	30	7.4	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Guangxi, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	45	71	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Guangxi, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	47	31	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Hunan, China	Domestic chicken eggs (*Gallus Gallus domesticus*)	Composite samples (n=90)	ng/g ww	81	30	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Hunan, China	Cow's milk	Composite samples (n=90)	ng/g ww	39	13	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Hunan, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	80	67	Not Measured	MDL (3 x SD background)	MDL (3 x SD background)	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
							3.2	2.0			
Hunan, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	36	26	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Guizhou, China	Domestic chicken eggs (*Gallus Gallus domesticus*)	Composite samples (n=90)	ng/g ww	80	62	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Guizhou, China	Cow's milk	Composite samples (n=90)	ng/g ww	47	11	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Guizhou, China	Human food (meat from food animals; terrestrial)	Composite samples (n=90)	ng/g ww	50	71	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Guizhou, China	Human food (aquatic sources)	Composite samples (n=90)	ng/g ww	45	53	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Mean from 9 provinces (Shanghai, Fujian, Jiangxi, Jiangsu, Zhejiang, Hubei, Guangxi,	Domestic chicken eggs (*Gallus Gallus domesticus*)	Mean from 9 Composite samples (n=90)	ng/g ww	64	46	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Hunan, Guizhou) China											
Mean from 9 provinces (Shanghai, Fujian, Jiangxi, Jiangsu, Zhejiang, Hubei, Guangxi, Hunan, Guizhou) China	Cow's milk	Mean from 9 Composite samples (n=90)	ng/g ww	38	12	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Mean from 9 provinces (Shanghai, Fujian, Jiangxi, Jiangsu, Zhejiang, Hubei, Guangxi, Hunan, Guizhou) China	Human food (meat from food animals; terrestrial)	Mean from 9 Composite samples (n=90)	ng/g ww	69	63	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)
Mean from 9 provinces (Shanghai, Fujian, Jiangxi, Jiangsu, Zhejiang, Hubei,	Human food (aquatic sources)	Mean from 9 Composite samples (n=90)	ng/g ww	55	36	Not Measured	MDL (3 x SD background) 3.2	MDL (3 x SD background) 2.0	Not measured	2D GCxGC ECNI-MS	Ciu *et al*. (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Guangxi, Hunan, Guizhou) China											
Norway /Scotland aqua-culture	Salmon (*Salmo salar*)	January 2016 Fresh/Frozen n=1	ng/g lw (converted from pg/µL)	228	358	Not measured	LOQ: 0.1-6	LOQ 0.4-1.2	Not measured	GC-ECNI-Orbitrap-HRMS	Krätschmer *et al*. (2018)
Norway /Scotland aqua-culture	Salmon (*Salmo salar*)	January 2016 Fresh/Frozen n=1	ng/g lw (converted from pg/µL)	195	372	Not measured	LOQ: 0.1-6	LOQ 0.4-1.2	Not measured	GC-ECNI-Orbitrap-HRMS	Krätschmer *et al*. (2018)
Norway /Scotland aqua-culture	Salmon (*Salmo salar*)	January 2016 Fresh/Frozen n=1	ng/g lw (converted from pg/µL)	194	115	Not measured	LOQ: 0.1-6	LOQ 0.4-1.2	Not measured	GC-ECNI-Orbitrap-HRMS	Krätschmer *et al*. (2018)
Norway /Scotland aqua-culture	Salmon (*Salmo salar*)	January 2016 Fresh/Frozen n=1	ng/g lw (converted from pg/µL)	1250	792	Not measured	LOQ: 0.1-6	LOQ 0.4-1.2	Not measured	GC-ECNI-Orbitrap-HRMS	Krätschmer *et al*. (2018)
Norway /Scotland aqua-culture	Salmon (*Salmo salar*)	January 2016 Fresh/Frozen n=1	ng/g lw (converted from pg/µL)	149	128	Not measured	LOQ: 0.1-6	LOQ 0.4-1.2	Not measured	GC-ECNI-Orbitrap-HRMS	Krätschmer *et al*. (2018)
Norway /Scotland aqua-culture	Salmon (*Salmo salar*)	January 2016 Fresh/Frozen n=1	ng/g lw (converted from pg/µL)	2260	694	Not measured	LOQ: 0.1-6	LOQ 0.4-1.2	Not measured	GC-ECNI-Orbitrap-HRMS	Krätschmer *et al*. (2018)
German markets, Mean of all samples	Salmon, farmed (*Salmo salar*), wild (*Oncorhynchus*	2014-2017	ng/g ww	14 (9.1; 0.97–170)	19 (13; 1.1-79)	Not measured	Values are procedural blank	Values are procedural blank	Not measured	GC/MS-ECNI-Orbitrap	Krätschmer *et al*. (2019)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
	gorbuscha and *Oncorhynchus keta*)	Mean of n=133 samples Mean (Median; minimum-maximum)					subtracted and corrected for internal standards	subtracted and corrected for internal standards			
German markets; Norwegian salmon	Salmon, farmed (*Salmo salar*), wild (*Oncorhynchus gorbuscha* and *Oncorhynchus keta*)	Norwegian salmon 2014-2017 n=74 Mean (Median; minimum-maximum)	ng/g ww	13 (9.6; 1.2-170)	21 (15; 1.1-78)	Not measured	Values are procedural blank subtracted and corrected for internal standards	Values are procedural blank subtracted and corrected for internal standards	Not measured	GC/MS-ECNI-Orbitrap	Krätschmer *et al*. (2019)
German markets; Scottish salmon	Salmon, farmed (*Salmo salar*), wild (*Oncorhynchus gorbuscha* and *Oncorhynchus keta*)	Scottish salmon 2014-2017 n=7 Mean (Median; minimum-maximum)	ng/g ww	7.9 (8.1; 2.2-12)	14 (9.3; 1.6-43)	Not measured	Values are procedural blank subtracted and corrected for internal standards	Values are procedural blank subtracted and corrected for internal standards	Not measured	GC/MS-ECNI-Orbitrap	Krätschmer *et al*. (2019)
German markets; Danish salmon	Salmon, farmed (*Salmo salar*), wild (*Oncorhynchus gorbuscha* and *Oncorhynchus keta*)	Danish salmon 2014-2017 n=14 Mean (Median; minimum-maximum)	ng/g ww	8.5 (6.0; 1.5-18)	15 (10; 1.7-43)	Not measured	Values are procedural blank subtracted and corrected for internal standards	Values are procedural blank subtracted and corrected for internal standards	Not measured	GC/MS-ECNI-Orbitrap	Krätschmer *et al*. (2019)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
German markets; Chilean salmon	Salmon, farmed (*Salmo salar*), wild (*Oncorhynchus gorbuscha* and *Oncorhynchus keta*)	Chilean salmon 2014-2016 n=5 Mean (Median; minimum-maximum)	ng/g ww	47 (40; 9.9-98)	39 (33; 11-79)	Not measured	Values are procedural blank subtracted and corrected for internal standards	Values are procedural blank subtracted and corrected for internal standards	Not measured	GC/MS-ECNI-Orbitrap	Krätschmer *et al.* (2019)
German markets; Wild salmon	Salmon, farmed (*Salmo salar*), wild (*Oncorhynchus gorbuscha* and *Oncorhynchus keta*)	Wild salmon 2014-2017 n=11 Mean (Median; minimum-maximum)	ng/g ww	5.3 (3.2; 0.97-12)	7.6 (4.6; 1.1-23)	Not measured	Values are procedural blank subtracted and corrected for internal standards	Values are procedural blank subtracted and corrected for internal standards	Not measured	GC/MS-ECNI-Orbitrap	Krätschmer *et al.* (2019)
German markets; other salmon	Salmon, farmed (*Salmo salar*), wild (*Oncorhynchus gorbuscha* and *Oncorhynchus keta*)	Other salmon 2014-2017 n=22 Mean (Median; minimum-maximum)	ng/g ww	11 (9.7; 3.1-29)	22 (18; 4.2-70)	Not measured	Values are procedural blank subtracted and corrected for internal standards	Values are procedural blank subtracted and corrected for internal standards	Not measured	GC/MS-ECNI-Orbitrap	Krätschmer *et al.* (2019)
South-China (e-waste polluted area)	Free range Chicken eggs (Gallus gallus domesticus)	2013 n=38, 2g dw of homogenised sample Mean (Median; minimum-maximum)	ng/g lw	2680 (926; 477-26200)	6100 (1030; 125-90700)	Not measured	MDL (3 x SD background) 30-45	MDL (3 x SD background) 30-45	Not measured	GC-ECNI-MS	Zeng *et al.* (2018)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
South-China (e-waste polluted area)	Free range Chicken eggs (Gallus gallus domesticus)	2016 n=30, 2g dw of homogenised sample Mean (Median; minimum-maximum)	ng/g lw	10100 (1490; 611-111000)	6830 (999; 297-91100)	Not measured	MDL (3 x SD background) 30-45	MDL (3 x SD background) 30-45	Not measured	GC-ECNI-MS	Zeng *et al*. (2018)
China, average of 20 provinces	Meat from markets (terrestrial)	2011 Lipid % = 54.2 N value not reported apart from 1800 households mean±sd	ng/g ww	129±4.1	5.7±0.59	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Beijing, China	Meat from markets (terrestrial)	2011 Lipid % = 37.7 N value not reported apart from 1800 households mean±sd	ng/g ww	118±6.1	3.2±0.28	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Shanghai, China	Meat from markets (terrestrial)	2011 Lipid % = 52.7 N value not reported apart from 1800 households mean±sd	ng/g ww	58±3.6	0.8±0.13	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Hebei, China	Meat from markets (terrestrial)	2011 Lipid % = 46.1 N value not reported apart from 1800 households mean±sd	ng/g ww	207±9.7	23.7±2.3	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Henan, China	Meat from markets (terrestrial)	2011 Lipid % = 33.2	ng/g ww	260±10.9	5.2±0.74	Not measured	MDL (3 x SD background)	MDL (3 x SD background)	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
		N value not reported apart from 1800 households mean±sd					0.6	0.2			
Liaoning, China	Meat from markets (terrestrial)	2011 Lipid % = 45.1 N value not reported apart from 1800 households mean±sd	ng/g ww	140±7.5	11.2±2.2	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Jilin, China	Meat from markets (terrestrial)	2011 Lipid % = 57.1 N value not reported apart from 1800 households mean±sd	ng/g ww	40.6±1.7	1.2±0.26	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Heilongjiang, China	Meat from markets (terrestrial)	2011 Lipid % = 65.5 N value not reported apart from 1800 households mean±sd	ng/g ww	21.6±2.4	0.3±0.05	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Hunan, China	Meat from markets (terrestrial)	2011 Lipid % = 62.5 N value not reported apart from 1800 households mean±sd	ng/g ww	43.6±2.9	1.7±0.38	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Fujian, China	Meat from markets (terrestrial)	2011 Lipid % = 49.6 N value not reported apart from 1800 households mean±sd	ng/g ww	121±3.9	11.4±1.3	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Zhejiang, China	Meat from markets (terrestrial)	2011 Lipid % = 44.2 N value not reported apart from 1800 households mean±sd	ng/g ww	469±13.6	23.8±1.5	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Jiangsu, China	Meat from markets (terrestrial)	2011 Lipid % = 43.4 N value not reported apart from 1800 households mean±sd	ng/g ww	62.3±4.1	2.7±0.37	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Jiangxi, China	Meat from markets (terrestrial)	2011 Lipid % = 57.2 N value not reported apart from 1800 households mean±sd	ng/g ww	15.7±1.3	0.4±0.13	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Ningxia, China	Meat from markets (terrestrial)	2011 Lipid % = 82.6 N value not reported apart from 1800 households mean±sd	ng/g ww	139±12.0	8.3±0.84	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Guangdong, China	Meat from markets (terrestrial)	2011 Lipid % = 46.2 N value not reported apart from 1800 households mean±sd	ng/g ww	152±11.0	6.3±0.42	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Neimenggu, China	Meat from markets (terrestrial)	2011 Lipid % = 53.9 N value not reported apart from 1800 households	ng/g ww	171±0.91	2.2±0.51	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
		mean±sd									
Shanxi, China	Meat from markets (terrestrial)	2011 Lipid % = 64.9 N value not reported apart from 1800 households mean±sd	ng/g ww	121±8.3	1.7±0.46	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Hubei, China	Meat from markets (terrestrial)	2011 Lipid % = 57.2 N value not reported apart from 1800 households mean±sd	ng/g ww	68.6±6.8	0.5±0.12	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Guangxi, China	Meat from markets (terrestrial)	2011 Lipid % = 48.9 N value not reported apart from 1800 households mean±sd	ng/g ww	43.8±5.8	1.6±0.37	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Sichuan, China	Meat from markets (terrestrial)	2011 Lipid % = 63.2 N value not reported apart from 1800 households mean±sd	ng/g ww	222±14.0	5.9±0.91	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Qinghai, China	Meat from markets (terrestrial)	2011 Lipid % = 73.2 N value not reported apart from 1800 households mean±sd	ng/g ww	107±8.4	2.1±0.42	Not measured	MDL (3 x SD background) 0.6	MDL (3 x SD background) 0.2	Not measured	GCxGC-ECNI-HRTOF-MS TIC	Huang *et al*. (2018)
Baltic Sea, benthic food web, Darsser Ort,	Blue mussel (*Mytilus edulis*)	2015 Soft body n=100 pooled Lipid % = 1.40	ng/g lw	72	210	120	LOQ: 63	LOQ: 98	LOQ: 6.3	APCI-QTOF-MS	De Wit *et al*. (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Arkona Basin											
Baltic Sea, benthic food web, Darsser Ort, Arkona Basin	Viviparous eelpout (*Zoarces viviparous*)	2015 Muscle n=47 pooled Lipid % = 1.52	ng/g lw	52	130	130	LOQ: 34	LOQ: 52	LOQ: 3.4	APCI-QTOF-MS	De Wit *et al*. (2020)
Neimenggu, China, Industrial area	Cow's milk	n=10 mean (median; minimum-maximum)[12] Lipid % =4.23 (4.20; 3.80-4.60)[1]	ng/g lw	1088 (1040; 490-1870)	63.88 (57; 6.8-170)	Not measured	MDL (blank + 3δ) 12	MDL (blank + 3δ) 6.8	Not measured	GCxGC-MS/MS-NCI	Dong *et al*. (2020)
Neimenggu, China, non-CP production area	Cow's milk	n=10 mean (median; minimum-maximum)[1] Lipid % =3.98 (4.00; 3.40-4.60)[1]	ng/g lw	490 (535; 130-700)	71.38 (81.5; 6.8-126)	Not measured	MDL (blank + 3δ) 12	MDL (blank + 3δ) 6.8	Not measured	GCxGC-MS/MS-NCI	Dong *et al*. (2020)
Hebei, China	Cow's milk	n=9 mean (median; minimum-maximum)[1] Lipid % =3.22 (3.10; 2.40-4.30)[1]	ng/g lw	2174.44 (1860; 1420-3210)	329.11 (330; 72-520)	Not measured	MDL (blank + 3δ) 12	MDL (blank + 3δ) 6.8	Not measured	GCxGC-MS/MS-NCI	Dong *et al*. (2020)

[12] Calculated by the Environment Agency, from raw data.

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Shandong, China	Cow's milk	n=10 mean (median; minimum-maximum)[1] Lipid % =3.74 (3.90; 2.40-4.20)[1]	ng/g lw	1355 (1190; 930-2720)	180.2 (170; 56-330)	Not measured	MDL (blank + 3δ) 12	MDL (blank + 3δ) 6.8	Not measured	GCxGC-MS/MS-NCI	Dong *et al*. (2020)
Henan, China	Cow's milk	n=10 mean (median; minimum-maximum)[1] Lipid % =3.43 (3.40; 2.40-4.30)[1]	ng/g lw	1363 (1330; 1140-1610)	260.8 (230; 63-800)	Not measured	MDL (blank + 3δ) 12	MDL (blank + 3δ) 6.8	Not measured	GCxGC-MS/MS-NCI	Dong *et al*. (2020)
Hubei, China	Cow's milk	n=9 mean (median; minimum-maximum)[1] Lipid % =3.46 (3.60; 2.70-4.00)[1]	ng/g lw	2518.89 (2260; 1200-5770)	102.78 (100; 16-250)	Not measured	MDL (blank + 3δ) 12	MDL (blank + 3δ) 6.8	Not measured	GCxGC-MS/MS-NCI	Dong *et al*. (2020)
Hebei, China	Cow's feed (silage)	Similar congener pattern to that found in milk. n=9 mean (median; minimum-maximum)[1] Moisture content % =72 (72; 66-79)[1]	ng/g dw	750 (740; 330-1120)	36 (25; 18-69)	Not measured	MDL (blank + 3δ) 10	MDL (blank + 3δ) 4.5	Not measured	GCxGC-MS/MS-NCI	Dong *et al*. (2020)
Average across 18 provinces, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=18 Mean (minimum-maximum Lipid % = 7.2 (1.2-13.2)	ng/g ww	1472 (215-4200)	80.5 (9.0-586)	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Beijing, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 6.4	ng/g ww	934	77.4	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Fujian, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 2.2	ng/g ww	880	34.4	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Guangdong, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 8.2	ng/g ww	1379	586	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Guangxi, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 12.6	ng/g ww	4200	301	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Hebei, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 5.3	ng/g ww	215	11.9	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Henan, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 11.4	ng/g ww	551	33.2	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Heilongjiang, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 10.5	ng/g ww	730	21.7	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Hubei, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 1.2	ng/g ww	385	9.0	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Hunan, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 8.6	ng/g ww	3476	32.0	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Jilin, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 3.9	ng/g ww	503	19.8	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Jiangsu, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 7.6	ng/g ww	1362	26.1	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Liaoning, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 8.0	ng/g ww	2913	56.9	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Neimenggu, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 4.4	ng/g ww	1053	30.8	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Ningxia, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 5.2	ng/g ww	238	39.6	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Qinghai, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 8.8	ng/g ww	1172	36.3	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Shanxi, China	Composite Aquatic foods sample[1]	Composite aquatic foods sample n=1 Lipid % = 13.2	ng/g ww	2795	54.0	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Shanghai, China	Composite aquatic foods[1]	Composite aquatic foods sample n=1 Lipid % = 5.5	ng/g ww	2778	39.8	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Sichuan, China	Composite Aauatic foods[1]	Composite aquatic foods sample n=1 Lipid % = 7.3	ng/g ww	935	38.8	Not measured	MDL (blank + 3δ) 2	MDL (blank + 3δ) 1	Not measured	GCxGC-ECNI-TOF-MS	Wang *et al*. (2018)
Iqaluit, Nanavut, Canada; Kagnitsuatsia	Arctic char (*Salvelinus alpinus*)	Male n=20 Female **n=16** Combined n=36 Mean±SD (minimum-maximum)	ng/g ww	6.8±9.6 (ND-38.8) 9.1±23.0 (ND-96.0) 7.8±17.0 (ND-96.0)	6.2±8.1 (ND-29.0) **7.6±14.2 (ND-54.5)** 6.8±11.1 (ND-54.5)	Not measured	0.2	0.1	Not measured	GC-HRMS	Dick *et al*. (2010)
Iqaluit, Nanavut, Canada, Peterhead inlet	Arctic char (*Salvelinus alpinus*)	n=3 Mean±SD (minimum-maximum)	ng/g ww	1.6±2.8 (ND-4.9)	3.7±1.8 (2.79-6.45)	Not measured	0.2	0.1	Not measured	GC-HRMS	Dick *et al*. (2010)
Iqaluit, Nanavut, Canada, Iqalu-gaajuruluit lake	Arctic char (*Salvelinus alpinus*)	n=1	ng/g ww	12.1	13.3	Not measured	0.2	0.1	Not measured	GC-HRMS	Dick *et al*. (2010)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Iqaluit, Nanavut, Canada, Old military dump	Ninespine stickleback (*Pungitius pungitius*)	2 pooled samples of n=30 Mean±SD (minimum-maximum)	ng/g ww	12.2±2.2 (10.7-13.8)	24.9±10.9 (17.2-32.7)	Not measured	0.2	0.1	Not measured	GC-HRMS	Dick *et al*. (2010)
Longtang Town, Qingyuan County, Guangdong province	Chinese watersnake (*Enhydris chinensis*)	Muscle **n=7** Egg n=3 Muscle lipid % =0.75±0.22 Egg lipid % =14±2.3 Mean (minimum-maximum)	µg/g lw	**70 (29-250)** 18 (8.4-81)	**93 (37-200)** 14 (8.2-23)	Not measured	Not reported	Not reported	Not measured	GC/MS-ECNI	Guan *et al*. (2020)
Longtang Town, Qingyuan County, Guangdong province	Common carp (*Cyprinus carp*io)	n=4 Lipid % =1.2±0.22 Mean (minimum-maximum)	µg/g lw	28 (27-29)	45 (32-58)	Not measured	Not reported	Not reported	Not measured	GC/MS-ECNI	Guan *et al*. (2020)
Longtang Town, Qingyuan County, Guangdong province	Oriental river prawn (*Macrobrachium niponense*)	n=4 Lipid % =1.4±0.07 Mean (minimum-maximum)	µg/g lw	7.8 (6.1-9.5)	6.4 (2.8-7.0)	Not measured	Not reported	Not reported	Not measured	GC/MS-ECNI	Guan *et al*. (2020)
Longtang Town, Qingyuan County, Guangdong province	White-breasted waterhen (Anaurornis *phoenicurus*)	Eggs n=6 Lipid % =11±0.69 Mean (minimum-maximum)	µg/g lw	1.8 (1.2-2.5)	2.8 (2.3-5.0)	Not measured	Not reported	Not reported	Not measured	GC/MS-ECNI	Guan *et al*. (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Norwegian coastline, Sklinna & Røst (remote colonies)	Common eider (*Somateria mollisima*)	May-June 2012 Sklinna **2 pooled samples of n=3** Røst 4 pooled samples of n=3 Individual pool values separated by semi-colon	ng/g ww	**2.46;<2.00** 2.45; 4.76; 2.51; <2.00	**1.00; 0.97** 1.07; 17.5; 1.70; 0.79	Not measured	Signal to noise ration 3:1	Signal to noise ration 3:1	Not measured	GC-MS/MS	Huber *et al*. (2015)
Norwegian coastline, Sklinna & Røst (remote colonies)	European shag (*Phalacrocorax aristotelis aristotelis*)	May-June 2012 **Sklinna 2 pooled samples of n=3** Røst 4 pooled samples of n=3 Individual pool values separated by semi-colon	ng/g ww	**<2.00; <2.00** <2.00; <2.00; <2.00; <2.00	**<0.76; 0.97** 7.12; 2.71; 1.76; 0.80	Not measured	Signal to noise ration 3:1 2.00	Signal to noise ration 3:1 0.76	Not measured	GC-MS/MS	Huber *et al*. (2015)
Norwegian coastline, Sklinna & Røst (remote colonies)	European herring gull (*Larus argentatus*)	May-June 2012 Sklinna **2 pooled samples of n=3** Røst 4 pooled samples of n=3 Individual pool values separated by semi-colon	ng/g ww	**<2.65; <2.00** 2.66; <2.00; <2.00; 2.06	**1.21; 1.18** 1.19; <0.76; <0.76; <0.76	Not measured	Signal to noise ration 3:1	Signal to noise ration 3:1	Not measured	GC-MS/MS	Huber *et al*. (2015)
Oslofjord, Oslo, Norway, Inner fjord, Søndre Skjælholmen (high pollution)	Urban herring gulls (*Larus argentatus*)	Paired egg and blood samples Blood **n=15 pooled** Egg n=15 pooled Mean±sd (minimum-maximum) δ^{13}C blood -24.45±0.35	ng/g ww	**50.3±32.4 (14.0-108)** 35.0±24.9 (13.0-91)	**28.3±23.8 (8.00-76.0)** 29.1±19.8 (6.00-68.0)	Not measured	MDL (3 x SD background) All samples above LOD	MDL (3 x SD background) All samples above LOD	Not measured	GC/Q-ToF-ECNI-MS	Knudtzon *et al*. (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
		δ13C egg -25.79±0.75 δ15N blood 8.43±0.73 δ15N egg 8.92±1.08									
Oslofjord, Oslo, Norway, Outer fjord, Store Revlingen (low pollution)	Urban herring gulls (*Larus argentatus*)	Paired egg and blood samples Blood **n=15 pooled** Egg n=15 pooled Mean±sd (minimum-maximum) δ^{13}C blood -23.79±1.01 δ13C egg -24.98±1.15 δ15N blood 10.01±1.14 δ^{15}N egg 10.89±1.37	ng/g ww	**30.3±49.0 (5.0-200)** 42.0±46.3 (18.0-178)	**38.9±64.6 (6.00-200)** 69.6±160 3.00-630	Not measured	MDL (3 x SD background) All samples above LOD	MDL (3 x SD background) All samples above LOD	Not measured	GC/Q-ToF-ECNI-MS	Knudtzon *et al.* (2021)
Rhône river basin, France, Chéran river	Common Barbel (*Barbus barbus*)	Muscle n=3 Lipid % =1.7±0.6 mean±SD	ng/g lw	842±224	7123±2802	Not measured	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determined for each congener	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determined for each congener	Not measured	GC/Q-ToF-ECNI-MS	Labadie *et al.* (2019)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Rhône river basin, France, Usses river	Common Barbel (*Barbus barbus*)	Muscle n=5 Lipid % =2.0±0.9 mean±SD	ng/g lw	644±713	4615±3823	Not measured	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determined for each congener	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determined for each congener	Not measured	GC/Q-ToF-ECNI-MS	Labadie *et al.* (2019)
Rhône river basin, France, Combeauté river	Common Barbel (*Barbus barbus*)	Muscle n=4 Lipid % =3.3±0.7 mean±SD	ng/g lw	796±291	5423±1539	Not measured	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determined for each congener	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determined for each congener	Not measured	GC/Q-ToF-ECNI-MS	Labadie *et al.* (2019)
Rhône river basin, France, Rhône river	Common Barbel (*Barbus barbus*)	Muscle n=5 Lipid % =5.9±0.8 mean±SD	ng/g lw	379±395	904±866	Not measured	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determine	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determine	Not measured	GC/Q-ToF-ECNI-MS	Labadie *et al.* (2019)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
							d for each congener	d for each congener			
Rhône river basin, France, Morge canal	Common Barbel (*Barbus barbus*)	Muscle n=5 Lipid % =1.4±0.3 mean±SD	ng/g lw	862±517	3292±1644	Not measured	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determined for each congener	MDL: SD of blank x Student's t-value at 99th percentile for n-1 degrees of freedom determined for each congener	Not measured	GC/Q-ToF-ECNI-MS	Labadie *et al*. (2019)
Freshwater lakes Canada, Kusawa lake	Lake trout	2010-2011 n=10 Mean±SD Lipid % = 10.4±5.0	ng/g lw	22.0±17.6	13.4±11.0	Not measured	Blank corrected as significantly lower blank than sample conc.	Blank corrected as significantly lower blank than sample conc.	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)
Freshwater lakes Canada, Columbia river	Walleye	2010-2011 n=10 Mean±SD Lipid % =4.9±0.9	ng/g lw	110.2±114.9	28.8±23.5	Not measured	Blank corrected as significantly lower blank than sample conc.	Blank corrected as significantly lower blank than sample conc.	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)
Freshwater lakes Canada, Lake Athabasca	Lake trout	2010-2011 n=10 Mean±SD Lipid % = 12.3±6.7	ng/g lw	93.2±114.0	45.2±16.6	Not measured	Blank corrected as significantly lower	Blank corrected as significantly lower	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
							blank than sample conc.	blank than sample conc.			
Freshwater lakes Canada, Lake Superior	Lake trout	2010-2011 n=10 Mean±SD Lipid % = 13.5±5.5 $\delta^{13}C$= -27.6±1.0 δ15N= 9.6±0.6	ng/g lw	22.4±19.4	32.1±28.8	Not measured	Blank corrected as significantly lower blank than sample conc.	Blank corrected as significantly lower blank than sample conc.	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)
Freshwater lakes Canada, Lake Huron	Lake trout	2010-2011 n=10 Mean±SD Lipid % = 14.0±3.7 $\delta^{13}C$= -25.9±1.0 $\delta^{15}N$= 12.7±0.7	ng/g lw	25.6±23.6	100.1±118.8	Not measured	Blank corrected as significantly lower blank than sample conc.	Blank corrected as significantly lower blank than sample conc.	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)
Freshwater lakes Canada, Lake Erie	Lake trout	2010-2011 n=10 Mean±SD Lipid % = 20.3±3.0 $\delta^{13}C$= -26.3±0.5 $\delta^{15}N$= 17.8±0.3	ng/g lw	12.2±7.2	57.1±39.2	Not measured	Blank corrected as significantly lower blank than sample conc.	Blank corrected as significantly lower blank than sample conc.	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)
Freshwater lakes Canada, Lake Ontario	Lake trout	2010-2011 n=10 Mean±SD Lipid % = 14.1±3.1 $\delta^{13}C$= -26.7±0.6 $\delta^{15}N$= 17.5±0.4	ng/g lw	37.2±20.8	91.4±41.9	Not measured	Blank corrected as significantly lower blank than sample conc.	Blank corrected as significantly lower blank than sample conc.	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Freshwater lakes Canada, St. Lawrence river	Walleye	2010-2011 n=10 Mean±SD Lipid % = 6.6±1.6 $\delta^{13}C$= -20.9±0.3 $\delta^{15}N$= 14.7±0.3	ng/g lw	83.8±50.6	88.4±79.4	Not measured	Blank corrected as significantly lower blank than sample conc.	Blank corrected as significantly lower blank than sample conc.	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)
Freshwater lakes Canada, Kejimikujik lake	Brook trout	2010-2011 n=10 Mean±SD Lipid % = 4.7±2.9	ng/g lw	288.0± 300.7	129.6±160.5	Not measured	Blank corrected as significantly lower blank than sample conc.	Blank corrected as significantly lower blank than sample conc.	Not measured	HR-ECNI-MS	Basconcillo *et al*. (2015)
Norway, Svalbard	Polar bear (*Ursus maritimus*)	2012 n=20 plasma samples Lipid %=0.9 mean±sd	ng/mL plasma	3.99±2.91	2.20±1.84	Not measured	MDL not reported, 95% of samples above detection limit	MDL not reported, 95% of samples above detection limit	Not measured	GC-HRMS	Norwegian Climate and pollution Agency (Klif; 2013)
Norway, Kongsfjord, Svalbard	Kittiwake (*Rissa tridactyla*)	2012 n=12 eggs Lipid %=8.1	ng/g ww	7.83±8.26	4.91±4.88	Not measured	MDL not reported, 67% of samples above detection limit	MDL not reported, 100% of samples above detection limit	Not measured	GC-HRMS	Klif 2013
Norway, Kongsfjord, Svalbard	Common eiders (*Somateria mollissima*)	2012 n=12 eggs Lipid %=17.4	ng/g ww	3.23±1.77	4.24±4.07	Not measured	MDL not reported, 83% of samples above	MDL not reported, 100% of samples above	Not measured	GC-HRMS	Klif 2013

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
							detection limit	detection limit			
Norway, Kongsfjord, Svalbard	Glaucous gull (*Larus hyperboreus*)	2012 n=12 plasma samples Lipid %=14.4	ng/mL plasma	3.95±1.99	8.87±9.88	Not measured	MDL not reported, 75% of samples above detection limit	MDL not reported, 67% of samples above detection limit	Not measured	GC-HRMS	Klif 2013
Norway, Kongsfjord, Svalbard	Ringed seal (*Phoca hispida*)	2010 n=10 plasma samples Lipid %=0.7	ng/mL plasma	4.96±2.70	2.91±2.39	Not measured	MDL not reported, 100% of samples above detection limit	MDL not reported, 90% of samples above detection limit	Not measured	GC-HRMS	Klif 2013
Norway, Svalbard	Atantic cod (*Gadus morhua*)	2012 n=10 liver samples Lipid %=50.5	ng/g ww	10.3±10.7	0.94	Not measured	MDL not reported, 100% of samples above detection limit	MDL not reported, 10% of samples above detection limit	Not measured	GC-HRMS	Klif 2013
Norway, Svalbard	Polar cod (*Boreogadus saida*)	2012 1 pooled whole fish sample Lipid %=1.7	ng/g ww	2.28	1.51	Not measured	MDL not reported, 100% of samples above detection limit	MDL not reported, 100% of samples above detection limit	Not measured	GC-HRMS	Klif 2013
Washington USA, Clayton Beach	Sand Lance (fish; *Ammodytes personatus*)	05/12/2010 n=9 pooled Moisture %= 77.9 Lipid %= 2.19	**ng/g** ww ng/g lw	**270** 12300	**175** 7990	**38** 1760	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Washington USA, Clayton Beach	Sand Lance (fish; *Ammodytes personatus*)	16/02/2011 n=10 pooled Moisture %= 76.8 Lipid %= 1.36	**ng/g** ww ng/g lw	**152** 11200	**<125** <9200	**23.9** 1760	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)
Washington USA, Eagle harbour	Sand Lance (fish; Ammodytes *personatus*)	09/05/2012 n=9 pooled Moisture %= 74.3 Lipid %= 4.55	**ng/g ww** ng/g lw	**<126** <2770	**<126** <2770	**<22.6** <496	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)
Washington USA, Eagle harbour REP	Sand Lance (fish; *Ammodytes personatus*)	09/05/2012 n=9 pooled Moisture %= 74.9 Lipid %= 4.57	**ng/g ww** ng/g lw	**207** 4530	**137** 3000	**24.2** 529	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)
Washington USA, Eagle harbour LG	Sand Lance (fish; *Ammodytes personatus*)	09/05/2012 n=5 pooled Moisture %= 74.4 Lipid %= 4.38	**ng/g** ww ng/g lw	**376** 8590	**305** 6960	**54.3** 1240	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)
Washington USA, Point Monroe	Sand Lance (fish; *Ammodytes personatus*)	15/06/2012 n=10 pooled Moisture %= 72.5 Lipid %= 7.58	**ng/g ww** ng/g lw	**341** 4500	**265** 3500	**48.4** 639	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)
Washington USA, Liberty Bay	Sand Lance (fish; *Ammodytes personatus*)	17/06/2012 n=19 pooled Moisture %= 75.8 Lipid %= 4.54	**ng/g ww** ng/g lw	**<125** <2760	**<125** <2760	**<22.5** <496	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)
Washington USA, Agate Pass	Sand Lance (fish; *Ammodytes personatus*)	18/06/2012 n=22 pooled Moisture %= 76.0 Lipid %= 3.86	**ng/g** ww ng/g lw	**166** 4300	**143** 3710	**23.8** 617	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)
Washington USA, Nisqually	Sand Lance (fish; *Ammodytes personatus*)	18/06/2014 n=23 pooled Moisture %= 76.7 Lipid %= 4.16	**ng/g** ww ng/g lw	**140** 3370	**<125** <3000	**<22.6** <543	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Washington USA, Lopez Island	Sand Lance (fish; *Ammodytes personatus*)	14/08/2014 n=35 pooled Moisture %= 78.4 Lipid %= 2.59	**ng/g** ww ng/g lw	**159** 6140	**<124** <4790	**<22.2** <859	125ng/g ww	125ng/g ww	22.5ng/g ww	HRGC-LRMS	Conn *et al.* (2020)
Washington USA, Lake Washington	Common Carp (*Cyprinus carpio*)	Muscle, n=1 Lipid %= 2.3	ng/g ww **ng/g** lw[1]	194 **8434.8**	107 **4652.2**	18.2 **791.3**	1 **43.48**	1 **43.48**	1 **43.48**	LR-GC/MS	Johnson *et al.* (2012)
Washington USA, Lower Columbia River	Common Carp (*Cyprinus carpio*)	Muscle, n=5 Lipid %= 4.0	ng/g ww **ng/g lw[1]**	242 6050	132 3300	30.7 767.5	1 **25**	1 **25**	1 **25**	LR-GC/MS	Johnson *et al.* (2012)
Washington USA, Lower Yakima River	Common Carp (*Cyprinus carpio*)	Muscle, n=4 Lipid %= 4.6	ng/g ww **ng/g** lw[1]	459 9978.3	190 4130.4	39.2 852.2	1 **21.7**	1 21.**7**	1 **21.7**	LR-GC/MS	Johnson *et al.* (2012)
Washington USA, Lake Spokane	Common Carp (*Cyprinus carpio*)	Muscle, n=3 Lipid %= 2.4	ng/g ww **ng/g** lw[1]	340 **14166.7**	208 **8666.7**	28.9 **1204.2**	1 **41.7**	1 **41.7**	1 **41.7**	LR-GC/MS	Johnson *et al.* (2012)
Washington USA, Lake Washington	Largescale sucker (*Catostomus macrocheilus*)	Whole fish, n=5 Lipid %= 9.9	ng/g ww **ng/g** lw[1]	895 **9040.4**	663 **6697.0**	108 **1090.9**	1 **10.1**	1 **10.1**	1 **10.1**	LR-GC/MS	Johnson *et al.* (2012)
Washington USA, Lower Columbia River	Largescale sucker (*Catostomus macrocheilus*)	Whole fish, n=3 Lipid %= 6.1	ng/g ww **ng/g** lw[1]	391 **6409.8**	259 5647.1	53.2 1057.6	1 16.**4**	1 **16.4**	1 **16.4**	LR-GC/MS	Johnson *et al.* (2012)
Washington USA, Lower Yakima River	Largescale sucker (*Catostomus macrocheilus*)	Whole fish, n=5 Lipid %= 8.5	ng/g ww **ng/g** lw[1]	541 **6364.7**	480 5647.1	89.9 2444.4	1 11.**8**	1 11.**8**	1 **11.8**	LR-GC/MS	Johnson *et al.* (2012)

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Washington USA, Lake Spokane	Largescale sucker (*Catostomus macrocheilus*)	Whole fish, n=5 Lipid %= 2.7	ng/g ww **ng/g** lw[1]	353 13074.1	245 9074.1	66.0 2444.4	1 **37.0**	1 **37.0**	1 **37.0**	LR-GC/MS	Johnson *et al.* (2012)
St Lawrence Estuary, Eastern Canada	Beluga whale (*Delphinapterus leucas)*	September 2015&2016 n=40 male skin and blubber samples mean±SD (minimum-maximum)	ng/g ww **ng/g** lw[1]	6545± 1325 (<MDL-30745) **60348± 11740 (<MDL-272578**	Not measured	Not measured	MDL: S/N=3 MQL: S/N=10	Not measured	Not measured	GC/MS-ECNI	Simond *et al.* (2020)
Western Hudson Bay	Polar bear (*Ursus maritimus*)	2013-2014 n=17 Liver and subcutaneous fat samples Adult females n=1, lipid % =91 **Adult males n=12, lipid % = 84±8.7** Subadults male and female n=4, lipid % =85±12 Mean (95% confidence)	ng/g lw	28.2 163 (111-240) 303 (160-571)	Not measured	Not measured		Not measured	Not measured	HRGC-HRMS	Letcher *et al.* (2018)
Southern Hudson Bay	Polar bear (*Ursus maritimus*)	2013-2014 n=24 Liver and subcutaneous fat samples Adult females n=5, lipid % =84±2.6 **Adult males n=10, lipid % = 88±5.0**	ng/g lw	136 (31-598) 117.5 (50.7-272) 163 (81.1-326)	Not measured	Not measured	MDL: S/N 3:1	Not measured	Not measured	HRGC-HRMS	Letcher *et al.* (2018)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
		Sub-adults male and female n=9, lipid % =85±8.4 Mean (95% confidence)									
Liaodong Bay, North China	Bastard halibut (*Cleisthenes herzensteini*)	n=5 Lipid % =1.94 Moisture % =78.28 Trophic level =3.81 mean±sd	ng/g lw	8596± 2751	706.5± 240.2	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Turbot (*Scophthalmus maximus*)	n=1 Lipid % =0.91 Moisture % =79.77 Trophic level =3.87 mean±sd	ng/g lw	4035± 1735	5097± 2242	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Ray (*Rajiformes*)	n=8 Lipid % =0.84 Moisture % =92.50 Trophic level =3.53 mean±sd	ng/g lw	2233± 938	109.0± 44.6	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Navadon Septentrionalis (*Thamnaconus modestus*)	n=3 Lipid % =0.54 Moisture % =77.60 Trophic level =3.41 mean±sd	ng/g lw	1750± 612	375.9± 120.2	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Yellow Croaker (*Larimichthys polyactis*)	n=15 Lipid % =6.97 Moisture % =74.50 Trophic level =3.62 mean±sd	ng/g lw	1383± 567	55.19± 23.73	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Bass (*Cantharus*)	n=2 Lipid % =2.94 Moisture % =79.35 Trophic level =3.18 mean±sd	ng/g lw	974.5± 428.7	24.57± 10.31	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Capelin (*Mallotus-villosus*)	n=23 Lipid % =9.19 Moisture % =70.48 Trophic level =3.33 mean±sd	ng/g lw	863.0± 310.6	30.26± 11.49	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
Liaodong Bay, North China	Spanish Mackerel (Spanish *lacertus*)	n=3 Lipid % =4.19 Moisture % =75.38 Trophic level =3.65 mean±sd	ng/g lw	660.2± 257.4	53.92± 22.64	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Abalone (Abalone)	n=10 Lipid % =0.70 Moisture % =76.27 Trophic level =2.98 mean±sd	ng/g lw	440.2± 184.8	63.48± 24.75	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Cod (*Gadus*)	n=3 Lipid % =0.71 Moisture % =81.85 Trophic level =3.56 mean±sd	ng/g lw	376.3± 169.3	22.37± 9.17	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Jellyfish (*Rhopilema*)	n=3 Lipid % = 0.12 Trophic level = 2.31 Mean	ng/g lw	2622	448.2	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Conch neptunea (*Neptunea cumingi Crosse*)	n=10 Lipid % =3.94 Trophic level = 2.61 mean±sd	ng/g lw	648.2	64.97	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Clam (Clam)	n=33 Lipid % = 7.19 Trophic level = 2.99 mean±sd	ng/g lw	1033	185.1	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	*Patinopecten yessoensis* (invertebrate)	n=20 Lipid % = 4.10 Trophic level = 3.05 mean±sd	ng/g lw	2347	335.8	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)
Liaodong Bay, North China	Mantis shrimp (*Oratosquilla oratoria*)	n=12 Lipid % = 11.67 Trophic level = 3.78 mean±sd	ng/g lw	3343	16.72	Not measured	MDL: blank+3sd 9.4	MDL: blank+3sd 7.0	Not measured	GCxGC-ECNI-HRTOF-MS	Huang *et al*. (2018)

Location	Species	Year /Comment	Units	Conc[m] SCCP	Conc[m] MCCP	Conc[m] LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
North East Atlantic Ocean, Iceland	Greenland shark (*Somniosus microcephalus*)	April 2001-October 2003 n=15 female liver samples Lipid % = 55 (46-75) median (min-max)	ng/g lw	430 (<MDL-5200)	Not measured	Not measured	MDL: Blank+3sd 55	Not measured	Not measured	GC-HRMS-ECNI	Strid *et al*. (2013
Melville bay, Greenland	Narwhal (*Monodon Monoceros*)	2018 Adult males n=2 Muscle **Cl%=51** Blubber Cl%=64 (min-max)	ng/g lw	**(<22-31)** (<5.2-16)	**(<**48) (<10)	**(<2.4)** (<0.41-0.66)	Mean blank +3sd **26** 5.8	Mean blank +3sd **41.5** 9.15	Mean blank +3sd **2.05** 0.46	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)
Maniitsoq & Nuuk, Greenland	Harbour porpoise (*Phocoena phocoena*)	2018 Calf-adult n=5 Blubber Median (min-max) Mean Cl%=61%	ng/g lw	13 (<6.1-24	<15 (<9.8-18)	<0.76 (<0.48-1.1)	Mean blank +3sd 8.8	Mean blank +3sd 14.1	Mean blank +3sd 0.70	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)
Nuuk, Greenland	Blue mussel (*Mytilus edulis*)	2020 Soft tissue n=2 pooled samples (min-max) Mean Cl%=55	ng/g lw	(69-300)	(87-250)	(26-67)	Mean blank +3sd 15	Mean blank +3sd 24.5	Mean blank +3sd 1.2	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)
Nuuk, Greenland	Iceland scallop (*Chlamys islandica*)	2018 Soft tissue n=1 pooled sample Cl%=52	ng/g lw	<68	120	10	Mean blank +3sd 68	Mean blank +3sd 110	Mean blank +3sd 5.3	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)
Tasiilaq, Greenland	Killer whale (*Orcinus orca*)	2016 N=1 adult female Muscle **Cl%=53** Blubber Cl%=57	ng/g lw	**20** 9.7	**35** <14	**2.0** <0.67	Mean blank +3sd **7.4** 8.5	Mean blank +3sd **12** 14	Mean blank +3sd **0**.58 0.67	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)
Tasiilaq, Greenland	Minke whale (*Balaenoptera acutorostrata*)	2017 **n=1 female fetus muscle Cl%=52**	ng/g lw	**6.0** 20	**19** 85	**0.73** 2.9	Mean blank +3sd **4.9**	Mean blank +3sd **7.9**	Mean blank +3sd **0**.39	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)

Location	Species	Year /Comment	Units	Conc^{m} SCCP	Conc^{m} MCCP	Conc^{m} LCCP	LOD/Q SCCP	LOD/Q MCCP	LOD/Q LCCP	Method	Reference
		n=1 adult female muscle Cl%=51					15	24	1.2		
Tasiilaq, Greenland	Pilot whale (*Globicephala melas*)	2018 Calf-adult n=3 Muscle **Cl%=53** Blubber Cl%=58 Median (min-max)	ng/g lw	**26 (8-32)** 8.3 (<5.4-27)	**37 (20-50)** <12 (<8.6-17)	**1.6 (0.61-3.3)** (<0.67)	Mean blank +3sd **8.13** 7.13	Mean blank +3sd **12.83** 11.53	Mean blank +3sd **0.63** 0.56	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)
Iceland	Greenland shark (*Somniosus microcephalus*)	2001-2003 Adult females n=2 Liver (min-max) Mean Cl%=56)	ng/g lw	(3.2-15)	(5.0-5.1)	(0.45-0.92)	Mean blank +3sd 2.8	Mean blank +3sd 4.45	Mean blank +3sd 0.22	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)
Mollösund, Skagerrak, Swedish west coast	Killer whale (*Orcinus orca*)	2018 Adult male n=1 Muscle **Cl%=48** Blubber Cl%=59	ng/g lw	**570** 280	**270** 74	**930** 32	Mean blank +3sd **83** 5.5	Mean blank +3sd 130 8.8	Mean blank +3sd **6.5** 0.44	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)
Öresund, Swedish west coast	Harbour porpoise (*Phocoena phocoena*)	2016-2018 Adult both sexes n=3 Blubber Mean Cl%=63% Median (min-max)	ng/g lw	79 (25-110)	17 (14-18)	12 (11-13)	Mean blank +3sd 6.1	Mean blank +3sd 1.57	Mean blank +3sd 0.63	UPLC-APCI-Orbitrap-MS	Yuan *et al*. (2021)

20 Appendix I: Mammalian Toxico-kinetics Data

Table I.1 Summary of toxicokinetics from dossier

Method and test substance	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
No guideline **C_{22-26} 43% Cl wt. (liquid)**	Rat	13 week repeated dose toxicity study, 18 rats each sex, single radiolabelled dose (oral) either 100 or 3750 mg/kg following either having received 100, 3750 or 0 mg/kg dose unlabelled daily for 13 weeks. 3 animals per sex euthanised at 0.5, 1, 2, 7, 28 and 90 days.	It was found that between 82 and 95 per cent of the administered radioactivity was recovered in the faeces during the seven-day collection period, most of which was recovered during the first two days. Between 0.1 and 0.8 per cent of the radiolabel was excreted in the urine. Blood concentrations of radioactivity in animals from the two dose groups were very similar. Also, the inter-group differences in the concentration of radioactivity for any given tissue were much less than the differences between the administered doses. Tissue radioactivity levels were initially greatest in the liver but by 90 days a redistribution to adipose tissue had occurred. This study suggests that absorption of the LCCP product may be saturable, but the extent of systemic absorption and systemic elimination of LCCP could not be determined from this study.	None given	ECHA (2022)
No guideline **C_{22-26} 70% Cl**	Rat	13 week repeated dose toxicity study, 18 rats each sex, single radiolabelled dose (oral) either 100 or 3750 mg/kg	It was found that between 61 and 88 percent of the administered radioactivity was recovered in the faeces during the seven-day collection period. Only a very small proportion of the radioactivity (<0.1–1 per cent) was excreted in the urine. The highest levels of radioactivity were found in the liver,	None given	ECHA (2022)

Method and test substance	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
wt. (solid)		following either having received 100, 3750 or 0 mg/kg dose unlabelled daily for 13 weeks. 3 animals per sex euthanised at 0.5, 1, 2, 7, 28 and 90 days.	gonads and adipose tissue seven days after dosing, with lower levels being found in the brain, kidney, blood and heart. As was the case with the $C_{22–26}$, 43%Cl wt. LCCP study, the extent of systemic absorption and systemic elimination could not be determined.		
^{14}C-labelled C_{18} 50-53% Cl wt.	Rat (F)	Single oral dose 500mg/kg	After 24 h, 1% of the radioactive dose was recovered in the urine, 1.5% in the expired air and 22% in the faeces. After 96 h, 1.9% of the radioactive dose was recovered in the urine, 3.3% in the expired air, 5% in body tissue and 76% in the faeces.	None given	ECHA (2022)
Two substances ^{14}C-labelled C_{18} 50-53% Cl wt. (CP-LH) and C_{28} 47% Cl (CP-LL)	Rat	Single dose, dermal 5-7 of each sex, 66 mg/cm^2 approximately equivalent to 2000mg/kg body weight	Only 0.7% (males) and 0.6% (females) of the C_{18} dose was absorbed after 96 h. Only 0.02% of the C_{28} dose was absorbed in males whereas in females the level was not detectable. This indicates that increasing chain length leads to decreased permeability. Of the absorbed C_{18} dose, 40% was exhaled as $^{14}CO_2$, and 20% was excreted in urine and 20% in faeces. These results indicate that rat skin acts as an effective barrier to chlorinated paraffins containing eighteen or more carbons and more than 40% chlorine by weight. The dermal absorption of the Cl_{18}	None given	ECHA (2022)

Method and test substance	Species	Brief study details	Results	Reliability (Klimisch) score	Reference
			chlorinated paraffin was estimated to be nearly 100 times less than the oral absorption. Based on current toxicity results from rodent experiments and these present findings, chlorinated paraffins of the type tested would be expected to have little or no effect in animals as a result of dermal exposure. In a review of limited comparative *in vivo* data from man and rat (Wester and Maibach, 1983) noted that percutaneous absorption is generally greater in the rat. Thus, it is reasonable to suggest that chlorinated paraffins are unlikely to be systemically toxic to humans by skin contact under normal conditions of production and use.		

Table I.2 Summary of mammalian repeated dose toxicity endpoints

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Reference
Repeated dose oral toxicity, EPA OPPTS 870.3100 (90-Day Oral Toxicity in Rodents) **C_{20-30}, 70% Cl wt. (solid) (unstabilized). Electrofine S70.** **GLP**	Rat (F344)	Administered at nominal concentrations of 0, 100, 900 and 3 750 mg/kg/day in diet for 13 weeks 15 animals per sex per dose	Non treatment related mortality, elevated liver enzymes at 3 750mg/kg/day, liver weight increase at 3750 mg/kg/day (Females; hypertrophy and fat vacuolisation) **NOAEL 900 mg/kg/day** **LOAEL 3 750 mg/kg/day**	1 (key study) This study appears to be a duplicate of the IRDC study below	Unnamed (1984) cited in ECHA (2021b)
Repeated dose oral toxicity, EPA OPPTS 870.3100 (90-Day Oral Toxicity in Rodents) **Equivalent to EPA OPP 82-1 (90-Day Oral Toxicity)** **GLP**		Administered at nominal concentrations of 0, 100, 900 and 3 750 mg/kg/day by oral gavage in corn oil daily for 13 weeks	Several mortalities occurred in study but were attributed to handling/dosing errors. Dose-related evidence of liver changes (females only) characterised as granulomatous inflammation, necrosis and positive fat staining. The significance of an increased incidence of nephrosis and interstitial pneumonia in high dose male animals was described as obscure. Inflammatory changes and necrosis in the liver of female rats occurred at all doses, with increased intensity of Oil-red O staining. Mean absolute and relative organ weights were also increased. Male rats and the **NOAEL was established at the top dose (3 750 mg/kg/day). Effects in female rats, primarily in the liver, were observed at all dose levels and thus a LOAEL was established at 100 mg/kg/day.**	1 (key study) This study appears to be a duplicate of the IRDC study below	Unnamed (1984) cited in ECHA (2021b)
CPs with an average chain length of C_{23}, 43% Cl wt. Molecular Weight 560 (average)	Rat (F344/N) Mouse (B6C3F1)	Oral gavage in corn oil 13 weeks 5 days per week RAT: 0, 235, 469, 938, 1 875, 3 750mg/kg bw	Mortalities in mice (assumed non treatment related, gavage related injury) Rats: dose dependent granulomatous inflammation of the liver was observed in female rats of all treated groups; these liver changes were not observed in the male rats.	2	US NTP (1980) cited in ECHA (2021b)

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Reference
GLP		MOUSE: 0, 469, 938, 1 875, 3 750, 7 500 mg/kg bw 10 animals per sex per dose	Mice: no compound-related histopathology was observed. **Mice: NOAEL 7 500mg/kg/day** **Male Rat: NOAEL 3 750mg/kg/day** **Female Rat: no NOAEL, LOAEL 235mg/kg/day**		
Repeated dose chronic toxicology study, liquid LCCP (C_{23} 43% Cl wt.) **Corn oil oral gavage**	Rat (F344/N)	50 rats of each sex. Male: 0, 1 875 or 3 750mg/kg bodyweight 5 days per week for 103 weeks Female: 0, 100, 300 or 900mg/kg bodyweight 5 days per week for 103 weeks	In contrast to the absence of chemically related toxicity in mice, a dose-related inflammation of the liver was observed in female rats (but not in male rats) in the 13-week studies and in male and female rats at 6 and 12 months in the 2-year studies. A no-observed-effect-level was not established for this effect. The chronic **LOAEL for effects in the liver was 1 875 mg/kg bw/day in male rats and 100 mg/kg bw/day in female rats. The NOAEL for chronic toxicity in mice was 5 000 mg/kg/day.**	None given	US NTP (1985) cited in ECHA (2021b)
13-week repeated dose toxicology study of a liquid grade LCCP (C_{22-26}, 43% Cl wt.) **GLP**	Rat	corn oil by gavage daily for 13 weeks to groups of fifteen Fischer rats of each sex at dose levels of 0, 100, 900 or 3 750 mg/kg/day	As seen in the NTP study, liver effects were observed in female rats. There was evidence of liver toxicity in females of all treated groups (increased absolute and relative liver weight, granulomatous inflammation, necrosis, and positive fat staining. There were no effects in the livers of treated male rats, although trace/mild nephrosis was reported in male rats receiving 3750 mg/kg/day. The **NOAEL for male rats from this study was 900 mg/kg bw/day, LOAEL 3 750mg/kg/day for male rats.** **LOAEL for female rats was 100 mg/kg bw/day (no NOAEL could be established).**	See note above (first two studies in this table) Stated range and molecular formulae do not agree	IRDC (1984a) cited in ECHA (2021b)
13-week repeated dose toxicology study of a solid grade LCCP containing higher levels of	Rat	13-weeks via diet to 15 Fischer rats of each sex at concentrations resulting in dose levels	There were no treatment-related mortalities or clinical signs seen in this study. Increased food consumption was noted at the high dose level, possibly due to nutritional displacement caused by the high concentrations of test substance in the diet (up to 5.8%). High dose male animals showed slightly	None given Stated range and molecular	IRDC (1984b) cited in ECHA (2021b)

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Reference
chlorine (C_{22-28}, 70% Cl wt.)		of 0, 100, 900 or 3 750 mg/kg/day. (initial concentrations of solid LCCP product in the diet were 1 000, 9 000 and 37 500 ppm in the low-, mid-, and high-dose groups respectively; Week 13 concentrations for low-, mid- and high-dose group males were approximately 1682, 14 525 and 57 386 ppm, respectively; Week 13 concentrations for the low-, mid- and high-dose group females were approximately 1 393, 11 649 and 46 997 ppm, respectively.)	reduced body weight gain. There was evidence of a mild effect on the liver in the high-dose animals only. This was characterized by slightly elevated liver enzyme levels in serum, increased liver weights, hepatocellular hypotrophy, and cytoplasmic fat vacuolation. The microscopic changes were more prominent among females. Liver microsomal determinations were generally consistent with these findings. The liver inflammation and necrosis observed in studies of liquid grade LCCPs were not seen in this study. One important methodological difference was bolus gavage dosing of the liquid LCCPs. For this 70% chlorination solid LCCP product, effects in the liver occurred only at a very high exposure level of 3 750 mg/kg/day (concentrations in the diet up to 5.8%). Based on the findings of this study, a **NOAEL of 900 mg/kg/day was identified for male and female rats based on the observation of slight liver effects at the higher dose level of 3 750 mg/kg/day.** These values are considered to be the most relevant for evaluating human safety.	formulae do not agree See note above (first two studies in this table)	

One repeated dose toxicity study disregarded, given a klimisch score of 3 (unreliable) by registrant

Table I.3 Summary of mutagenicity endpoints

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Environment Agency comments	Reference
Bacterial Reverse Mutation Assay, OECD TG 471 **GLP**	Salmonella typhimurium TA 1535, TA 1537, TA 98 and TA 100.	Exposure at 156, 313, 625, 1 250, 2 500, 5 000 µg/plate With and without metabolic activation. Met activation: Arachlor-induced rat liver post mitochondrial supernatant. Positive and negative control Test material: Cereclor 42 (C_{22-26}, 42% Cl wt., liquid) 0.25-2 500µg/ml	Negative (no adverse effects reported at these concentrations). The test article is not mutagenic with or without metabolic activation under the test conditions.	1 (key study)	No data presented.	Unnamed (1981) cited in ECHA (2021b)
Sister chromatid exchange assay in mammalian cells OECD TG 479 (Galloway SM *et al*., 1985)	Chinese hamster ovary	With and without metabolic activation (S9 mixture 1250-5000 µg/plate Unnamed Constituent (C_{23} avg, 43% Cl. Wt.) Liquid Chlorowax 500C (Same as used for NTP testing	Increased chromosomal aberrations were seen following exposure to 5 000 µg/plate, oily droplets formed at doses >057 µg/mL EU REACH Registrant conclusion: Interpretation of results (migrated information): ambiguous with and without activation Both positive and negative results were reported from this study, though the	1 (key study)	Arbitrary concentration /plate? If oily droplets formed then different methodology should be attempted ie different vehicle. For example 0.1% ethanol can be used with hydrophobic substances	Chromosome aberration and Sister Chromatid Exchange Test Results with 42 Chemicals. Ander, B.E., Zeiger, E., Shelby, M.D., Resnick, M.A., Gulati, D.K., Ivett, J.L., Loveday, K.S., 1990. cited in ECHA (2021b)

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Environment Agency comments	Reference
			results are somewhat difficult to interpret based on the note that oily droplets formed and study was run at a potentially cytotoxic dose. *In vivo* data provided a definitive basis to determine that LCCP is not genotoxic to mammalian cells.			
***In vitro* gene mutation study in bacteria** **Bacterial reverse mutation assay**	*Salmonella typhimurium* TA97, TA98, TA100, TA1535 Arochlor 1254-induced postmitochondrial supernatant (S-9 mix) from either male Sprague-Dawley rats or male Syrian hamsters.	Unnamed constituent C_{23} (avg) 43% Cl wt. (liquid) tested at 100, 333, 1 000, 3 333, 10 000 ug/plate with and without metabolic activation (s-9 mix)	Negative (no further detail given)	2 (Supporting study)	Arbitrary concentration / plate Little information given	Unnamed (1986) "Comparative Toxicity and Carcinogenicity of two Chlorinated Paraffins in F344/N Rats and B6C3F1 Mice" Bucher, JR *et al* Fund. Appl. Toxicol., 9 cited in ECHA (2021b)
***in vitro* gene mutation study in bacteria** **Preincubation method (Haworth *et al*, 1983).**	*S. typhimurium* TA 1535, TA 1537, TA 98 and TA 100	Unnamed Constituent C_{23} (avg) 43% Cl wt. (liquid). Chlorowax 500C. Used at 33, 100, 333, 1 000, 3 333, 10 000	Negative (no further detail given)	1 (reliable without restriction; supporting study)	Arbitrary /plate concentration, no density of cells, no actual comparable concentration	"Salmonella Mutagenicity Tests III. Results from the testing of 255 chemicals." Zeiger, E.

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Environment Agency comments	Reference
		µg/plate with and without metabolic activation (S-9 mix)				1987 Environ. Muta., 9, Suppl. 9:1-110 cited in ECHA (2021b)
***in vitro* gene mutation study in bacteria** **bacterial reverse mutation assay**	Salmonella typhimurium TA98, TA100, TA1535, TA1538	C_{22-26}; 42% Cl wt. (liquid). Cereclor 42. Used at 4, 20, 100, 500 and 2 500 µg/plate with or without metabolic activation (s-9 mix)	Negative (no further details given)	2 (reliable with restrictions; supporting study)	Arbitrary /plate concentration, no density of cells, no actual comparable concentration	The Toxicological Effects of Chlorinated Paraffins in Mammals. Birtley, R.D.N. *et al.* 1980 Toxicol. Appl. Pharmacol., 54, 514-525 cited in ECHA (2021b)
***in vitro* gene mutation study in bacteria** **OECD Guideline 471 (Bacterial Reverse Mutation Assay)** **GLP**	Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538	Unnamed Constituent C_{18-20}; 40% Cl wt. (liquid). Chlorparaffin 40 NV. No dose provided With and without metabolic activation	Negative (no further details given)	4 (not assignable; supporting study)	Not enough information for evaluation	Unnamed: (1989) cited in ECHA (2021b)
***in vitro* gene mutation study in bacteria** **OECD Guideline 471 (Bacterial Reverse Mutation Assay)**	Salmonella typhimurium TA98, TA100, TA1535, TA1538	Unnamed Constituent C_{20-23}; 42% Cl wt. (liquid). No dose provided, with or without met activation	Negative (no further details given)	4 (not assignable; supporting study)	Not enough information for evaluation	Unnamed; cited in ECHA (2021b)
***in vivo* mammalian somatic cell study: cytogenicity / bone**	Rat Fischer 344 (male)	Oral gavage of Unnamed Constituent C_{20-30}; 70% Cl (solid), in	No increases in the frequency of chromosomal abnormalities were	1 (reliable without	Positive control administered via alternative route to treatments,	Unnamed (1983) cited in ECHA (2021b)

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Environment Agency comments	Reference
marrow chromosome aberration **OECD Guideline 475 (Mammalian Bone Marrow Chromosome Aberration Test)**		vehicle (1% carboxymethylcellulose in water), at 0,500,1500, 5000 mg/kg/day, 8 animals per dose plus positive control of cyclophosphamide (40 mg/kg), i.p. inj on day 5 and 6 of study	observed in the treated groups when compared to the controls.	restriction; key study)	therefore no indication of whether vehicle was appropriate and influenced absorption of target chemical. *In vivo* effects may be seen in organs other than bone marrow.	
***in vivo* mammalian somatic cell study: cytogenicity / bone marrow chromosome aberration** **OECD Guideline 475 (Mammalian Bone Marrow Chromosome Aberration Test)**	Rat Fischer 344 (male)	Unnamed Constituent C22-26; 43% Cl (liquid) administered via oral gavage in corn oil vehicle for 5 days at 0, 500, 5000 mg/kg bodyweight 8 animals per concentration. Plus positive control of cyclophosphamide (40mg/kg) ip inj on day 5 and 6 of study	Not genotoxic to rat bone marrow at doses up to 5000 mg/kg/day.	1 (reliable without restriction; key study)	Positive control administered via alternative route to treatments, therefore no indication of whether vehicle was appropriate and influenced absorption of target chemical. *In vivo* effects may be seen in organs other than bone marrow.	Unnamed (1983) cited in ECHA (2021b)

No further studies found in literature

Table I.4 Summary of carcinogenicity endpoints

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Environment Agency comments	Reference
carcinogenicity: oral Equivalent or similar to EPA OPP 83-2 (Carcinogenicity) US NTP GLP	Mouse B6C3F1	Chlorinated Paraffins Average Chain Length: C23 43% Cl wt. via oral gavage in corn oil for 103 weeks 5 days per week at 0, 2 500, 5 000 mg/kg bodyweight, 50 animals per dose	The incidences of malignant lymphoma in male mice and hepatocellular carcinoma in female mice both showed a positive trend although only the incidence of malignant lymphoma in male mice exposed to 5 000 mg/kg bw was statistically significant different from controls. An increased incidence of malignant lymphoma in male mice was reported at the highest dose tested, 5 000 mg/kg/day. The significance of the increased incidence of malignant lymphoma in male mice is unclear. Malignant lymphoma is a commonly occurring tumour in this strain of mouse and the effect was not seen in female mice. Given the very high dose and the limited nature of the finding it appears the study shows just limited evidence of carcinogenicity for long-chain chlorinated paraffin in the mouse. Overall, while there were some positive findings from this study, they occurred at an exposure level that is so high (5000 mg/kg/day) that the relevance of this property to a human health hazard assessment is doubtful. IARC conclusion for LCCP is Class 3.	2 (reliable with restrictions; key study)	The data appears to show a trend of increased occurrence in malignant lymphoma in males at 2 500 and 5 000 mg/kg bw/day. There, in the females, also appears to be an increase int eh occurrence of carcinomas. A repeat study would increase statistical power and likely result in statistical significance for these effects even at the lower doses.	Unnamed (1986)
carcinogenicity: oral test procedure in accordance	Rat (Fischer 344), male	Chlorinated Paraffins Average Chain Length: C_{23} 43% Cl wt.; applied	The primary nonneoplastic lesion associated with chlorinated paraffins (C_{23}, 43% Cl wt.) administration was a diffuse lymphohistiocytic inflammation in the liver and in the pancreatic and mesenteric lymph nodes of male and female rats. Splenic congestion was a	2 (Reliable with restrictions; key study)	In each study non neoplastic effects were seen at lowest concentrations. This adds	Unnamed (1986) cited in ECHA (2021b)

Method	Species	Brief study details	Results	Reliability (Klimisch) score provided under EU REACH	Environment Agency comments	Reference
with national standard methods with acceptable restrictions US National Toxicology Program GLP	and female	via oral gavage in corn oil, for 103 weeks, 5 days per week at 0,1875, 3750 mg/kg bodyweight in males and 0, 100, 300 and 900 mg/kg bodyweight 70 of each sex 10 rats from each group terminated at 6 and 12 months	secondary effect. These lesions occurred in most animals of all treated groups, earlier and at lower doses in female rats than in male rats. Description (incidence and severity): The incidence of adrenal medullary phaeochromocytomas was increase in treated female rats compared to controls, although there was no evidence of hyperplasia. The increase was statistically significantly different in the group receiving 900 mg/kg bw (Table 1). Non neoplastic treatment effects in male at LOAEL 1875 mg/kg bw/ day (lowest test conc) Treatment effects in female loael 100 mg/kg bw /day (lowest dose)		evidence to the STOT RE 1 classification	Comparative Toxicity and Carcinogenicity of two Chlorinated Paraffins in F344/N Rats and B6C3F1 Mice Bucher, J.R. *et al* Fund. Appl. Toxicol., 9

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