Substance Name: Tricosafluorododecanoic acid

EC Number: 206-203-2

CAS Number: 307-55-1

MEMBER STATE COMMITTEE

SUPPORT DOCUMENT FOR IDENTIFICATION OF

TRICOSAFLUORODODECANOIC ACID

AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS vPvB PROPERTIES

Adopted on 13 December 2012

CONTENTS

TABLES

PREFACE

In four provided dossiers, the intrinsic properties of four perfluorinated carboxylic acids (PFCAs) are assessed: C11-14-PFCAs. Many studies are only available for structurally similar shorter chain PFCAs such as C8-PFCA and C9-PFCA. In those cases where studies on the particular substance are missing, studies from either shorter or longer chain PFCAs are used in the provided dossiers by applying read-across. Read-across is based on the structural similarities and on the physicochemical properties, which follow a regular pattern. All PFCAs contain a carboxylic acids group and a perfluorinated carbon chain. The only difference is the number of CF2-groups in this chain. Details on the read-across approach, i.e. showing the trend of physicochemical properties and the structural similarities are given in Annex I.

Substance Name(s): Tricosafluorododecanoic acid

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The substance is identified as a vPvB according to Article 57 (e).

Summary of how the substance meets the CMR (Cat 1A or 1B), PBT or vPvB criteria, or is considered to be a substance giving rise to an equivalent level of concern

A weight of evidence determination according to the provisions of Annex XIII of REACH is used to identify the substance as vPvB. All available information (such as results of standard tests, monitoring and modelling, information from the application of the category and analog approach (grouping, read-across) and (Q)SAR results) was considered together in a weight of evidence approach. The individual results have been considered in the assessment with differing weights depending on their nature, adequacy and relevance. The available results are assembled together in a single weight of evidence determination.

Persistence:
Tricosafluorododecanoic acid (C_{12}-PFCA) has no abiotic degradation studies available. Only one standard screening study is available.

Read across approach within C_8-C_{14}-PFCAs can be applied for the persistence assessment of these substances. C_{8-14}-PFCAs contain a highly similar chemical structure, a perfluorinated carbon chain and a carboxylic acid group. The compounds differ only in the number of CF_2-groups. As a result of comparing the experimental and estimated physico-chemical data of C_8-PFCA (the analogue substance) with experimental and estimated data on C_{11-14}-PFCAs it can be assumed that with increasing chain length water solubility decreases and the sorption potential increases (See Table 14 of the support document). It can be with a sufficient reliability stated that the behaviour of these chemicals follow a regular pattern.

Due to both structural similarity and a regular pattern of physico-chemical properties, C_{8-14}-PFCAs may be considered as a group or a category of substances for the purpose of the PBT/vPvB assessment and the read-across approach can be applied within this group.

In general, the persistence of C_{11}-C_{14}-PFCAs can be explained by the shielding effect of the fluorine atoms, blocking e.g. nucleophilic attacks to the carbon chain. High electronegativity, low polarizability and high bond energies make highly fluorinated alkanes to the most stable organic compounds. It is not expected that the carboxylic group in PFCAs alters this persistence of these chemicals. This fact is confirmed by a hydrolysis study which obtained a DT_{50} of >92 years for C_8-PFCA in water. Screening studies of $C_{8,9,12,14}$-PFCAs showed no biodegradation within 28 days. Non-standard abiotic degradation tests with C_8-PFCA could not detect any degradation products under environmentally relevant conditions. Furthermore, screening biodegradation studies on $C_{8,9,12,14}$-PFCAs and one non-standard anaerobic biodegradation simulation test with C_8-PFCA provide evidence of high persistence. Additionally, elements of non-standard higher tier aerobic biodegradation studies on C_8-PFCA provide further support that no biodegradation in water, soil and sediment occurs.

Therefore, based on the information summarized above it is concluded that C_{12}-PFCA is not degraded in the environment and thus fulfils the P- and vP- criteria in accordance with the criteria and provisions set out in Annex XIII of REACH.

Bioaccumulation:

Regarding the bioaccumulation potential for C_{12}-PFCA the available experimental BCF-values of C_{12}-PFCA are above 5000. A number of field-BMFs and TMFs are available for C_{12}-PFCA and they provide evidence that biomagnification of this substance takes place in nature between

different trophic levels of food chains and from the bottom to the top of food chains (See Table 15 of the support document). Due to the structural similarity and the regular pattern of physico-chemical properties within the group of C_{11-14}-PFCAs, read across can be applied within the group. The available field bioaccumulation data of C_{12}-PFCA and the other substances of the group provide further support to assume that C_{12}-PFCA biomagnifies in the food chain. Thus, it is concluded the B as well as the vB-criteria -are met in accordance with the criteria and provisions set out in Annex XIII of REACH.

Conclusion:

In conclusion, C_{12}-PFCAs is identified as a vPvB-substance according to Art. 57 (e) of REACH and by applying a weight of evidence determination using expert judgement by comparing all relevant and available information listed in Section 3 of Annex XIII of REACH with the criteria set out in Section 1 of the same Annex.

The substance has not yet been registered under REACH.

Justification

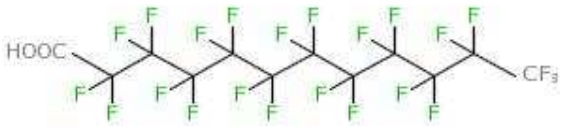
1 Identity of the substance and physical and chemical properties

1.1 Name and other identifiers of the substance

Table 1: Substance identity

EC number:	206-203-2
EC name:	Tricosafluorododecanoic acid
CAS number (in the EC inventory):	307-55-1
CAS number:	307-55-1
CAS name:	Dodecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-tricosafluoro-
IUPAC name:	Tricosafluorododecanoic acid
Index number in Annex VI of the CLP Regulation	-
Molecular formula:	$C_{12}HF_{23}O_2$
Molecular weight range:	614.0984 g/mol
Synonyms:	Dodecanoic acid, tricosafluoro-C_{12}-PFCA Perfluorododecanoic acid Perfluorolauric acid

Structural formula:



1.2 Composition of the substance

Name: Tricosafluorododecanoic acid

Description: Mono-constituent substance

Degree of purity: Registration dossiers or other information on concentration ranges and on any impurities are not available.

1.3 Physico-chemical properties

The following physico-chemical properties are mainly obtained by calculation. No further information regarding the given values or other properties is available.

Table 2: Overview of physicochemical properties

Property	Value	Remarks	Reference
Physical state at 20°C and 101.3 kPa	*solid*	*According to melting point*	
Melting/freezing point	*112 – 114 °C*	*Experimental result*	*Huang B-N, Haas A., Lieb M., 1987*
Boiling point	*249 °C*	*Data from SRC PhysProp Database* *"PhysProp" data were obtained from Syracuse Research Corporation of Syracuse, New York (US)*	*Data from SRC PhysProp Database, 02/2012* *"PhysProp" data were obtained from Syracuse Research Corporation of Syracuse, New York (US)*
Vapour pressure	*0.0043 mm Hg*	*Estimated value*	
	9.40E-3 Torr at 25°C		Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)
Water solubility	*4.81 E-006 mg/l*	*Estimated value*	
	2.9E-5 g/L pH 1 at 25°C *2.2E-4 g/L pH 2 at 25°C* *2.0E-3 g/L pH 3 at 25°C* *0.014 g/L pH 4 at 25°C* *0.034 g/L pH 5 at 25°C* *0.039 g/L pH 6 at 25°C* *0.040 g/L pH 7 at 25°C* *0.041 g/L pH 8-10 at 25°C*		*Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)*
Partition coefficient n-octanol/water	*10.16*	*Estimated value*	
	logP 9.363±0.888 at 25°C	The value was most likely calculated for the non-ionised form.	*Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)*
Dissociation constant	*0.52±0.10 pH:*	-	*Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)*
[enter other property, if relevant, or delete row]	-	-	

The above presented experimentally determined or calculated values are in good agreement with the physical chemical information, which is available for the homologues of PFCAs. With increasing chain length the melting and boiling point increase, while no significant change can be found for the vapour pressure and dissociation constant for the $C_{11\text{-}14}$-PFCAs based on the calculations given in Table 3. The water solubility is predicted to decrease with increasing chain length. This is in agreement with the fact that the polarity of the substances decreases with an increasing chain length. It should be emphasised here that it is not possible to assess the

calculated values of C_{11-14}-PFCAs because there are factors like special conformation of the molecules which have an influence on the real values, but which have not been taken into account for the calculation.

However, the calculated values have dimensions which would be theoretically expected for the C_{11-14} PFCAs.

2 Harmonised classification and labelling

C_{12}-PFCA is not classified according to Annex VI of Regulation (EC) No 1272/2008 (CLP Regulation).

Twenty-seven notifications (4 aggregated notifications) have been submitted to the C&L Inventory.

Table 3: Notified classification and labelling according to CLP criteria for C_{12}-PFCA (query from October 2012)

Classification		Labelling		
Hazard Class and Category Code(s)	**Hazard Statement Code(s)**	**Hazard Statement Code(s)**	**Pictograms**	**Signal Word Code(s)**
Skin Irrit. 2 Eye Irrit. 2 STOT SE 3	H315 H319 H335	H315 H319 H335	GHS07	Wng
		H314	GHS05	Dgr
Acute Tox. 4 Acute Tox. 4 Skin Irrit. 2 Eye Irrit. 2 Acute Tox. 4 STOT SE 3	H302 H312 H315 H319 H332 H335	H302 H312 H315 H319 H332 H335	GHS07	Wng
Met. Corr. 1 Skin Corr. 1B Eye Dam. 1 Aquatic Acute 1 Aquatic Chronic 1	H290 H314 H318 H400 H410	H290 H314 H318 H400 H410	GHS09 GHS05	Dgr

3 Environmental fate properties

3.1 Degradation

3.1.1 Abiotic degradation

3.1.1.1 Hydrolysis

There are no studies on the hydrolysis of C_{12}-PFCA available. Based on the data given in Annex 1, results of studies of structurally similar substances of the same chemical group could be used to evaluate the hydrolysis of C_{12}-PFCA.

Two studies are available on shorter chain lengths PFCAs. Hydrolysis of perfluorinated octanoic acid (C_8-PFCA; PFOA) and its ammonium salt (APFO) (CAS-No: 335-67-1, 3825-26-1) and perfluorinated nonanoic acid (C_9-PFCA; PFNA) (CAS No: 375-95-1) were analyzed. The studies are summarized in the following:

C_8-PFCA is hydrolytically stable under relevant environmental conditions. One study has been discussed in the OECD SIDS Initial Assessment Report for C_8-PFCA (PFOA), which has been copied here in italic letters (OECD, 2006):

The 3M Environmental Laboratory performed a study of the hydrolysis of APFO (3M Co., 2001a) (Realiability = 1)*. The study procedures were based on USEPA's OPPTS Guideline Document 835.2110; although the procedures do not fulfil all the requirements of the guideline, they were more than adequate for these studies. Results were based on the observed concentrations of APFO in buffered aqueous solutions as a function of time. The chosen analytical technique was high performance liquid chromatography with mass spectrometry detection (HPLC-MS).*

During the study, samples were prepared and examined at six different pH levels from 1.5 to 11.0 over a period of 109 days. Experiments were performed at 50 °C and the results extrapolated to 25 °C. Data from two of the pH levels (3.0 and 11) failed to meet the data quality objective and were rejected. Also rejected were the data obtained for pH 1.5 because ion pairing led to artificially low concentrations for all the incubation periods. The results for the remaining pH levels (5.0, 7.0, and 9.0) indicated no clear dependence of the degradation rate of PFOA on pH. From the data pooled over the three pH levels, it was estimated that the hydrolytic half-life of PFOA at 25°C is greater than 92 years, with the most likely value of 235 years. From the mean value and precision of PFOA concentrations, it was estimated the hydrolytic half-life of PFOA to be greater than 97 years.

A newer study showed no decomposition of C_{8-9}-PFCAs in hot water in absence of $S_2O_8^{2-}$. After the addition of $S_2O_8^{2-}$ to the reaction system efficient decomposition of PFCAs has been observed at 80 °C. After a reaction time of 6 hours, C_8-PFCA and C_9-PFCA were decomposed completely. The reaction products were mainly F^- and CO_2 at a yield of 77.5 % ((moles of F^- formed)/(moles of fluorine content in initial PFOA)) and 70.2 % ((moles of CO_2 formed)/(moles of carbon content in initial PFOA)), respectively for C_8-PFCA. For C_9-PFCA the reaction products were mainly F^- and CO_2 at a yield of 88.9 % and 75.2 %, respectively. Short chain PFCAs were a minor reaction product. However, at higher temperatures (150°C) 12.3% of the initial C_8-PFCA remained and the yields of F^- and CO_2 were 24.6 and 37.0 %, respectively (Hori et al., 2008) (Reliabilty = 2).

The water solubility of C_{12}-PFCA is lower than those of $C_{8,9}$-PFCA, which can be explained by the expanded fluorinated carbon chain (Annex 1). However, the stability of the PFCAs is mainly based on the stability of the highly fluorinated carbon chain (Siegemund et al., 2000). Since C_8-PFCA is hydrolytically stable, we estimate a comparable hydrolytically stability also for C_{12}-PFCA.

Based on the read across rationale described in Annex 1, data on C_8-PFCA is used as evidence for C_{12}-PFCA to conclude that it is hydrolytically stable under environmental conditions.

3.1.1.2 Phototransformation/photolysis

Direct photolysis of a carbon fluorine chain is expected to be very slow, with stability expected to be sustained for more than 1000 years (Environment Canada, 2012).

3.1.1.2.1 Phototransformation in air

There are no studies on phototransformation for C_{12}-PFCA in air available. However, studies on C_8-PFCA exist and are summarized below:

The following information was copied from the OECD SIDS Initial Assessment Report for C_8-PFCA (PFOA) (OECD, 2006):

Hurley et al. determined the rate constants of the reactions of OH radicals with a homologous series of perfluorinated acids (from trifluoroacetic acid to nonafluoropentanoic acid) in 700 Torr of air at 296 K (Hurley et al., 2004). For C_3 to C_5 chain length had no discernible impact on the reactivity of the molecule. The rate constant $k(OH + F(CF_2)_nCOOH) = (1.69\pm0.22)\times10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} for n = 2, 3, 4, respectively. Atmospheric lifetimes of $F(CF_2)_nCOOH$ with respect to reaction with OH radicals are estimated to be approximately 230 days for n = 1 and 130 days for n > 1. (Calculation of lifetime by comparison with CH_3CCl3 (half-life 5.99 years, $k = 1.0\times10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}). The authors conclude, that the major atmospheric loss mechanism of perfluorinated carboxylic acids is dry and wet (particle mediated) deposition which occur on a time scale which is probably of the order of 10 days. Reaction with OH is a minor atmospheric loss mechanism for perfluorinated carboxylic acids

3.1.1.2.2 Phototransformation in water

There are no studies on phototransformation in water for C_{12}-PFCA available. However, studies on C_{8-11}-PFCA exist and are summarized below:

The photochemical decomposition of long-chain PFCAs in water by use of persulfate ion ($S_2O_8^{2-}$) in water (C_9-PFCA) and in an aqueous/liquid CO_2 biphasic system (C_{9-11}-PFCAs) was examined by Hori et al. (Hori et al., 2005b) (Reliability = 2). In water and in the absence of $S_2O_8^{2-}$ (direct photolysis) C_9-PFCA decomposition of 64.5 % was determined. In the presence of $S_2O_8^{2-}$ the decomposition increased to 100%. The decompositions after 12 hours in the biphasic system were 100% for C_9-PFCA and C_{10}-PFCA, and 77.1% for C_{11}-PFCA. The reaction product was mainly F^- (66.2 %, 73.4 % and 46.35 % of (moles of F^- formed)/(moles of fluorine content in initial PFCA)) and the minor reaction products were short-chain PFCAs. Since the conditions in this study are not environmentally relevant, we did not describe this study in detail.

In addition to the study of Hori et al, further studies are available for C_8-PFCA (PFOA) and its ammonium salt APFO (see table 3).

Table 4: Summary of photodegradation studies for C_8-PFCA and its ammonium salt

Test Substance	Result	Remarks	Reliability	Reference
Ammonium salt of C_8-PFCA	No photodegradation	Direct photolysis	2	(OECD, 2006);(3M Co., 1979)
Ammonium salt of C_8-PFCA	No photodegradation	Direct and indirect (H_2O_2; synthethic humic water, Fe_2O_3) photolysis	1	(OECD, 2006);(3M Co., 2001b)
	Estimated half-life > 349 days	Indirect photolysis (Fe_2O_3)		
C_8-PFCA		Short wave length (<300 nm) used for irradiation → limited relevance for an aqueous environment	2	(Hori et al., 2004)
	44.9% of the initial PFOA was decomposed after 24 hours	Direct photolysis; 0.48 MPa O_2		
	35.5% of the initial PFOA was decomposed after 24 hours	Indirect photolysis (H_2O_2); 0.48 MPa O_2		
	100% of the initial PFOA was decomposed after 24 hours	Indirect photolysis (tungstic heteropolyacid photocatalyst); 0.48 MPa O_2		
C_8-PFCA		Short wave length (<300 nm) used for irradiation → limited relevance for an aqueous environment	2	(Hori et al., 2005a)
	16.8% of the initial PFOA was decomposed after 4 hours	Direct photolysis; 0.48 MPa O_2		
	100% of the initial PFOA was decomposed after 4 hours	Indirect photolysis ($S_2O_8^{2-}$); 0.48 MPa O_2		

The following information was copied from the OECD SIDS Initial Assessment Report for C_8-PFCA (PFOA) (OECD, 2006):

Direct photolysis of APFO was examined in two separate studies (3M Co., 1979; 3M Co., 2001b) and photodegradation was not observed in either study. In the 3M (1979) study, a solution of 50 mg/l APFO in 2.8 litres of distilled water was exposed to simulated sunlight at 22±2 ºC. Spectral energy was characterized from 290-600 nm with a max output at ~360 nm. Direct photolysis of the test substance was not detected.

In the 3M (3M Co., 2001b) study, both direct and indirect photolysis were examined utilizing techniques based on USEPA and OECD guidance documents. To determine the potential for direct photolysis, APFO was dissolved in pH 7 buffered water and exposed to simulated sunlight. For indirect photolysis, APFO was dissolved in 3 separate matrices and exposed to simulated sunlight for periods of time from 69.5 to 164 hours. These exposures tested how each matrix would affect the photodegradation of APFO. One matrix was a pH 7 buffered aqueous solution containing H_2O_2 as a well-characterized source of OH radicals. This tested the propensity of APFO to undergo indirect photolysis. The second matrix contained Fe_2O_3 in water that has been shown to generate hydroxyl radicals via a Fenton-type reaction in the presence

of natural and artificial sunlight. The third matrix contained a standard solution of humic material. Neither direct nor indirect photolysis of APFO was observed based on loss of starting material. Predicted degradation products were not detected above their limits of quantitation. There was no conclusive evidence of direct or indirect photolysis whose rates of degradation are highly dependent on the experimental conditions. Using the iron oxide (Fe_2O_3) photoinitiator matrix model, the APFO half-life was estimated to be greater than 349 days.

According to Hori et al., aqueous solutions of PFOA absorb light strongly from the deep UV-region to 220 nm (Hori et al., 2004). A weak, broad absorption band reaches from 220 to 270 nm (no absorption coefficient stated). The irradiation of a 1.35 mM PFOA solution (29.6 µmol) in water (under 0.48 MPa of oxygen) with light from a xenon-mercury lamp (no radiant flux stated) for 24 hours resulted in a ca. 44.9 % reduction (13.3 µmol) of PFOA concentration. Concentrations of CO_2 and fluoride increased simultaneously. Small amounts (0.1-5 µmol) of short chain perfluorinated hydrocarbon acids (C_2-C_7) were detected. The addition of the photocatalyst tungsten heteropolyacid ($[PW_{12}O_{40}]^-$) or persulfate ($S_2O_8^{2-}$) (Hori et al., 2005a) *accelerates the reaction rate. Due to the short wave length used for irradiation (< 300 nm) the photodegradation described may be of limited relevance for an aqueous environment but may be used as a technical process.*

3.1.1.2.3 Phototransformation in soil

No data available

3.1.1.3 Summary and discussion on abiotic degradation

In general, the perfluorinated carboxylates are very stable. Since there are no degradation studies (under relevant environmental conditions) on the C12-PFCA available, data from similar substances need to be considered and discussed. Based on the data given in Annex 1, results of studies of structurally similar substances of the same chemical group could be used to evaluate the abiotic degradation of C12-PFCA.

The data on C_8-PFCA indicate that abiotic degradation in the atmosphere is expected to be slow (atmospheric lifetime = 130 days; conclusion by analogy from short-chain perfluorinated acids). Under relevant environmental conditions C_8-PFCA is hydrolytically stable (DT_{50} > 92 years) and do not undergo direct photodegradation in natural waters. The estimated DT_{50} for indirect photolysis is 349 days.

Based on the read across rationale described in Annex 1, data on C_8-PFCA are used as evidence for C_{12}-PFCA to conclude that it is stable under environmental conditions and abiotic degradation is expected to be as low as for the chemically similar substance C_8-PFCA.

3.1.2 Biodegradation

3.1.2.1 Biodegradation in water

3.1.2.1.1 Estimated data

For the C_9-PFCA a half-life in water of 2477 days and a half-life in soil of 4954 days was estimated (Lambert et al. 2011).

3.1.2.1.2 Screening tests

There is one study available for the C_{12}-PFCA (Table 5). In a 28 day ready biodegradability test (OECD 301 C) using 100 mg/L C_{12}-PFCA, and 30 mg/L activated sludge non-biodegradability was demonstrated. For C_{12}-PFCA no biodegradation was observed (National Institute of Technology and Evaluation, 2007).

Table 5: Screening tests for C_{12}-PFCA.

Test substance	**Method**	**Result**	**Reliability**	**Reference**
C_{12}-PFCA	OECD 301 C	minus 16% in 28 days	2	(National Institute of Technology and Evaluation, 2002)

In summary, on the basis of the available screening test C_{12} PFCA is not readily biodegradable.

3.1.2.1.3 Simulation tests

For C12-PFCA no experimental degradation test is available. Based on the data given in Annex 1, results of studies of structurally similar substances of the same chemical group could be used to evaluate the hydrolysis of C_{12}-PFCA.

Therefore, test results for C_8-PFCA are discussed shortly in the following.

No environmental half-lives for C_8-PFCA have been reported, even in the cases where corresponding tests have been performed (see table 5).

Table 6: Summary of simulations tests of C_8-PFCA (PFOA) and its and ammonium salt (APFO) and sodium salt

Test substance	**Method**	**Result**	**Reliability**	**Reference**
C_8-PFCA	Closed-loop systems in laboratory scale; Aerobic and anaerobic conditions	No elimination	3	(Meesters and Schroeder, 2004; Schröder, 2003)
Ammonium salt of C_8-PFCA	Biodegradation in mixed bacterial culture and activated sludge Aerobic conditions	< 0.6 % of $^{14}CO_2$ was detected after 28 days	4	(Wang et al., 2005)
Sodium salt of C_8-PFCA	Microcosm study Aerobic conditions	No significant dissipation from water column after 35 days (initial concentration 0.3 mg/L; 1mg/L; 30 mg/L) 32% dissipation in 35 days (initial concentration 100 mg/L)	3	(Hanson et al., 2005)
C_8-PFCA/ ammonium salt of C_8-PFCA	1.Preliminary screening: C_8-PFCA serves as an electron acceptor under anaerobic conditions (in combination with different inocula) 2. Hypothesis refinement: ^{14}C C_8-PFCA serves as an electron acceptor under anaerobic conditions	No significant consumption of the initial C_8-PFCA during 110 – 259 days No loss of ammonium salt of C_8-PFCA No production of $^{14}CO_2$ No detection of radiolabel transformation products	2	(Liou et al., 2010)

In the OECD SIDS Initial Assessment Report it was concluded that C_8-PFCA (PFOA) is not expected to undergo biodegradation (OECD, 2006). The following text in italic letters was copied from there:

Schroeder (2003), and Meesters and Schroeder (2004) investigated the biochemical degradation of PFOA in sewage sludge in laboratory scale reactors. After 25 days under aerobic conditions PFOA (initial concentration 5 mg/l) was not eliminated by metabolic processes, mineralization processes or by adsorption (Meesters and Schroeder, 2004; Schröder, 2003).

Wang et al. studied the biodegradation of fluorotelomer alcohols. However, ^{14}C-labelled C_8-PFCA ammonium salt was used as starting material in this study, too. The authors analyzed the headspace of sealed vessels containing mixed bacterial cultures and vessels containing

activated sludge from a domestic sewage treatment plant under continuous air flow. The mixed bacterial culture from industrial wastewater treatment sludge was enriched using 8:2 telomere alcohol and ^{14}C-labelled C_8-PFCA ammonium salt, respectively. However, for using C_8-PFCA ammonium salt as a starting material no detailed information are available from the report. The authors describe that potential biodegradation products were separated and quantified by LC/ARC (on-line liquid chromatography/accurate radioisotope counting). Transformation products were identified by quadrupole time of flight mass spectrometry. Only <0.6 % of $^{14}CO_2$ was detected after 28 days. The report contains no graphs or further data to re-evaluate this statement. Although the study seems to be very well documented for ^{14}C labelled 8:2 FTOH, we can only flag the study with a reliability of 3-4, since details on C_8-PFCA ammonium salt are not available. The documentation for the results obtained with C_8-PFCA is missing in the report. However the result indicates that C_8-PFCA ammonium salt is not biodegradable within 28 days (Wang et al., 2005).

Hanson et al. performed a microcosm study. Microcosms were approximately 1.2 m deep with a water depth of 1 m, a diameter of 3.9 m, and a surface area of 11.95 m². Each microcosm had a capacity of approximately 12m³ of water. Sediment consisted of a 1:1:1 mixture of sand, loam and organic matter (mainly composted manure). The total carbon content of the sediment was 16.3%. Microcosms were circulated for 2 weeks from a well-fed irrigation pond prior to the experiments. Nominal concentrations of 0.3, 1, 30, and 100 mg/L C_8-PFCA, as the sodium salt, plus controls were added to the microcosms. Each exposure was randomly assigned to three separate microcosms from a total of 15 microcosms. Immediately prior to treatment, water flow into each microcosm from the main irrigation pond ceased, creating a closed system relative to the other microcosms and the irrigation pond.

Water chemistry and PFOA analysis were taken at the same time on a regularly basis. Temperature and dissolved oxygen content were measured daily. Water samples were collected with a metal integrated water column sampler. Integrated subsamples from at least 4 randomly selected locations in each microcosm were collected to a total volume of 4 L. Samples were stored at 4 °C until analysis. Water samples were analyzed by ion chromatography. The mobile phase was 0.5 mM NaOH, 5 % methanol, and 5% acetonitrile with a flow rate of 0.4 mL/min. Injection volumes varied from 5, 10, 75, and 200 µl for the 100, 30, 1 and 0.3 mg/L microcosms, respectively. For each set of samples analyzed five standards and one quality control sample were included at the beginning of each run and again at the end. Radioactive labelling was not performed. Over a 35-day field study C_8-PFCA showed no significant dissipation from the water column. However, at the highest concentration (100 mg/L) a partitioning from the water column into other compartments is suspected (32% dissipation in 35 days) (Hanson et al., 2005). Since the documentation of the procedure was insufficient in our opinion the study is not reliable (reliability 3).

Liou et al. investigated the anaerobic biodegradability of C_8-PFCA respectively its ammonium salt. In a two-phase experiment (preliminary screening, hypothesis refinement) the use of C_8-PFCA as a physiological electron acceptor (electron donator: acetate, lactate, ethanol or hydrogen gas) was studied. Additionally, the possibility of co-metabolism of C_8-PFCA during reductive dechlorination of trichloroethene and during various physiological conditions (aerobic, nitrate-reducing, iron-reducing, sulfate reducing, and methanogenic) was analyzed. Five different inoculums were used (from a municipal waste-water treatment plant, industrial site sediment, an agricultural soil, and soils from two fire training areas). Environmental samples used as inoculum sources in the biodegradation experiments were aseptically gathered (sterile spatula) placed in 0.5 L sterilized canning jars (filled to the brim), stored on ice in the field, and maintained at 4 °C before being transferred to an anaerobic hood where samples were degassed and dispensed as slurries in biodegradation assays. Soils and sludges were gathered from: the Ithaca sewagetreatment plant; a water-saturated drainage ditch adjacent to the DuPont Chambers Works waste treatment facility in Salem County, New Jersey, previously shown to carry out reductive dechlorination (Fung et al., 2009); the Cornell agricultural field station (Collamer silt loam, Ithaca, NY), the Ithaca fire training facility, and the Rochester, NY fire training facility (the latter two sites were chosen due to potential contamination with fluorinated fire retardant chemicals) (Liou et al., 2010).

For the serum bottle –based biodegradation assays treatments occurred in triplicats (160 ml serum bottles with 100 mL of media; live ± C_8-PFCA and abiotic controls, autoclaved for 1 h). For the ^{14}C-PFOA experiments, 15-mL serum bottles were utilized (50% O_2-free N_2 headspace, 50% inoculated anaerobic test medium) with non-radioactive C_8-PFCA and ^{14}C- C_8-PFCA (4.5 lCi/mL test medium) to give a final concentration of 100 mg/L C_8-PFCA medium. For establishing the various terminal electron-accepting processes, a standard anaerobic procedure was used. The anaerobic mineral salts buffer (plus vitamins and trace minerals) was used as diluents for the various inoculums sources (5% wt/volume) with addition of electron donors (10 mM sodium acetate ± 40 mM sodium lactate or 0.6 mM ethanol or 2 atm H_2) or electron acceptors [O_2 as air headspace or O_2- free N_2 headspace in each serum bottle with additions of 30 mM nitrate or 4 mg/mL FeOOH or 10 mM sulfate or 0.4 mM trichloroethene (TCE) or no addition (for the methanogenic treatment)]. Samples (1.0 mL) were periodically removed from each serum bottle, placed in 4-mL glass vials sealed with Al-backed caps, immediately mixed with an equal volume of methanol and stored at _20 °C until analysis. Accumulated batches of samples from serum vials were analyzed for concentrations of PFOA, ^{14}C- C_8-PFCA, fluoride, nitrate, sulfate, and potential C_8-PFCA transformation products. Headspace gases were sampled with a gas-tight syringe (250 mL) and analyzed for TCE, vinyl chloride and methane. In the radiotracer study, dissolved ^{14}C activity in the anaerobic medium and in the 0.4 N KOH solution retrieved from the internal reservoir to trap $^{14}CO_2$ were determined by scintillation counting. To assay potential microbial inhibition by C_8-PFCA, triplicate serum- bottle assays inoculated with 5% Ithaca sewage were prepared, as above. Anaerobic preparations (±100 ppm C_8-PFCA) were assayed for methanogenesis. Aerobic preparations containing 15 ppm naphthalene were sampled as above and analyzed by high-performance liquid chromatography (HPLC). After filtration through nylon acrodisc filters, naphthalene was separated at room temperature. Methanol–water (1:1) was the mobile phase at a flow rate of 1.5 mL/ min. The eluent was monitored by UV VIS at 340 nm. Quantification was done by comparison to authentic standards (Liou et al., 2010). C_8-PFCA quantification was performed by LC/MS/MS following a standard procedure. Potential C_8-PFCA metabolites were screened by applying LC/MS.

In no combination of the inoculum source, electron donator or physiological conditions a significant percentage of the initial C_8-PFCA (100 ppm and 100 ppb) was consumed (110 - 259 days). In a test with ^{14}C labelled C_8-PFCA ammonium salt (inoculum = sewage), no loss of C_8-PFCA ammonium salt was detected, no $^{14}CO_2$ was produced and no radiolabelled C_8-PFCA ammonium salt transformation product was indicated. Co-metabolism of C_8-PFCA during reductive dechlorination of trichlorethene was suggested by a drop in C_8-PFCA concentration in the 100 ppb treatment after a 65-d incubation. However, extensive analysis failed to determine corroborating transformation products. In summary, under conditions which were examined in this study, C_8-PFCA is environmentally persistent (Liou et al., 2010). This study is assessed with reliability 3 due to significant methodological deficiencies.

Although for aerobic conditions no reliable study is available, it can be concluded that the above-mentioned studies support that C_8-PFCA is not biodegradable under aerobic conditions. In the environment aerobic as well as anaerobic conditions occur. Hence, simulations tests under both conditions are necessary for assessing the persistence. In conclusion, the degradation simulation studies on C_8-PFCA demonstrate the high persistence of the compound. Based on the read across rationale described in Annex 1, data on C_8-PFCAs can be used as evidence of persistence for C_{12}-PFCA.

3.1.2.2 Biodegradation in sediments

No data available

3.1.2.3 Biodegradation in soil

There are no degradation studies on C_{12}-PFCA available. Based on the data given in Annex 1, results of studies of structurally similar substances of the same chemical group could be used to evaluate the hydrolysis of C_{12}-PFCA. A number of studies are available for C_8-PFCA (PFOA) which were already discussed in the OECD SIDS Initial Assessment Report. The following text was copied from there (italic letters) (OECD, 2006):

Moody and Field (1999) conducted sampling and analysis of samples taken from groundwater 1 to 3 meters below the soil surface in close proximity to two fire-training areas with a history of aqueous film forming foam use. Perfluorooctanoate was detected at maximum concentrations ranging from 116 to 6750 µg/l at the two sites many years after its use at those sites had been discontinued. These results suggest that PFOA can leach to groundwater (Moody and Field, 1999).

Extensive site specific monitoring of soil and ground water concentrations of PFOA and related substances was conducted by 3M, DuPont Daikin and others. PFOA in soil has been shown to persist for decades and to be a long term source of groundwater and surface water contamination (see for example (DuPont Co., 2003; 3M Co., 2005)).

At the DuPont Washington Works site soil contaminated by perfluorochemical waste has been shown to contain ppm levels of PFOA 3 decades after application ceased. The underlying groundwater also contains ppm levels of PFOA (DuPont Co., 1999).

Extensive field monitoring data generated by 3M at the Decatur, AL site have also shown that PFOA is persistent in soils. Soil samples were collected from a former sludge application area of the 3M Decatur, AL facility also show soil contamination and underlying groundwater contamination up to ppm levels decades after application ceased.

Moody et al. investigated groundwater at a former fire-training area at Wurtsmith Air Force Base which was used between 1950s and 1993. Before sampling, the soil and groundwater in the area has been studied in detail. Groundwater samples were collected from two types of monitoring wells. All samples were collected in high density polypropylene bottles. Samples were shipped on ice without preservation and stored at 4 °C prior to analysis. Perfluorocarboxylate concentrations were measured as described in the following: Strong anion exchange disks were used to extract perfluorocarboxylates (6 to 8 carbons) from groundwater. The perfluorocarboxylates were simultaneously eluted from the disks and derivatized to their methyl esters by treatment with iodomethane for direct analysis by electron impact gas chromatography-mass spectrometry (GC-MS). A single analysis was conducted for each groundwater sample. The detection limit (defined as a signal-to-noise ratio greater than 3) and quantification limit (defined as a signal-to-noise ratio greater than 10) for perfluorocarboxylates were 3 and 13 mg/ L, respectively, using 2-chlorolepidine as the internal standard. Additionally, electron capture negative chemical ionization GC-MS was employed to confirm the identity of PFOA, in groundwater samples (Moody et al., 2003). Depending on the location of sampling, the concentrations of C_8-PFCA were between 8 and 105µg/L in groundwater. The authors estimated that perfluorinated surfactants had been in the groundwater for at least five years and possibly for as long as 15 years. This showed that degradation of C_8-PFCA was negligible under the environmental conditions at this site (for both soil and groundwater) (Reliability = 2) (Moody et al., 2003).

The anaerobic biodegradability of C_8-PFCA and its ammonium salt, respectively, in soil from two fire training areas was investigated by Liou et al. (see above 3.1.2.1.3 Simulation tests). No significant amount of the initial PFOA was dissipated after 259 days.

In conclusion, the available data on C_8-PFCA demonstrate the high persistence of the compound. Based on the read across rationale described in Annex 1, data on C_8-PFCAs can be used as evidence of persistence for C_{12}-PFCA.

3.1.2.4 Summary and discussion on biodegradation

A screening study proves that C_{12}-PFCA is not readily biodegradable.

Results from non standard degradation studies of C_8-PFCA, used for read-across approach as described in Annex1, indicate that the structurally similar compound is not biodegradable. The results of one non-standard aerobic biodegradation simulation test, one non-standard anaerobic biodegradation simulation test and field monitoring data on C_8-PFCA from contaminated sites provide evidence that no biodegradation in water, soil and sediment occurs. Since the stability of PFCAs is in general mainly based on the stability of the fluorinated carbon chain it can be concluded that also for C_{12}-PFCA no biodegradation in water, soil and sediment can be expected. Thus, it can be assumed that C_{12}-PFCA is not biodegradable.

3.1.3 Summary and discussion on degradation

In conclusion, for C_{12}-PFCA there is only one study available showing that the substance is not readily biodegradable. Therefore, data from chemically similar compounds should be considered in a read-across approach (please see Annex 1 for further details). The degradation potential of substances differing only in the number of carbons in the fluorinated carbon chain has been analyzed in some studies. Generally, it is known that the bond between carbon and fluorine is one of the most stable ones in organic chemistry.

A number of studies for the shorter chain C_8-PFCA show that this substance is very persistent and does not undergo abiotic or biotic degradation at all under environmental conditions. Moreover, also for the C_9-PFCA, it was shown that no readily biodegradation occurs. Phototransformation was analysed for $C_{8\text{-}11}$-PFCA (please see the Data Matrix in Annex 1). However, the test was not obtained under relevant environmental conditions. The persistence is mainly based on the common structural feature: the fluorinated carbon chain.

Abiotic degradation

The data on C_8-PFCA indicate that abiotic degradation in the atmosphere is expected to be slow (atmospheric lifetime = 130 days). The hydrolytic half-life of C_8-PFCA at 25°C is greater than 92 years, with the most likely value of 235 years under relevant environmental conditions *(3M Co., 2001a)*. No photodegradation of C_8-PFCA has been observed in studies conducted under relevant environmental conditions. The estimated DT_{50} for indirect photolysis is 349 days.

Biotic degradation

A standard screening tests is available for C_{12}-PFCA. No biodegradation at all has been observed within 28 days. For C_8-PFCA test results differ from "no biodegratation" to 13% biodegradation of the ammonium salt. Thus, it can be concluded that $C_{8,12}$-PFCAs are not readily biodegradable.

For C_8-PFCA a non-standard aerobic biodegradation simulation test, one non-standard anaerobic biodegradation simulation test and field monitoring data from contaminated sites provide evidence that no biodegradation in water, soil and sediment occurs.

Conclusion

PFCAs are synthetic compounds which contain a structural feature: a perfluorinated carbon chain combined with a carboxylic group. The chemical structure of these compounds differs only in the number of perfluorinated carbons in the carbon chain.

The stability of organic fluorine compounds has been described in detail by Siegemund et al., 2000: When all valences of a carbon chain are satisfied by fluorine, the zig-zag-shaped carbon skeleton is twisted out of its plane in the form of a helix. This situation allows the electronegative fluorine substituents to envelope the carbon skeleton completely and shield it

from chemical attack. Several other properties of the carbon-fluorine bond contribute to the fact that highly fluorinated alkanes are the most stable organic compounds. These include polarizability and high bond energies, which increase with increasing substitution by fluorine. The influence of fluorine is greatest in highly fluorinated and perfluorinated compounds. Properties that are exploited commercially include high thermal and chemical stability (Siegemund et al., 2000).

Based on their molecular properties it is, thus, not surprising, that researchers could not measure degradation of the intensively studied C_8-PFCA or its salts. Considering the organic chemistry of this substance group it seems to be very likely that a carbon chain being some CF_2-groups longer is as persistent as a shorter chain C_8-PFCAs. We therefore conclude that C_{9-14}-PFCAs are as resistant to degradation as it has been shown for C_8-PFCA.

In summary, using the described read across approach, we conclude that C12-PFCA is a very persistent synthetic compound which is resistant to abiotic and biotic degradation.

3.2 Environmental distribution

3.2.1 Adsorption/desorption

Not relevant for the SVHC identification of the substance in accordance with Article 57 (e).

3.2.2 Volatilisation

Not relevant for the SVHC identification of the substance in accordance with Article 57 (e).

3.2.3 Distribution modelling

Not relevant for the SVHC identification of the substance in accordance with Article 57 (e).

3.3 Bioaccumulation

3.3.1 Aquatic bioaccumulation

3.3.1.1 Bioconcentration factor BCF

Bioconcentration is the process by which a chemical is accumulated by an organism as a result of exposure to the chemical in water – it often refers to a condition usually achieved under laboratory and steady state conditions. The BCF is typically calculated as the ratio of the measured chemical concentrations in the organism and the water once a steady state has been achieved:

$$BCF = \frac{C_{Biota}}{C_{Water}}$$

The BFC can alternatively be determined kinetically by using the uptake rate k_1 and the depuration rate k_2:

$$BCF = \frac{k_1}{k_2}$$

There are two studies available which determined the BCFs of C_{12}-PFCA.

In the first study carp were exposed to C_{12}-PFCA (National Institute of Technology and Evaluation, 2007). The test was conducted in accordance with the OECD 305 guideline. The test was conducted in a flow through test system, the concentration of the test substance were 1 µg/L and 0.1µg/L and below the predicted water solubility value. The concentrations were analytically checked via HPLC-MS. The pH was within the range 7.7 to 7.8. The uptake period was 60 days. The depuration period was 45 days. Steady state BCFs were in the range from 10000 - 16000 for C_{12}-PFCA (Table 7).

In the second study rainbow trout were exposed in a flow-through system for 12 days followed by a depuration time of 33 days in fresh water to determine tissue distribution and bioconcentration (Martin et al., 2003a). For determination of bioconcentration, juvenile fish (5-10g) were exposed simultaneously to PFCAs of varying chain length. No adverse effects were observable based on fish mortality, growth and liver somatic index. The exposure concentration of each PFCA was analytically checked. PFCA concentrations were stable throughout the uptake phase. For C11-PFCA the measured concentration was 0.20 µg/L with a relative standard deviation of 30%. There was an initial decrease between 0.25 h and 24 h which is considered to be caused by the rapid uptake of the PFCAs. At 7 occasions during uptake period and 9 occasions during depuration phase, three fish from the exposure tank and one fish from the control were removed to determine the kinetics of uptake and depuration. The BCFs (carcass, blood and liver) were determined on the basis of the uptake and depuration kinetics and results are given in Table 7. All tissue concentrations were corrected for growth dilution. Additionally, for the tissue distribution study, four immature trout (30 – 48 g) were exposed in separate tanks but under the same uptake conditions (Martin et al., 2003a).This tissue distribution study showed that unlike lipophilic organic compounds PFCAs did not preferentially accumulate in adipose tissue. Hence a lipid-normalisation of the BCFs would not be reasonable. C_{11}-C_{14}-PFCA concentrations were highest in blood, kidney, liver and gall bladder and low in the gonads, adipose and muscle tissue. Within the blood, the plasma contained between 94 – 99 % of PFCA, with only a minor fraction detectable in the cellular fraction. Recovery from hearts and spleen was low (<10%). Based on high blood, liver and gall bladder concentrations and slow depuration the authors assume that PFCA enter the enterohepatic recirculation in fish. That means the compounds are continuously transferred between the different organs (Martin et al., 2003a).

BCFs were calculated for different body compartments. Though, bioaccumulation should preferably be based on whole body. According to the authors carcass BCFs closely approximate the whole-body BCF. However, compartment-specific BCFs can be more relevant if there is a potential for direct organ-specific toxicity. PFCAs cause hepatomegaly in rodents (Kudo et al., 2000) which is an indicator for hepatotoxicity. This study investigated PFCAs with 7–10 carbon chain lengths. PFCAs having a longer perfluorinated carbon chain showed a more potent induction of hepatomegaly. However due to its structural similarity, with additional fluorinated carbons, it can be assumed that also C_{12}-PFCA may be hepatotoxic. Thus, from a toxicological perspective, BCFs based on concentrations in individual organs, such as the liver, may be more relevant when the potential for direct organ-specific toxicity (i.e., liver toxicity) is being predicted. No statistically significant difference was found between the liver somatic index of exposed and control fish. However, bioaccumulation tests are not designed for showing toxic effects. The calculated kinetic BCFs are summarized in Tabe 8.

BCF values may be estimated using biomagnifications data. Based on the assumption the elimination kinetics are the same regardless of the uptake pathway, a kinetic BCF can be calculated. For this the measured elimination-rate from a fish feeding study and a modelled uptake rate for uptake through the gills is used. There are various mechanistic models available to roughly estimate the uptake rate. An overview is given in Crookes and Brooks

(2011). These models depend on physical-chemical input parameters such as the log K_{OW}. As this parameter cannot be sufficiently estimated for PFCAs these approaches should not be used (Weisbrod et al., 2009). However, based on a study with in vivo and isolated perfused gills Sijm et al. suggested an approach, which is independent of the log K_{OW} and describes an uptake rate dependent on fish weight only (Sijm et al. 1995). This approach has been suggested as potentially suitable for the estimation of an uptake rate and the calculation of a BCF from biomagnifications data (Crookes and Brooks 2011). Another approach similar to the Sijm approach has also been considered as potentially suitable. Barber et al. (2003) compared and reviewed models and methods for predicting bioconcentration in fish by comparing the predictability of these models using a set of experimental bioconcentration data. As a result an allometric equation, also independent of the log K_{OW}, was derived using 517 data points. Using the elimination rate values for C_{11}-PFCA measured by Martin et al. 2003b (please find details of the study in section 3.3.1.3)and taking into account growth i.e. increase of weight over time the calculated BCFs range between 7725-8210 for carcass and 8068-8575 for liver based on the allometric equation derived by Sijm et al. (1995). Based on the allometric equation from Barber et al. (2003), BCFs range between 7589-7879 for carcass and 7927-8575 for liver. The calculated BCFs from BMFs of the fish feeding study (Martin et al., 2003b) are larger than the measured BCFs (Martin et al., 2003a) but in a similar order of magnitude. The elimination rates were different in the two studies of Martin et al. (Martin et al., 2003a; Martin et al., 2003b), which may be due to the different fish size and may explain the differences.

A recently published comparison of BCFs and biomagnification factors (BMFs) investigated 9 substances in a laboratory fish feeding study with carp (Inoue et al. 2012). Five substances showed BCFs larger than 5000 but only two of these substances were likely to biomagnify. Based on linear regression conducted with their data the authors suggest that a BMF of 0.31 indicates a high bioaccumulation potential. We used the linear regression to calculate BCFs based on BMFs of the study by Martin et al (Martin et al., 2003b) (please find details of the study in section 3.3.1.3). Again, the calculated BCFs from BMFs of the fish feeding study (Martin et al., 2003b) are smaller than the measured BCF (Martin et al., 2003a) but in a similar order of magnitude. However the results of this calculation may only be seen as equivocal evidence. Only nine data points were used to derive the linear regression and as the authors state themselves the results of the study are highly suggestive and more data would be necessary to support their findings.

The calculated kinetic BCFs are summarized in Table 8.

Table 7: Bioconcentration factors (BCF) of C_{12} –PFCA.

Species/foodweb	**BCF**	**Reliability**	**Reference**
Rainbow trout (carcass)	18000 ± 2700	2	(Martin et al., 2003a)
Rainbow trout (blood)	40000 ± 4500		
Rainbow trout (liver)	18000 ± 2900		
Carp (whole)	10000-16000	2	(National Institute of Technology and Evaluation, 2007)

Table 8: Calculated BCFs based on elimination rate and BMF values for C_{12}-PFCA. The BMFs were measured by Martin et al. 2003b (please find details of the study in section 3.3.1.3).

Species/foodweb	**BCF**	**Reliability**	**Reference**
Juvenile rainbow trout (Carcass)	7725-8210	2	(Sijm et al., 1995; Martin et al., 2003b)
Juvenile rainbow trout (Liver)	8068-8575	2	
Juvenile rainbow trout (Carcass)	7589-7879	2	(Barber et al., 2003; Martin et al., 2003b)

Juvenile rainbow trout (Liver)	7927-8575	2	
Juvenile rainbow trout (Carcass)	5761-7327	3	(Inoue et al., 2012; Martin et al., 2003b)

Conclusion:

All reported BCFs are above 5000 indicating a high bioaccumulation potential of the C_{12}-PFCA.

3.3.1.2 Bioaccumulation factors (BAFs)

In field studies on bioaccumulation of chemicals bioaccumulation factors (BAF) are measured. The BAF is typically measured in the field as the ratio of the chemical concentrations in the organism and the water:

$$BAF = \frac{C_{Biota}}{C_{Water}}$$

where chemical concentration in the organism (C_{Biota}) is usually expressed in units of gram of chemical per kilogram of organism. The weight of the organism can be expressed on a wet weight basis or appropriately normalized, if needed, (e.g.,lipid- or protein-normalized) (Conder et al., 2011). BCFs are measured under controlled laboratory conditions, whereas BAF is a field measurement and therefore different from BCF. Moreover, the chemical exposure is not only limited to water but all routes including diet.

Labadie et al. (2011) investigated the partitioning of various PFCAs in the Orge River, an urban tributary of the Seine River. Bioaccumulation and tissue distribution was studied in European chup, a common cyprinid in European freshwater and a benthopelagic fish. Five adult fish were collected in April 2010. The sex of each individual fish was analysed according to gonad morphology. Whole liver, gills and gonads were taken along with portions of muscle. Water and sediment samples were taken as triplicates at the same site. Large inter-individual variations, not sex-related, were observed. In agreement with the findings made by Martin et al. (2003a) tissue distribution shows that C_{12}-PFCA is especially accumulated in blood and liver. All values are above 5000. The results of this study are summarized in table 9.

Species	**Log BAF**	**BAF**	**Reliability**	**Reference**
Chup(*Leuciscus cephalus*) plasma	6.7±0.1	5011872	2	Labadie et al. (2011)
Chup(*Leuciscus cephalus*) liver	5.7±0.4	501187		
Chup(*Leuciscus cephalus*) gills	5.7±0.2	501187		
Chup(*Leuciscus cephalus*) gonads	5.5±0.1	316228		
Chup(*Leuciscus cephalus*) muscle	5.0±0.1	100000		

Table 9 Bioaccumulation factors (BCF) of C_{12} –PFCA

3.3.1.3 Biomagnification factors (BMFs)

Besides bioconcentration also biomagnification describes the potential of a chemical to bioaccumulate. Biomagnification factors (BMFs) can be measured in the laboratory in a fashion similar to that used in the OECD and US-EPA bioconcentration test protocols. Organisms are exposed to a chemical preliminary via diet. The BMF test typically includes an uptake phase, where levels of chemicals are followed over time, ideally until the chemical concentration in the

organism no longer changes with time (i.e., reaching the steady-state). If a steady-state cannot be reached in the experiment, the uptake phase is followed by a depuration phase where organisms are exposed to uncontaminated food. The rate of decline in chemical concentration over time measured in the depuration phase can then be used to derive the chemical uptake rate from which a hypothetical steady-state concentration can be estimated (Conder et al., 2011).

The laboratory-derived dietary BMF is calculated using the ratio of the chemical concentrations in the test animals at steady-state and their diet:

$$BMF = \frac{C_{biota}}{C_{diet}}$$

where chemical concentration in the organism (C_{biota}) and its diet (C_{diet}) are appropriately normalized, if needed, (e.g., lipid- or protein-normalized) (Conder et al., 2011).

BMF values based on field studies are based on the ratio of the concentration in the predator and the prey:

$$BMF_{(field)} = \frac{C_{predator}}{C_{prey}}$$

There are several uncertainties concerning field based BMFs similar to field based trophical magnifacation factors which regard food webs. There are biological, ecological factors which can influence the outcome of a BMF. Additionally as there is no standard procedure so far how to conduct such filed studies and therefore different study designs may too have an influence. The uncertainties of field studies have been addressed and discussed by Borga et al. (2012). As the authors actually refer to field based trophical magnifacation factors a summery of the discussion has been included in chapter 3.3.1.4 trophic magnifacation factors.

Problems arise with increasing body size of predators because analysis is based on tissue or serum samples. Whole-body analysis is not feasible for ethical reasons, i.e. a whole whale would be needed, and due to the challenging logistics with respect to sampling and laboratory constraints. Therefore, some of the derived BMF-values are restricted to certain tissue samples rather than whole body samples. BMF values based on liver samples may be over estimative. From a toxicological perspective concentrations in individual organs, such as the liver, may be more relevant when the potential for direct organ-specific toxicity (i.e., liver toxicity) is being predicted. Whole body values may be estimated if the tissue mass fraction is known for the organism regarded. There may however be some uncertainties due to inter individual and geographical differences (Houde et al., 2006).

Martin et al. (2003b) exposed juvenile rainbow trout (*Oncorhynchus mykiss*) for 34 days to PFCAs in the diet, followed by a 41 day depuration period. Though, the authors describe their results as BAF the results of this study should rather be assigned as BMFs according to the above mentioned definition as uptake only derived from the diet. During the uptake period, animals were daily fed with spiked food at a rate of 1.5 % food per body weight. Spiked food concentrations were 1.1 µg/g for C_{12}-PFCA. Water samples collected before and after feeding revealed no traces of PFCAs in water. At 6 occasions during uptake period and during depuration period, fish were removed to determine the kinetics of uptake and depuration. The authors estimated the steady state to less than 34 days. Carcass and liver concentrations were determined by using liquid chromatography-tandem mass spectrometry, and kinetic rates were calculated to determine bioaccumulation parameters. Bioaccumulation (carcass) increased with increasing chain length but was not larger than one: 0.43 ± 0.062 for C_{12}-PFCA (see also Table 78). This indicates that a dietary exposure will not result in biomagnification in juvenile trout. The authors assume that the lack of observed biomagnification was likely due to the small size of fish used in the study, resulting in more rapid chemical elimination to water, relative to body size and and that their natural feeding rate is too low. This more rapid chemical elimination

would reduce the BMF stronger than what would be observed for larger species or size classes (Martin et al., 2003b).

Furthermore BMFs were estimated from field studies. Studies are described below and results are shown in Table 10.

Transfer of PFCAs was elucidated in Lake Ontario including one 4-membered pelagic food chain (Martin et al., 2004). Whole body samples were collected. Two macroinvertebrates (*Diporeia* and *Mysis*) were considered as primary prey whereas rainbow trout inhabited the top predator´s position. Lake trout samples were taken at various locations and years (1980-2001) in Lake Ontario. Seven samples were selected every three years (i.e. 7 individual fish samples per year). Forage fish species, including sculpin, smelt, and alewife, were collected on October 9th 2002 at an offshore site near Niagara-on-the-Lake, Lake Ontario. Due to the inherent uncertainties correlated with constitution of diet 4 individual combinations of rainbow trout and its prey were regarded. As this study was conducted with fish uptake of PFCAs may not have occurred exclusively over diet but also over the gills. Thus, the factors may be more accurately addressed as BAF. A striking finding of this study was the unexpectedly high content of PFCAs in the benthic invertebrate *Diporeia* occupying the lowest trophic level. The mechanism leading to this exceptional accumulation still needs to be unravelled. The author's hypothesis is that sediments are a major source for PFCAs. Results are given in Table 10.

Tomy et al. also investigated beluga whale, ringed seal, fish pelagic amphipod and arctic copepod of the Western Canadian Arctic. The animals selected were from the sample archived repository at Fisheries and Oceans, Canada. Blubber and liver of beluga (n = 10, all males,) from Hendrickson Island and ringed seal (n = 10, all males) from Holman Island were collected in 2007 and 2004, respectively. Fish species collected in 2004 and 2005 included the marine pelagic Arctic cod (n = 10) from the Amundsen Gulf, the marine coastal Pacific herring (n = 10) from the Mackenzie Shelf and the anadromous Arctic Cisco (n = 9) from the Mackenzie estuary. The marine pelagic amphipod *Themisto libellula* (pooled samples, n = 2) and the marine Arctic copepod *Calanus hyperboreus* (pooled samples, n = 5) were collected in 2004 from the eastern Beaufort Sea and Amundsen Gulf region. As the authors state themselves differences in sampling years may influence the interpretation of the food web transfer. On the other hand the Arctic as a remote area may be less prone to temporal changes and the existence of point sources there is unlikely. The derived BMF-values (see Table 11) are restricted to the liver and the resulting BMF may be over estimative. From a toxicological perspective concentrations in individual organs, such as the liver, may be more relevant when the potential for direct organ-specific toxicity (i.e., liver toxicity) is being predicted (Tomy et al., 2009).

Houde et al. examined PFCA serum concentrations in bottlenose dolphins at two different habitats, Charleston Harbor and its tributaries (i.e., the Cooper, Ashley, and Wando rivers) and the Stono River estuary, South Carolina, and in Sarasota Bay, Florida. Marine water (n=18), surface sediment (n=17), Atlantic croaker(n=3), pinfish(n=4), red drum (n=8), spotfish (n=10) , spotted seatrout (n=11), striped mullet (n=8), and bottlenose dolphin samples (n=24) were collected around the Charleston Harbor area. Marine water(n=10), surface sediment (n=8), zooplankton 8n03), sheephead (n= 3), pigfish (n= 10), pinfish (n=10), striped mullet (n=9), spotted seatrout (n=8), and bottlenose dolphin samples 8n=12) were collected at Sarasota Bay. Dolphin plasma, skin, and teeth were collected from both locations. Additionally, dolphin tissue samples (i.e., liver, kidney, muscle, lungs, heart, thyroid, and thymus) were collected of recently deceased bottlenose dolphins from Sarasota Bay (2002, n = 1, male, 233.5 kg) and Charleston (2003, n = 1, female, 708.4 kg). Additional liver (n = 6) and kidney (n = 6) samples collected from stranded bottlenose dolphins were available at Sarasota Bay. The authors claim that utilization of serum or liver concentrations of dolphins will overestimate the BMF by a factor of 10 - 30. Whole body concentrations were estimated on the basis of tissue distribution. Samples were collected between 2002 and 2004. Unfortunately, concentrations in other representative fish species originated from different years, thus, entailing additional uncertainty when assessing BMF through the food chain. Wastewater treatment plant discharges in the Charleston area may have resulted in non–

steady state concentrations in the food web. On the other hand it may be assumed that media and biota were continuously exposed to PFCA in this area throughout the years. The results are summarized in Table 8 (Houde et al., 2006).

Butt et al. conducted a study in the Canadian Arctic. Ringed seal liver samples (n=10 per site) were provided by local hunters from 11 different locations in the Canadian Arctic. The age of the animals was determined via tooth aging and for a few samples the age was estimated using length-age correlations. Stable isotope analysis was done with ^{15}N to ^{14}N and ^{13}C to ^{12}C. Based on liver samples from polar bears obtained from another study and ringed seal data measured in this study BMFs were calculated (see Table 8). The polar bear sample sites were associated with ringed seal populations. However, the sample collection year for ringed seal populations varied from 2002 to 2005, and it is possible that interpretation of spatial trends may be confounded by temporal variations of PFCA concentration within seal populations (Butt et al., 2008).

Various predator prey relationships in the Westerschelde (Netherlands) were investigated by van Heuvel-Greve and co-workers. Samples of harbour seal plasma (n=3) and whole body samples of herring, seabass and flounder (n=4 per species) as well as zooplankton were collected in 2007 and 2008. The trophic level was estimated based on stable isotope (^{15}N) analysis. BMFs were considerable for harbour seal as well as for the sediment dwelling flounder (Environment Canada, 2012; van den Heuvel-Greve et al., 2009).

Table10: Available BMF data of C_{12}-PFCA; if not indicated otherwise BMFs refer to whole body

Location	**Species/foodweb**	**BMF**	**Reference**	**Reliability**
Canadian Arctic	Polar bear (liver)/ ringed seal (liver)	2.3-3.6	Butt et al. 2008	2
US, South Carolina, Charleston	Seatrout /pinfish	0.1	Houde et al. 2000	2
US, South Carolina	Dolphin(whole, estimated)/striped mullet	0.2		
US, South Carolina	Dolphin(whole, estimated)/pinfish	0.1		
US, South Carolina	Dolphin(whole, estimated)/red drum	0.4		
US, South Carolina	Dolphin(whole, estimated) / atlantic croaker	1.8		
US, South Carolina	Dolphin(whole, estimated) / spotfish	0.6		
US, South Carolina	Dolphin(whole, estimated) / seatrout	0.6		
US Sarasota Bay, Florida	striped mullet / zooplankton	89		
US Sarasota Bay, Florida	Pigfish/ zooplankton	2.5		
US Sarasota Bay, Florida	Sheephead/ zooplankton	156		
US Sarasota Bay, Florida	Pinfish/ zooplankton	2.5		
US Sarasota Bay, Florida	Seatrout/ zooplankton	35		
US Sarasota Bay, Florida	Seatrout/striped mullet	0.4		
US Sarasota Bay, Florida	Seatrout/pigfish	14		
US Sarasota Bay, Florida	Seatrout / sheephead	0.2		
US Sarasota Bay, Florida	Seatrout/pinfish	14		

US Sarasota Bay, Florida	Dolphin(whole, estimated)/striped mullet	0.1		
US Sarasota Bay, Florida	Dolphin (whole, estimated)/pigfish	2.0		
US Sarasota Bay, Florida	Dolphin(whole, estimated)/ sheephead	0.0		
US Sarasota Bay, Florida	Dolphin(whole, estimated)/pinfish	2.0		
US Sarasota Bay, Florida	Dolphin/seatrout	0.1		
Western Canadian Arctic	Ringed seal (liver)/ arctic cod (liver)	0.1	Tomy et al. 2009	2
Western Canadian Arctic	Beluga whale (liver)/ arctic cod (liver)	3.2		
Western Canadian Arctic	Beluga whale (liver)/ Pacific herring (liver)	7.9		
Western Canadian Arctic	Beluga whale (liver)/ arctic cisco (liver)	4.0		
Western Canadian Arctic	Arctic cod (liver)/ marine arctic copepod (whole body)	1.2		
Western Canadian Arctic	Arctic cod (liver)/ marine pelagic amphipod (whole body)	1.3		
Lake Ontario	Lake trout /alewife	1.9	Martin et al. 2004	2
Lake Ontario	Lake trout/ smelt	1.0		
Lake Ontario	Lake trout / sculpin	0.28		
Lake Ontario	Lake trout / prey (weighted)	1.6		
Laboratory	juvenile rainbow trout(Carcass)	0.43 ±0.062	Martin et al. 2003b	2

Conclusion:

The biomagnification potential of C_{12}-PFCAs was investigated in several field studies and one laboratory study. Field studies investigating the biomagnifications potential between different predator/prey-relationships showed BMFs well above one indicating biomagnification. Biomagnification was greater in homeotherms than in poikilotherms. Especially for dolphin, beluga whale, polar bear, arctic cod and seatrout, sheephead, and striped mullet BMFs greater than one have been reported.

3.3.1.4 Trophic magnification factors (TMFs)

The trophic magnification factor (TMF) is a measure to evaluate biomagnification occurring in food webs. In the Guidance Document on Information Requirements, Chapter R.7.10.1.1, TMF is defined as the concentration increase in organisms with an increase of one trophic level. Again, a TMF greater than one indicates accumulation within the food chain.

There are several uncertainties concerning TMFs. These have been addressed and summarized by Borga et al. (2012). There are biological factors such as the differences between

poikilotherms and homeotherms, sex, different energy requirements, different abilities to metabolize chemicals and slow or fast growing organisms.

Steady state between a consumer and its diet is assumed. However, as opportunistic feeders wild animals vary their diet over seasons or with life stage and point sources may influence observed TMFs. Additionally, apart from the diet there always is the possibility of a direct uptake of the substance under scrutiny and the relative importance of food versus e.g. water exposure can influence the magnitude of the TMF. The position in the food web is quantified using relative abundances of naturally occurring stable isotopes of N ($^{15}N/^{14}N$, referred to as $\delta^{15}N$). However the relative abundance of these isotopes und thus the determination of the trophical level and TMF is influenced by the physiology of the organism and its life trait history. Rapid growth with a higher protein demand for new tissue leads to lower enrichment factors than those with slower growth rates. Insufficient food supply and fasting and starvation leads to catabolism of body proteins and an increase of ^{15}N in organisms relative to those organisms with adequate food supply. There is no standard procedure for the conductance of TMF field studies. Hence, the conductance and sampling may vary between different studies. Disproportionate sampling of the food web or unbalanced replication of samples may significantly influence the TMF.

As already discussed in the BMF chapter sample collection is often restricted to tissue or serum samples with increasing body size of predators due to ethical reasons and due to the challenging logistics with respect to sampling and laboratory constraints.

Martin et al. examined PFCA contents in the food web from Lake Ontario in Canada (Martin et al., 2004). Adult lake trout (top predator) were collected at various years and locations in Lake Ontario. Samples of prey fish (sculpin, smelts and alewifess) and macroinvertebrates (*Mysis sp., Diporeia sp.*) were collected at one location in October 2002. A more detailed study description is given in chapter 3.3.1.3. Lake trout samples analyzed represented individual whole fish homogenates. The other species were processed as composites of whole individuals. TMFs are shown in Table11.

Houde et al. investigated the food web of bottlenose dolphins. The authors sampled different biota, i.e. croaker, pinfish, spotfish, spotted seatrout, striped mullet and samples from bottlenose dolphins, as well as water and surface sediment. Sample collection was conducted between 2002 and 2004. Based on stable isotope (^{15}N) analysis the trophic level of each biota sample was determined. PFCAs were analysed in plasma and liver of dolphins and afterwards a whole body burden was calculated. For prey whole body homogenates were analysed for PFCA (Houde et al., 2006). A more detailed study description is given in chapter 3.3.1.3. For results see Table 11.

Kelly et al. measured PFCAs in the Canadian Arctic marine food web. The authors used concentrations in sediment and in different organisms (lichens, macroalgae, bivalves, fish) and tissues and organs (stomach contents, liver, muscle, blubber and/or milk) of common eider ducks, and beluga whales and ringed seals to calculate TMFs. Sample collection was conducted between 1999 and 2003 along the eastern Hudson Bay coastline in close proximity to the Inuit village Umiujaq. PFCAs were measured in different tissues/fluids of the beluga whale including blood, muscle liver, milk and also in foetuses. The authors could show that PFCAs especially accumulate in protein rich compartments such as blood and liver and that the TMF of PFCAs correlates with the partitioning behaviour between protein and water and protein and air. Comparisons of different food webs show that the TMF is below one in the case of piscivorous food webs if air breathing organisms are excluded but becomes larger than one if air breathing organisms are taken into account (see Table 11) (Kelly et al., 2009).

Loi et al. investigated a subtropical food web in a nature reserve including phytoplankton, zooplankton, gastropod, worm and shrimp, and liver samples of fish and water bird. Samples were collected between 2008 and 2010. Surface water (n =12), sediment (n = 6), phytoplankton in general [pooled samples (p) = 3], zooplankton [mainly amphipods and copepods (p = 2)], gastropods (p = 3), worms (p = 10 of 3 families: Capitellidae, p = 5; Nephtyida, p = 3; Sabellidae, p=2), shrimps [p = 4 of 2 species: black tiger prawn (Penaeus

monodon), p = 2; sand prawn (Metapenaeusensis), p = 2], fish [n=21 of five species: greymullet (Mugil cephalus), n = 5; ladyfish (Elops saurus), n = 6; Mozambique tilapia (Oreochromis mossambicus), n = 5; small snakehead (Channa asiatica), n =3; flag-tailed glass perchlet (Ambassis miops), p = 2 with each pool consisting of 27 individuals] were collected from a tidal shrimp pond. Surface water and sediment samples were collected concurrently with the biota samples. BSAF were calculated based on the assumption that sediment was the major exposure pathway for worms. The study investigated PFCAs with different chain length. C_{12}-PFCA was detected in sediment only (Loi et al., 2011).

Table 10: Available Trophic Magnification Factors (TMF) for C_{12} PFCA; if not indicated otherwise TMFs refer to whole body.

Location	Species/foodweb	TMF	Reference	Reliability
US, South Carolina	Dolphin plasma croaker, pinfish, spotfish, spotted seatrout	0.7 ± 0.8	Houde et al. 2006	2
US, South Carolina,	Whole dolphin burden, croaker, pinfish, spotfish, spotted seatrout	0.6 ± 0.8		
Hudson Bay (north-eastern Canada	Sediment/ macroalgae/ bivalves/ fish/ seaduck/ beluga whale	3.89 - 5.87 2.34 - 3.76 (protein corrected)	Kelly et al. 2009	2
Hudson Bay (north-eastern Canada	Sediment/ macroalgae/ bivalves/ fish	0.71 - 1.44 (protein corrected)		
Lake Ontario	Diporeia/slimy sculpin	No significant association with trophic level	Martin et al. 2004	2
Lake Ontario	Mysis/alewife/rainbow smelt/lake trout	No significant association with trophic level		
Mai Po Marshes Nature Reserve in Hong Kong	Tidal shrimp pond brackish food web	1.38	Loi et al., 2011	2

Conclusion:

A number of field studies are available which analyzed the trophic magnification potential of C_{12}-PFCA. For food chains of beluga whale and in a subtropical pelagic food web TMFs greater than one have been reported, indicating trophic biomagnification. Trophical magnification was greater if the food chain contained homeotherms. TMFs were smaller in the case of piscovorous food webs and if air breathing organisms are excluded but became larger if air breathing organisms were taken into account (Kelly et al., 2009). Thus, C_{12}-PFCA biomagnifies in some food webs analyzed within the food chain.

3.3.1.5 Terrestrial bioaccumulation

Müller et al. conducted a terrestrial food web study consisting of lichen and plants as well as tissue samples (liver muscle and kidney) from caribou, and wolves from two remote northern areas in Canada. Liver, muscle, and kidney samples (n=7 Porcupine herd food web and n=10 for the Bathurst food web) from two caribou herds were collected; from the Porcupine herd in northern Yukon Territory and the Bathurst herd in the Northwest Territories (NWT)/western Nunavut . Wolf (n=6 Porcupine herd food web and n=10 for the Bathurst food web) lichen, and plant samples were collected in the same region as the caribou. Plant samples included cottongrass, aquatic sedge, willow, moss, and mushrooms. Liver and muscle samples were collected from the sampled wolves. Lichen, moss and mushrooms were collected as a whole

grass and willow without roots. Plant samples are from the same season (Summer 2008 in Porcupine or Summer 2009 in Bathurst) whereas wolf and caribou samples are from different years (2007 and 2010 in Porcupine and 2008 and 2007 in Bathurst). This food web is considered as relatively well documented example (Kelly and Gobas, 2003). The study illustrates a considerable carry over between plants and caribou. Caribou are a major human food source in numerous arctic communities. This food-chain may also be considered comparable to the pasture-cow food-chain in temperate regions. The results of the study, BMFs as well as TMFs are shown in Table 9.

Tissue concentrations and whole body concentrations were used for calculations. Tissue based BMFs differ considerably. Therefore it is concluded that BMFs based on whole body concentrations are more appropriate (Müller et al., 2011).

Table 11: BMF and TMF values for C_{12}-PFCA for a terrestrial food chain (Müller et al., 2011)

	Food chain	**Location**	
		Porcupine	**Bathurst**
BMF	Caribou (whole)/ lichen	2.9	11
BMF	Caribou(whole)/ lichen	4.5	8
BMF	Wolf (whole)/ caribou (whole)	1.2	1.4
TMF	Wolf (whole)/ caribou (whole)/ lichen	1.4	2.2
TMF	Wolf (whole)/ caribou (whole) / vegetation	1.3	2.0

Conclusion:

The terrestrial BMF and TMF of C_{12}-PFCAs are greater than one for the remote Arctic food chain lichen – caribou – wolf, indicating trophic biomagnification.

3.3.2 Summary and discussion of bioaccumulation

For C_{12}-PFCA reported BCFs are well above the trigger value of 5000 according to REACH Annex XIII. Thus, it can be concluded that C_{12}-PFCA is a very bioaccumulative substances. Moreover, BMF and TMF- values greater than one have been reported for a number of food chains, indicating a potential for biomagnification.

4 Human health hazard assessment

Not relevant for the SVHC identification of the substance in accordance with Article 57 (e).

5 Environmental hazard assessment

Not relevant for the SVHC identification of the substance in accordance with Article 57 (e).

6 Conclusions on the SVHC Properties

6.1 PBT, vPvB assessment

6.1.1 Assessment of PBT/vPvB properties – comparison with the criteria of Annex XIII

A weight of evidence determination according to the provisions of Annex XIII of REACH is used to identify the substance as vPvB. All available information (such as results of standard tests, monitoring and modelling, information from the application of the category and analog approach (grouping, read-across) and (Q)SAR results) was considered together in a weight of evidence approach. The individual results have been considered in the assessment with differing weights depending on their nature, adequacy and relevance. The available results are assembled together in a single weight of evidence determination.

6.1.1.1 Persistence

PFCAs are synthetic compounds which contain a structural feature: a perfluorinated carbon chain combined with a carboxylic group. The perfluorinated carbon chain is a synthetic feature, there are no natural sources known. The chemical structure of these compounds differs only in the number of perfluorinated carbons in the carbon chain.

The stability of organic fluorine compounds has been described in detail by Siegemund et al., 2000: When all valences of a carbon chain are satisfied by fluorine, the zig-zag-shaped carbon skeleton is twisted out of its plane in the form of a helix. This situation allows the electronegative fluorine substituents to envelope the carbon skeleton completely and shield it from chemical attack. Several other properties of the carbon-fluorine bond contribute to the fact that highly fluorinated alkanes are the most stable organic compounds. These include polarizability and high bond energies, which increase with increasing substitution by fluorine. The influence of fluorine is greatest in highly fluorinated and perfluorinated compounds. Properties that are exploited commercially include high thermal and chemical stability (Siegemund et al., 2000).

Comparing the physico-chemical properties of C_{8-14}-PFCAs it becomes obvious that with increasing chain length water solubility decreases and the sorption potential increases. This trend is based on the increasing number of CF_2-groups in the molecular structure. The molecular reason for the persistence of highly fluorinated chemicals is the shielding effect of the substituted fluorine atoms described by Siegemund et al., 2000. Thus, using the described read across approach (please see Annex 1 for further details), we conclude that C_{12}-PFCA is a very persistent synthetic compound which is resistant to abiotic and biotic degradation and fulfils both, the P and the vP criteria of Annex XIII.

Abiotic degradation

The data on C_8-PFCA indicate that abiotic degradation in the atmosphere is expected to be slow (atmospheric lifetime = 130 days). The hydrolytic half-life of C_8-PFCA at 25°C is greater than 92 years, with the most likely value of 235 years under relevant environmental conditions *(3M Co., 2001a)*. No photodegradation of C_8-PFCA has been observed in studies conducted under relevant environmental conditions. The estimated DT_{50} for indirect photolysis is 349 days.

Biotic degradation

A standard screening test is available for C_{12}-PFCA. No biodegradation at all has been detected for within 28 days. For C_8-PFCA test results differ from "no biodegratation" to 13% biodegradation of the ammonium salt. Thus, it can be concluded that $C_{8,12}$-PFCAs are not readily biodegradable.

For C_8-PFCA a non-standard aerobic biodegradation simulation test, one non-standard anaerobic biodegradation simulation test and field monitoring data from contaminated sites provide evidence that no biodegradation in water, soil and sediment occurs.

Conclusion

Henicosafluoroundecanoic acid (C_{11}-PFCA) has no degradation studies available.

Read across approach within C_8-C_{14}-PFCAs can be applied for the persistence assessment of these substances. $C_{8\text{-}14}$-PFCAs contain a highly similar chemical structure, a perfluorinated carbon chain and a carboxylic acid group. The compounds differ only in the number of CF_2-groups. As a result of comparing the experimental and estimated physico-chemical data of C_8-PFCA (the analogue substance) with experimental and estimated data on $C_{11\text{-}14}$-PFCAs it can be assumed that with increasing chain length water solubility decreases and the sorption potential increases (See Table 15 of the support document). It can be with a sufficient reliability stated that the behaviour of these chemicals follow a regular pattern.

Due to both structural similarity and a regular pattern of physico-chemical properties, $C_{8\text{-}14}$-PFCAs may be considered as a group or a category of substances for the purpose of the PBT/vPvB assessment and the read-across approach can be applied within this group.

In general, the persistence of C_{11}-C_{14}-PFCAs can be explained by the shielding effect of the fluorine atoms, blocking e.g. nucleophilic attacks to the carbon chain. High electronegativity, low polarizability and high bond energies make highly fluorinated alkanes to the most stable organic compounds. It is not expected that the carboxylic group in PFCAs alters this persistence of these chemicals. This fact is confirmed by a hydrolysis study which obtained a DT_{50} of >92 years for C_8-PFCA in water. Screening studies of $C_{8,9,12,14}$-PFCAs showed no biodegradation within 28 days. Non-standard abiotic degradation tests with C_8-PFCA could not detect any degradation products under environmentally relevant conditions. Furthermore, screening biodegradation studies on $C_{8,9,12,14}$-PFCAs and one non-standard anaerobic biodegradation simulation test with C_8-PFCA provide evidence of high persistence. Additionally, elements of non-standard higher tier aerobic biodegradation studies on C_8-PFCA provide further support that no biodegradation in water, soil and sediment occurs.

Therefore, based on the information summarised above, it is concluded that C_{11}-PFCA is not degraded in the environment and thus fulfils the P- and vP- criteria in accordance with the criteria and provisions set out in Annex XIII of REACH.

6.1.1.2 Bioaccumulation

Regarding the bioaccumulation potential for C_{12}-PFCA the available experimental BCF-values are above 5000. A number of field-BMFs and TMFs are available for C_{12}-PFCA and they provide evidence that biomagnification of this substance takes place in nature between different trophic levels of food chains and from the bottom to the top of food chains (see Table 15). Due to the structural similarity and the regular pattern of physico-chemical properties within the group of $C_{11\text{-}14}$-PFCAs, read across can be applied within the group. The available field bioaccumulation data of C_{12}-PFCA and the other substances of the group provide further support to assume that C_{12}-PFCA biomagnifies in the food chain. Thus, it is concluded the B as well as the vB-criteria -are met in accordance with the criteria and provisions set out in Annex XIII of REACH.

6.1.1.3 Toxicity

Not relevant for the SVHC identification of the substance in accordance with Article 57 (e).

6.1.2 Summary and overall conclusions on the PBT, vPvB properties

C_{12}-PFCA is not readily biodegradable. Further degradation studies are not available. Applying the read across approach, data from structurally similar compounds can be used to evaluate the degradation potential of the substance. $C_{8\text{-}14}$-PFCAs contain a highly similar chemical structure, a perfluorinated carbon chain and a carboxylic acid group. The compounds differ only in the number of CF_2-groups.

Comparing the physico-chemical properties of $C_{8\text{-}14}$-PFCAs it becomes obvious that with increasing chain length water solubility decreases and the sorption potential increases. This trend is based on the increasing number of CF_2-groups in the molecular structure. According to the read-across approach these chemicals follow a regular pattern as a result of structural similarity. Those substances may therefore be considered as a group or a category of substances and the read-across approach can be applied.

In general, the persistence of long chain PFCAs can be explained by the shielding effect of the fluorine atoms, blocking e.g. nucleophilic attacks to the carbon chain. High electronegativity, low polarizability and high bond energies make highly fluorinated alkanes to the most stable organic compounds. It is not expected that the substitution of a functional group – the carboxylic group in PFCAs– alters this persistence of these chemicals. This fact is confirmed by a study which obtained a DT_{50} of >92 years for C_8-PFCA in water. Screening studies of $C_{8,9,12,14}$-PFCA showed no biodegradation within 28 days. Non-standard tests with C_8-PFCA could not detect any degradation products under environmentally relevant conditions. Moreover, a monitoring study showed that C_8-PFCA remained in soil and groundwater, years after application of fire fighting foam which contained PFCAs.

Therefore, we conclude that C_{12}-PFCA is not degraded in the environment and thus fulfils the P- and vP-criteria under REACH.

The available BCF-values of C_{12}-PFCA are above 5000. Thus, the B as well as the vB-criteria according to Annex XIII of REACH are fulfilled.

In conclusion, C_{12}-PFCAs is identified as a vPvB-substance according to Art. 57 (e) of REACH and by applying a weight of evidence determination using expert judgement by comparing all relevant and available information listed in Section 3 of Annex XIII of REACH with the criteria set out in Section 1 of the same Annex.

6.2 CMR assessment

Not relevant for the SVHC identification of the substance in accordance with Article 57 (e).

6.3 Substances of equivalent level of concern assessment

Not relevant for the SVHC identification of the substance in accordance with Article 57 (e).

Annex I - Read-across approach

In general, the read-across approach can be applied if substances whose physicochemical and/or toxicological and/or ecotoxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity. Those substances may be considered as a group or a category of substances. According to ECHA`s practical guide 6 "How to report read-across and categories" similarities may be due to a common functional group, common precursor or breakdown products, constant pattern in changing potency or common constituents or chemical class.

Structural similarities of C8-14 PFCAs and some salts

In Table 13 the chemicals structures of the C8-14-PFCAs are displayed. All PFCAs contain a carboxylic acids group and a perfluorinated carbon chain. The compounds differ only in the number of carbon atoms within the fluorinated carbon chain. Thus, we conclude, that all the C8-14-PFCAs belong to the same chemical class and contain not only a common functional group but are highly similar according to their chemical structure.

Table 123: CAS-Numbers and similarity of chemical structures of long chain PFCAs.

Name	Abbreviation	CAS-No	IUPAC Name	Chemical structure
PFOA	C_8-PFCA	335-67-1	Octanoic acid, pentadecafluoro-	$CF_3(CF_2)_6$-COOH
PFNA	C_9-PFCA	375-95-1	Nonanoic acid, heptadecafluoro-	$CF_3(CF_2)_7$-COOH
PFDA	C_{10}-PFCA	335-76-2	Decanoic acid, nonadecafluoro-	$CF_3(CF_2)_8$-COOH
PFUnDA	C_{11}-PFCA	2058-94-8	Undecanoic acid, heneicosafluoro-	$CF_3(CF_2)_9$-COOH
PFDoDA	C_{12}-PFCA	307-55-1	Dodecanoic acid, tricosafluoro-	$CF_3(CF_2)_{10}$-COOH
PFTrDA	C_{13}-PFCA	72629-94-8	Tridecanoic acid, pentacosafluoro-	$CF_3(CF_2)_{11}$-COOH
PFTeDA	C_{14}-PFCA	376-06-7	Tetradecanoic acid, heptacosafluoro-	$CF_3(CF_2)_{12}$-COOH

Dissociation of C_{8-14}-PFCAs and its salts in aqueous media

Under environmental conditions in aqueous media the free perfluorinated carboxylic acids (PFCAs) stay in equilibrium with their conjugate bases, the perfluorinated carboxylates. The fraction of each species depends on the acid dissociation constant (pK_a) and the pH of the environmental compartment. Salts of PFCAs, which are sometimes used in laboratory experiments, will be in equilibrium with the corresponding acid in aqueous phases as well. Currently used techniques for analysis and quantification of PFCAs in i.e. environmental samples are not able to distinguish between both of the species. Therefore, reported concentrations always include the acids as well as the bases. If reported concentrations are used for the determination of bioaccumulation factors or for experiments determining the persistency, aqueous phase concentrations include both species. Experimental determination of pK_a is difficult for PFCAs, i.e. because of the surface active properties. Calculated values should be taken with care, because for most of the models it is unclear whether PFCAs are

within their applicability domain. For assessing the intrinsic properties of the PFCA within this dossier the exact knowledge of the fraction of each species is not required, because both of the species will be available independently from the starting conditions.

Furthermore, due to the uncertainties of pK_a values it is not wise to calculate partition coefficients under environmental pH conditions. We would like to mention that there is an ongoing scientific discussion showing that the partitioning of PFCAs in the environment can be described by the properties of the neutral PFCAs only (Webster and Ellis 2011).

Physicochemical properties and partition coefficients of C_{8-14}-PFCAs and some salts

The experimental determination of i.e. partition coefficients is difficult for example because of the surface active properties of the ionic PFCAs. The presence of ionic PFCAs depends on the dissociation of PFCAs in aqueous media. Nevertheless, there are models available, i.e. COSMOtherm calculating partitioning coefficients of neutral PFCAs. COSMOtherm is a quantum chemistry-based method that requires no specific calibration. This calibration would be difficult because of missing measured data of PFCAs. Therefore COSMOtherm is expected to be able to estimate properties for PFASs. Studies have shown that properties estimated with COSMOtherm showed good agreement with the experimental data for a number of per- and polyfluorinated chemicals, i.e. C8-PFCA (Wang et al. 2011; Arp et al. 2006). Again, whether neutral PFCAs are present in aqueous media depends in the dissociation of the acids. Air-water as well as octanol-water partition coefficients are of course different for PFCAs with 8 to 14 carbon atoms but they show a clear increasing, trend with chain length (see Table 13 below, Wang et al., 2011). This can be explained by the increasing molecular volume with each additional CF_2-unit. The trend of the fate of PFCAs with chain length is supported by information on sorption of PFCAs on sediment. Sorption increases with increasing chain length (Higgins and Luthy, 2006) also under environmental conditions (Ahrens et al., 2010) (seeTable 14).

Table 134: Basic substance information and physical chemical properties relevant to justify read across in the PBT assessment.

Abbreviation	**C_8-PFCA**			**C_9-PFCA**	**C_{10}-PFCA**	**C_{11}-PFCA**	**C_{12}-PFCA**	**C_{13}-PFCA**	**C_{14}-PFCA**
Acronym	PFOA	APFO	NaPFO	PFNA	PFDA	PFUnDA	PFDoDA	PFTrDA	PFTeDA
IUPAC Name	**Octanoic acid, pentadecafluoro-**	**ammonium pentadeca-fluoro-octanoate**	**pentadeca octanoic acid sodium salt**	**Nonanoic acid, heptadeca-fluoro-**	**Decanoic acid, nonadeca-fluoro-**	**Undecanoic acid, heneicosa-fluoro-**	**Dodecanoic acid, tricosafluoro-**	**Tridecanoic acid, pentacosa-fluoro-**	**Tetradecanoic acid, heptacosa-fluoro-**
Chemical Structure	CF3(CF2)6-COOH	CF3(CF2)6-COO-$NH4^+$	CF3(CF2)6-COO-Na^+	CF3(CF2)7-COOH	CF3(CF2)8-COOH	CF3(CF2)9-COOH	CF3(CF2)10-COOH	CF3(CF2)11-COOH	CF3(CF2)12-COOH
CAS No	335-67-1	3825-26-1	335-95-5	375-95-1	335-76-2	2058-94-8	307-55-1	72629-94-8	376-06-7
	Physico-chemical data								
Molecular Weight g/mol	414.09	431.1		464.08	514.08	564.0909	614.0984	664.1059	714.11
Partitioning Coefficient logKow				2.3 – 2.48 (exp)	2.65 – 2.87 (exp)	3.19 – 3.41	logP 9.363±0.888 at 25°C (calc)	logP 10.093±0.901 at 25 °C (calc)	logP 10.823±0.914 at 25 °C (calc)
	5.30 (calc., COSMOtherm, Wang et al., 2011)			5.9 (calc., COSMOtherm, Wang et al., 2011)	6.5 (calc., COSMOtherm, Wang et al., 2011)	7.2 (calc., COSMOtherm, Wang et al., 2011)	7.8 (calc., COSMOtherm, Wang et al., 2011)	8.25 (calc., COSMOtherm, Wang et al., 2011)	8.90 (calc., COSMOtherm, Wang et al., 2011)
log K_{OA}	7.23 (calc., COSMOtherm, Wang et al., 2011)			7.50 (calc., COSMOtherm, Wang et al., 2011)	7.77 (calc., COSMOtherm, Wang et al., 2011)	8.08 (calc., COSMOtherm, Wang et al., 2011)	8.36 (calc., COSMOtherm, Wang et al., 2011)	8.63 (calc., COSMOtherm, Wang et al., 2011)	8.87 (calc., COSMOtherm, Wang et al., 2011)
log K_{AW}	-1.93 (calc., COSMOtherm, Wang et al., 2011)			-1.58 (calc., COSMOtherm, Wang et al., 2011)	-1.27 (calc., COSMOtherm, Wang et al., 2011)	-0.92 (calc., COSMOtherm, Wang et al., 2011)	-0.58 (calc., COSMOtherm, Wang et al., 2011)	-0.38 (calc., COSMOtherm, Wang et al., 2011)	0.03 (calc., COSMOtherm, Wang et al., 2011)
Dissociation constant	2.5 2.8 in 50% aqueous ethanol 1.5 - 2.8					0.52±0.10; (calculated)	0.52±0.10 (calculated)	0.52±0.10; (calculated)	0.52±0.10; (calculated)
Partition coefficients log Kd (sediment and overlapping dissolved phase)	0.04 (Ahrens et al., 2010)*			0.6 (Ahrens et al., 2010) *	1.8 (Ahrens et al., 2010) *	3.0 (Ahrens et al., 2010) *			
Log Koc (sediment organic	2.06 (Higgins and Luthy, 2006)#			2.39 (Higgins and Luthy, 2006) #	2.76 (Higgins and Luthy, 2006) #	3.3 (Higgins and Luthy, 2006) # 4.8 (Ahrens et			

Abbreviation	**C_8-PFCA**			**C_9-PFCA**	**C_{10}-PFCA**	**C_{11}-PFCA**	**C_{12}-PFCA**	**C_{13}-PFCA**	**C_{14}-PFCA**
Acronym	PFOA	APFO	NaPFO	PFNA	PFDA	PFUnDA	PFDoDA	PFTrDA	PFTeDA
carbon-normalized distribution coefficient)	1.09 (Ahrens et al., 2010) *			2.4 (Ahrens et al., 2010) *	3.6 (Ahrens et al., 2010) *	al., 2010) *			
Water solubility	9.5 g/L (25° C) 4.14 g/L (22°C)	0.033 mol/L, 14.2 g/L at 2.5 °C (Nielsen 2012)	0.036 mol/L at 8.0 °C at critical micelle concentration (Nielsen 2012)			1.2E-4 g/L; pH 1 at 25°C 9.0E-4 g/L; pH 2 at 25°C 8.5E-3 g/L; pH 3 at 25°C 0.056 g/L; pH 4 at 25°C 0.14 g/L; pH 5 at 25°C 0.16 g/L; pH 6-10 at 25°C (calculated)	2.9E-5 g/L pH 1 at 25°C 2.2E-4 g/L pH 2 at 25°C 2.0E-3 g/L pH 3 at 25°C 0.014 g/L pH 4 at 25°C 0.034 g/L pH 5 at 25°C 0.039 g/L pH 6 at 25°C 0.040 g/L pH 7 at 25°C 0.041 g/L pH 8-10 at 25°C (calculated)	7.3E-6 g/L; pH 1 at 25 °C 5.5E-5 g/L; pH 2 at 25 °C 5.1E-4 g/L; pH 3 at 25 °C 3.5E-3 g/L; pH 4 at 25 °C 8.6E-3 g/L; pH 5 at 25 °C 0.0100 g/L; pH 6-10 at 25 °C (calculated)	1.9E-6 g/L; pH 1 at 25°C 1.4E-5 g/L; pH 2 at 25°C 1.3E-4 g/L; pH 3 at 25°C 9.3E-4 g/L; pH 4 at 25°C 2.2E-3 g/L; pH 5 at 25°C 2.6E-3 g/L; pH 6-10 at 25°C (calculated)
Vapour pressure	4.2 Pa (25 °C) for PFOA extrapolated from measured data 2.3Pa (20 °C) for PFOA extrapolated from measured data 128 Pa (59.3 °C) for PFOA measured	0.0081 Pa at 20 °C, calculated from measured data <0.1 hPa at 20 °C 0.012 Pa at 25 °C 0.0028 Pa at 25 °C (Nielsen 2012)				0.6 to 99.97 kPa (112 to 237.7°C) (calculated)	9.40E-3 Torr at 25°C(calculated)	3.59E-3 Torr at 25°C (calculated)	1.37E-3 Torr at 25 °C (calculated)
	Stability								
Phototransformation in water DT50	No photodegradation detected under relevant env. conditions	No photodegradation detected under relevant env. conditions		No photodegradation tested under relevant env. conditions 100 % after 12 h by use of persulfate ion ($S_2O_8^{2-}$) in	No photodegradation tested under relevant env. Conditions 100 % after 12 h by use of persulfate ion	No photodegradation tested under relevant env. Conditions 77% after 12 h by use of persulfate ion ($S_2O_8^{2-}$) in			

Abbreviation	**C_8-PFCA**			**C_9-PFCA**	**C_{10}-PFCA**	**C_{11}-PFCA**	**C_{12}-PFCA**	**C_{13}-PFCA**	**C_{14}-PFCA**
Acronym	PFOA	APFO	NaPFO	PFNA	PFDA	PFUnDA	PFDoDA	PFTrDA	PFTeDA
				water	(S2O82-) in water	water			
Hydrolysis DT50	>97 yr								
Direct photolysis		No photo-degradation							
indirect photolysis		No photo-degradation (H2O2; synthethic humic water, Fe2O3) estimated half-life > 349 days (Fe2O3)							
ready biodegradability screening test	not readily biodegradable (OECD 301 C,F)	not readily biodegradable (OECD 301 B)		not readily biodegradable (OECD 301 F)			not readily biodegradable (OECD 301 C)		not readily biodegradable (OECD 301 C)
Simulation tests	No elimination by metabolic processes, mineralization or adsorption								
Biodegradation in soil, sediment	No degradation detected								

* pH of the water samples analyzed 7.1-8.3 Temp.: 15.3 – 17.7 °C

Table 145: Information on BCF, BMF and TMF of C_{9-14} PFCAs relevant to justify read across in the B assessment.

Abbreviation	**C_9-PFCA**	**C_{10}-PFCA**	**C_{11}-PFCA**	**C_{12}-PFCA**	**C_{13}-PFCA**	**C_{14}-PFCA**
Acronym	PFNA	PFDA	PFUnDA	PFDoDA	PFTrDA	PFTeDA
IUPAC Name	Nonanoic acid, heptadecafluoro-	Decanoic acid, nonadecafluoro-	Undecanoic acid, heneicosafluoro-	Dodecanoic acid, tricosafluoro-	Tridecanoic acid, pentacosafluoro-	Tetradecanoic acid, heptacosafluoro-
Chemical Structure	CF3(CF2)7-COOH	CF3(CF2)8-COOH	CF3(CF2)9-COOH	CF3(CF2)10-COOH	CF3(CF2)11-COOH	CF3(CF2)12-COOH
CAS No	375-95-1	335-76-2	2058-94-8	307-55-1	72629-94-8	376-06-7
Physico-chemical data						
Molecular Weight g/mol	464.08	514.08	564.0909	614.0984	664.1059	714.11
Partitioning Coefficient log K_{OW}	2.3 – 2.48 (exp)	2.65 – 2.87 (exp)		logP 9.363±0.888 at 25°C (calc)	logP 10.093±0.901 at 25 °C (calc)	logP 10.823±0.914 at 25 °C (calc)
	5.9 (calc., COSMOtherm, Wang et al., 2011)	6.5 (calc., COSMOtherm, Wang et al., 2011)	7.2 (calc., COSMOtherm, Wang et al., 2011)	7.8 (calc., COSMOtherm, Wang et al., 2011)	8.25 (calc., COSMOtherm, Wang et al., 2011)	8.90 (calc., COSMOtherm, Wang et al., 2011)
log K_{OA}	7.50 (calc., COSMOtherm, Wang et al., 2011)	7.77 (calc., COSMOtherm, Wang et al., 2011)	8.08 (calc., COSMOtherm, Wang et al., 2011)	8.36 (calc., COSMOtherm, Wang et al., 2011)	8.63 (calc., COSMOtherm, Wang et al., 2011)	8.87 (calc., COSMOtherm, Wang et al., 2011)
log K_{AW}	-1.58 (calc., COSMOtherm, Wang et al., 2011)	-1.27 (calc., COSMOtherm, Wang et al., 2011)	-0.92 (calc., COSMOtherm, Wang et al., 2011)	-0.58 (calc., COSMOtherm, Wang et al., 2011)	-0.38 (calc., COSMOtherm, Wang et al., 2011)	0.03 (calc., COSMOtherm, Wang et al., 2011)
BCF						
Lumbriculus variegatus / sediment	0.64 ± 0.05	0.06 ± 0.04				
Rainbow trout (carcass)			2700 ± 400	18000 ± 2700		23000 ± 5300
Rainbow trout (blood)		2700±350	11000 ± 1400	40000 ± 4500		30000 ± 4200
Rainbow trout (liver)		1100 ± 180	4900 ± 770	18000 ± 2900		30000 ± 6000
Carp (whole)			2300 - 3700	10000-16000		16000 - 17000
Juvenile rainbow trout (carcass) calculated*			4044-6326	5761-8210		10388-19294
Juvenile rainbow trout (liver) calculated*			5245-6071	7926-8576		17835-19294
BAF						
Chup(*Leuciscus cephalus*) plasma			1000000	5011872		
Chup(*Leuciscus cephalus*)			100000	501187		

liver						
Chup(*Leuciscus cephalus*) gills			79433	501187		
Chup(*Leuciscus cephalus*) gonads			63096	316228		
Chup(*Leuciscus cephalus*) muscle			19953	100000		
BMF	0.13-111	0.21-87	0.21 - 353	0.1 – 156	0.35 – 9	0.33 – 8.5
TMF	1.9-7.0	1.5-20	0.75 – 31.2	0.6 – 3.76	1.4 – 2.45	0.23 – 2.6

* Calculated BCFs based on BMF values for C_{11}-PFCA (0.28 ± 0.04), C_{12}-PFCA (0.43 ± 0.062) and C_{14}-PFCA (1.0 ± 0.25).

pH of sediment analysed: 5.7 to 7.6

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