



REPORT

# **PFBS in the Environment:** **Monitoring and Physical-Chemical Data Related to the** **Environmental Distribution of Perfluorobutanesulfonic Acid**

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## Executive Summary

The Norwegian Environment Agency is currently considering whether the substance perfluorobutanesulfonic acid (PFBS) and its salts fulfil the criteria of a substance of very high concern, on the basis of Article 57 in the REACH legislation. The Norwegian Geotechnical Institute was asked to conduct a literature review on relevant physicochemical properties and environmental monitoring data to assist in this evaluation.

### *Physicochemical Properties*

Physicochemical Properties of the potassium salt of PFBS (PFBS-K) and the neutral PFBS (PFBS) have been collected, both of which are currently registered in REACH (EC numbers 249-616-3 and 206-793-1, respectively). Many of the pure phase properties are extremely different between the salt and the neutral form, due to the influence of the crystal lattice energy of the salt. For environmental and biological distribution processes, however, the physicochemical properties of the neutral form are the most relevant, as well as their dependence on pH.

### *Degradation*

PFBS is a perfluoroalkylsulfonate, which are amongst the most stable and persistent organic molecules possible. No studies have observed degradation of PFBS (or other perfluoroalkylsulfonates) under environmental conditions, including atmospheric photolysis. Reductive defluorination in anaerobic environments has been proposed as a pathway for environmental degradation; however, conclusive proof of this occurring in the environment has yet to be documented.

### *Environmental Distribution*

*Adsorption/Desorption* – several studies have measured soil-water or sediment-water partitioning constants. The average log organic carbon-water partition coefficient, log  $K_{oc}$ , from these studies is 2.2. Based on this value, it can be derived for a soil containing ca. 1% organic carbon that the concentration in soil (ng/kg) would be similar to that in water (ng/L), implying substantial mobility in the case of flowing water.

*Volatilisation* - PFBS is an anionic acid with a pH dependant air-water partition coefficient, log  $K_{aw}$ , that is too low to measure and is predicted to be as low as -14.5 at pH 8. This indicates that volatilization from water is negligible, and that air-phase presence is due to direct PFBS emissions into the air of the substance itself or contaminated water droplets/particles.

*Distribution Modelling* - PFBS is expected to be mainly distributed in water, globally. This is confirmed by the monitoring data.

### *Monitoring Data*

The compilation of monitoring data included 84 studies that were selected randomly. It is not considered exhaustive, therefore all results are to be taken within the context of these 84 studies and not the entire literature.

*Humans* – PFBS has been reported in blood samples throughout the world; there is also indication this concentration has been increasing (Glynn et al., 2012).

*Atmosphere* – PFBS is primarily detected in rain samples, max 1.54 ng/L (Kwok et al., 2010), rather than air samples, which is anticipated based on the low log *K<sub>ow</sub>*.

*Biota* – PFBS has been detected in Arctic biota, indicating long range transport. However, levels found in Arctic biota are much smaller than longer chain perfluoroalkylsulfonic acids like perfluorohexanesulfonic acid (PFHxS) and perfluorooctanesulfonic acid (PFOS). It has also been detected in diverse marine, freshwater and terrestrial species. PFBS shows a tendency for enrichment in plants, likely due to uptake through the xylem.

*Marine water* – PFBS is ubiquitous in oceanic water, from the Arctic, maximum 0.11 ng/L (Kallenborn et al., 2004), to coastal waters, maximum 1.48 ng/L (Kwok et al., 2015).

*Fresh water* – PFBS is ubiquitous in fresh water systems, including Arctic snow and ice (max 2.15 ng/L). Areas away from suspected source zones (e.g. fluorochemical production facilities) could be contaminated up to 1450 ng/L (Skutlarek et al., 2006).

*Drinking water* -- In regions away from established PFAS source areas, substantial drinking water contamination can occur, with a France maximum of 15 ng/L (Schwanz et al., 2016), a German maximum of 26 ng/L (Wilhelm et al., 2010), an Italy maximum of 45 ng/L (IRSA-CNR, 2013), a Spain maximum of 69 ng/L (Ericson et al., 2009), a China maximum of 18 ng/L (Mak et al., 2009), and a Brazil maximum of 16 ng/L (Schwanz et al., 2016). These concentrations even exceed those of some known source zones, such as 19.0 ng/L measured in drinking water near a PFAS production facility in the Netherlands (Gebbink et al., 2017).

*Soils and Sediments* – Very little monitoring data could be found for soils and sediments; however, based on the proposed log *K<sub>oc</sub>*, the concentrations in typical soils and sediments (in ng/kg) would be similar to that found water (in ng/L).

*Waste water and Leachate* – Waste water and leachate are important emission sources to PFAS in the environment. The maximum waste water concentration of 26 ng/L (Ahrens et al., 2009b) was less than the maximum landfill leachate concentration 3410 ng/L (Lang et al. 2017).

### ***Temporal trends/Comparisons with other PFAS***

There are multiple indicators that PFBS concentrations in aquatic media are continuing to increase, to an extent they are beginning to surpass most other PFAS substances. This has been observed in several recent waste water emissions and various fresh water studies, in which PFBS is either the dominant PFAS or amongst the top three. Several biota studies are also noticing an increase in PFBS over time; however, concentrations

in biota remain much smaller than other PFAS, due in part to the low bioaccumulation potential.

***Data indicating long-range transport.***

The physicochemical properties for PFBS, in particular its extreme environmental persistence, along with its low log K<sub>oc</sub> and low log K<sub>ow</sub>, collectively indicate that PFBS should enrich in the arctic overtime if emissions continue. The monitoring data collectively supports this expectation. The major transport pathway for PFBS in the environment is expected to through water, based on physicochemical properties. The ubiquity of PFBS in marine and freshwater isolated from known sources is support for this expectation. PFBS also appears ubiquitously in drinking water and bottled water, showing that it too can survive transport through filters and advanced treatment processes.

***Bioaccumulation.***

PFBS has been quantified in several biological matrices; however, generally at smaller concentrations than PFHxS and PFOS. To some extent this is explained by quicker excretion rates for PFBS. However if animals and humans are continuously exposed to increasing environmental concentrations of PFBS, the excretion pathway is less relevant, as biota would reach equilibrium with elevated exposure concentrations.

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## Appendix

Latin names of biota mentioned in this study.

## Review and reference page

## 1 Introduction

This report presents an overview of the physicochemical properties, monitoring data and environmental distribution of the substance perfluorobutanesulfonic acid (PFBS), IUPAC name (1,1,2,2,3,3,4,4,4-Nonafluorobutane-1-sulfonic acid).

Having 4 carbons in its molecular structure, this substance is referred to as a short chain perfluoroalkylsulfonate (PFAS). It was introduced to the market on a larger scale after the phase out of perfluorooctanesulfonic acid (PFOS), which had 8 carbons in its molecular structure. PFOS has been restricted due to it being persistent, bioaccumulative and toxic in the environment (PFOS, 2004). Due to the increasing use of PFBS, and increasing number of reports of PFBS in the environment, the Norwegian Environment Agency is currently considering whether PFBS and its salts fulfil the criteria of a substance of very high concern, on the basis of Article 57 in REACH. The data in this report was generated to provide background information to this evaluation.

## 2 Physicochemical properties

PFBS being a short chain perfluoroalkylsulfonate (PFAS) having 4 carbons, has many general physicochemical properties that are similar to its longer chain-counterparts, such as the 6 carbon perfluorohexanesulfonic acid (PFHxS) PFHxS, 8 carbon perfluorooctanesulfonic acid (PFOS) and other longer chain counterparts. In water PFBS is a strong acid, and predominantly dissociated as an anion. PFBS has excellent surfactant properties, having a hydrophilic anionic sulfonate head group, and hydrophobic perfluorinated end group.

In the pure phase, PFBS can be present as neutral liquid (molecular formula  $C_4F_9SO_3H$ ) or as a crystalline salt (molecular formula  $C_4F_9SO_3^-X^+$ ). Under REACH both the neutral and potassium (K-salt) form have been registered (EC numbers 206-793-1 and 249-616-3, respectively). As is always the case, the pure phase properties like melting point, boiling point, density, physical state at STP, vapour pressure and water solubility are intrinsically dependant on whether they are determined for the neutral species or the salt. The properties of solid salts are dominated by the strength of the crystal lattice structure that the anions and cations arrange themselves in; therefore, for the PFBS anion, different counter-ions will result in different solid state properties (e.g.  $Na^+PFBS^-$  has different pure phase properties than  $K^+PFBS^-$ ). However, as neutral liquids do not have a crystal structure, their pure phase properties of PFBS-acid in the pure form are radically different than PFBS-salts.

For environmental partitioning properties, such as the octanol-water partition coefficient ( $K_{ow}$ ), air-water partition coefficient ( $K_{aw}$ ), octanol-air partition coefficient ( $K_{oa}$ ), and organic carbon-water coefficient ( $K_{oc}$ ), these by definition apply to the PFBS-acid/-anion only, and are independent of cation.

An important consideration however is that all properties involving water, such as water solubility,  $K_{ow}$ , and  $K_{aw}$ , are dependent on pH. PFBS is an acid, and in water dissociates from the neutral form  $C_4F_9SO_3H$  to the anionic  $C_4F_9SO_3^-$  form. Over ambient pH ranges of acids and bases, there is a convention to use the symbol "D" instead of "K" for partitioning processes, to indicate the pH dependant "*D*"istribution of both the neutral and ionic species combined are being considered in the D value. In other words, the symbols  $D_{ow}$  and  $D_{aw}$  can be thought of as the pH-dependant  $K_{ow}$  and  $K_{aw}$  values, respectively. In this nomenclature,  $K_{ow}$  and  $K_{aw}$  are reserved for the neutral form only, and  $D_{ow}$ ,  $D_{aw}$  and  $D_{oc}$  are used for all relative fractions of the neutral and ionic forms. The pH dependence is governed by the acid-dissociation constant,  $pK_a$ . For monoprotic acids like PFBS, this pH dependence can be quantified using the following equations:

$$D_{ow} = K_{ow} / (1 + 10^{(pH - pK_a)}) \quad (1)$$

$$D_{aw} = K_{aw} / (1 + 10^{(pH - pK_a)}) \quad (2)$$

An overview of the properties of the PFBS-K salt and PFBS is presented in Table 1. A discussion of specific properties is presented further below.

Table 1: Overview of physiochemical properties of PFBS and the PFBS-K salt

Property	Salt/Neutral Form	Description of key information	Reference/source of information
Physical state at 20°C and 101.3 kPa	PFBS-K salt	White powder	Experimental, REACH registration dossier, September 2018 (EC: 249-616-3)
	PFBS	liquid	Ullmann's Encyclopedia of Industrial Chemistry. 7th ed. (1999-2015). New York, NY: John Wiley & Sons
Melting/freezing point	PFBS-K salt	> 280 °C	Experimental, REACH registration dossier, September 2018 (EC: 249-616-3)
	PFBS	-21 °C	Experimental, REACH registration dossier, September 2018 (EC: 206-793-1)
Boiling point	PFBS-K salt	Decomposes before boiling	Experimental, REACH registration dossier, September 2018 (EC: 249-616-3)

Property	Salt/Neutral Form	Description of key information	Reference/source of information
	PFBS	198 °C	Experimental, REACH registration dossier, September 2018 (EC: 206-793-1); Kirk-Othmer Encyclopedia of Chemical Technology, 3rd edition (1978-1984) M Grayson (ed). Vol 10, p.952 (R A Geunther contributor). New York, John Wiley and Sons.
Vapour pressure	PFBS-K salt	< 1.22E-05 Pa at 20°C ± 1°C	Experimental, REACH registration dossier, September 2018 (EC: 249-616-3)
	PFBS	7 Pa at 20°C	Experimental, REACH registration dossier, September 2018 (EC: 206-793-1)
		2.8 Pa	(Wang et al., 2011) Estimated using COSMOtherm
Density	PFBS-K salt	2.248 g/cm <sup>3</sup> at 20 °C	Experimental, REACH registration dossier, September 2018 (EC: 249-616-3)
	PFBS	1.824 g/cm <sup>3</sup> at 20°C	Experimental, REACH registration dossier, September 2018 (EC: 206-793-1)
Water solubility	PFBS-K salt	54.6 g/mL at 22.5-24 °C	REACH registration dossier, September 2018 (EC: 249-616-3; 3M Environmental Laboratory (2001) Characterisation Study PFBS: a.) Primary Standard – Test Control Reference #TCR-99030-023 (lot 101), b.) Test Control Reference #TCR-00017-071 (Lot 102) Phase: Solubility Determination. 3M Environmental Laboratory Study #FACT-TCR009 (LIMS #E00-1877), 28 March 2001. 3M Environmental Laboratory Minnesota (unpublished report submitted by the 3M Corporation)

Property	Salt/Neutral Form	Description of key information	Reference/source of information
	PFBS	Fully miscible at 20°C	Experimental, REACH registration dossier, September 2018 (EC: 206-793-1). This conclusion is also expected over the entire ambient pH range based on an estimated water solubility of the neutral species (30 g/L) and the estimated pKa of -3.94
Partitioning coefficient soil/water (log Koc)	PFBS-K salt	< 2	REACH registration dossier, September 2018 (EC: 249-616-3)
	PFBS	2.2	Average of three experimental values, from (Kwadijk et al. 2010; Guelfo & Higgins, 2013; Vierke et al., 2014)
Dissociation constant pKa	PFBS	-3.94	(Wang et al., 2011) Estimated using COSMOtherm, which is one of the best models for PFAS (Goss, 2008). Estimations using the SPARC method gave a value of 0.14.
Partition coefficient n-octanol/water (log Kow / pH dependent Dow value)	PFBS-K salt	-1.8 at 23 °C	Experimental, REACH registration dossier, September 2018 (EC: 249-616-3)
	PFBS	3.9 (neutral form) -4.0 to 0.0 (pH 4) -7.0 to -3.0 (pH 7) -8.0 to -4.0 (pH 8)	Estimated using COSMOtherm (Wang et al. 2011) along with the estimated pKas -3.94 and 0.14, respectively, and the equation Dow = $(1/(1+10^{(pH - pKa)}))Kow$ (for monoprotic acids)  One experimental value is -0.34 in a 0.01 mol/L concentration (pH 1.7) at 23°C, from Experimental, REACH registration dossier, September 2018 (EC: 206-793-1)

Property	Salt/Neutral Form	Description of key information	Reference/source of information
Partition coefficient air/water (log Kaw/ pH dependant Daw value )	PFBS	-2.59 (pH << 0)	(Wang et al., 2011) estimated for neutral (nonionized species) using COSMOtherm
		-2.6 (neutral form) -10.5 to -6.5 (pH 4) -13.5 to -9.5 (pH 7) -14.5 to -10.5 (pH 8)	Estimated using log Kaw of -2.6 for the neutral species and pKa -3.94 and 0.14, respectively, and the equation $Daw = (1/(1+10^{(pH - pKa)}))Kaw$ (for monoprotic acids)
Partitioning coefficient n-octanol/air (log Koa)	PFBS	6.49	(Wang et al., 2011) estimated using COSMOtherm

### 3 Degradation

PFBS, like other perfluoroalkylsulfonates, are amongst the most stable and persistent organic molecules possible (Stock et al. 2010). The main reason for this is the thermodynamic stability of the C-F bonds (with bond dissociation energies of 484 kJ/mole or larger) and the F<sub>2</sub>CF-SO<sub>3</sub> bonds, which are amongst the strongest bonds that carbon can make. Under aerobic, environmental conditions, replacing them is thermodynamically unfavourable, requiring energies that are typically not available without additional energy or some form of catalysis (Vecitis et.al, 2009). Similarly, the S in the sulphonate end group is at its maximum oxidation state, and cannot be oxidized further.

Quinette et al. (2010) tested for the degradation of PFBS using advanced oxidation processes through ultraviolet radiation, hydrogen peroxide, or both, followed by conventional tests, such as the manometric respirometry test (OECD 301 F; OxiTop), closed-bottle test (OECD 301 D), and standardized fixed-bed bioreactor; the study concluded that "PFBS is not biodegradable", with no significant degradation being observed under test conditions. The most theoretically plausible degradation pathway for PFBS is through reductive defluorination, which occurs under anaerobic conditions (Parsons et al. 2008). Mechanistic pathways for reductive defluorination have been established (Park et al. 2009). Parsons et al. (2008) conducted a review of biodegradation studies of PFOS, and concluded that no biodegradation has been observed in aerobic conditions, though there has been some observations of degradation of PFOS under anaerobic conditions (though no metabolites was measured in these studies). It cannot be ruled out that some degradation of PFBS under anaerobic conditions can occur (e.g. in hypoxic groundwater, marine water or sediments); however, the rates of these under environmental conditions are unknown, and potentially very slow or negligible, and have yet to be observed in the environment.

Photolysis of perfluoroalkylsulfonates in the atmosphere is generally considered negligible under environmental conditions (Vecitis et al, 2009). An outlying study is one by Taniyasu et al. (2013) which reported observing photolysis in air at high altitudes (>2500m) of PFOS, which reacted via dealkylation to form PFBS via dealkylation. However, they also concluded that PFBS was more recalcitrant and stable. It should be noted that these PFOS results have been disputed by Wang et al. (2015), who argue that PFOS is too stable to undergo atmospheric photolysis. Nevertheless, PFBS in particular is considered to remain stable to photolysis under environmental conditions, and this has been supported by all studies thus far.

In conclusion, to date no studies have observed degradation of PFBS (or other perfluoroalkylsulfonates) under environmental conditions.

## 4 Environmental Distribution

### 4.1 Adsorption/Desorption

For organic ions, like PFBS, conceptualizing sorption/desorption to soil is more complex than neutral organic molecules. For neutral organic molecules, one has to consider mainly van der Waal type interactions (non-ionic sorption interactions). For ionic substances, one has to additionally consider ionic interactions between the substance and soil. Soils exhibit wide variation in their anion exchange capacity (AEC), and hence their ability to retain anionic-charged molecules like PFBS.

Though adsorption/desorption to soils is commonly normalized to the organic carbon fraction, i.e. Koc value, a common discussion point regarding the adsorption/sorption of ions is the role of clays and minerals (Droge et al 2013). Clays and minerals can have widely differing available surface areas for sorption and AEC values. It is therefore challenging to include a generic parameter to account for clay sorption.

Three studies that determined log Koc values for naturally occurring soils and sediments are Guelfo & Higgins (2013), Kwadijk et al. (2010) and Vierke et al. (2014). Guelfo & Higgins (2013) studied the sorption of different Aqueous Film Forming Foam to different types of soil, and reported a narrow band of log Koc values ( $1.79 \pm 0.10$ ), though a wide range of log Kd values (-0.55 to 0.21). Kwadijk et al. (2010) examined the sorption of PFAS contaminated areas in the Netherlands and derived a log Koc of 2.2, and a distribution of log Kd from  $1.42 \pm 0.50$ . Vierke et al. (2014) reported a log Koc of 2.7 from column tests. Here the average log Koc from these studies of 2.2 is considered.

One can infer from a log Koc of 2.2 (or a Koc of 158 l/kg) that PFBS is quite mobile in the aquatic environment. For instance, if we consider the definition of Koc

$$K_{OC} = c_{soil} / (c_{water} * f_{OC}) \quad (3)$$

Where  $c_{soil}$  (ng/kg) is the soil concentration,  $c_{water}$  (ng/L) is the water concentration and  $f_{OC}$  the fraction of organic carbon. At 1%  $f_{OC}$ :

$$c_{sediment} \text{ (ng/kg)} = K_{OC} * c_{water} * 0.01 \text{ organic carbon} = 1.58 c_{water} \text{ (ng/L)}$$

Therefore, the concentration of PFBS in water per L is expected to be roughly similar to soil or sediment per kg. As a result, when water flows through soil, the PFBS can be readily transported compared to substances with a higher log  $K_{OC}$  value.

## 4.2 Volatilisation

PFBS-K salts do not volatilize, but neutral PFBS does volatilize to ca 2.8-7 Pa. This implies that traces of PFBS fumes would be present in a room containing neutral PFBS and poor ventilation. For air-water partitioning, the pH dependant air-water partition coefficient,  $\log D_{aw}$ , is too low to measure and is predicted to be as low as -14.5 at pH 8 (Table 1). This indicates that volatilization from water is negligible; at pH 8, essentially all PFBS is ionic, and it would be exclusively in water.

Because of negligible volatilization of PFBS, its presence in the air would be primarily due to direct emissions of the substance or its salts into the air. Another possibility is through emissions of contaminated particles or water droplets (e.g. contaminated marine aerosols). When PFBS is in the atmosphere, it is expected to readily partition with surface water and water droplets (rain, cloud droplets, fog droplets, etc.) based on this extremely low  $\log K_{aw}/D_{aw}$  value, and therefore undergo efficient removal from the atmosphere via wet-deposition.

## 4.3 Distribution modelling

Distribution modelling of anionic substances like PFBS and other PFAS is not straightforward. Most distribution models were developed for neutral substances, wherein distribution modelling is generally described using three main partitioning coefficients:  $K_{ow}$ ,  $K_{oa}$  and  $K_{aw}$ . However, "octanol" as a surrogate phase for soil/sediment/aerosol organic matter, or biological membranes, is inappropriate for anionic substances like PFBS, because octanol cannot make ionic interactions. One approach that has been used with PFOS is to use the experimental  $K_{OC}$  value in distribution modelling, rather than the  $K_{ow}$  (Armitage et al. 2009), as the experimental  $K_{OC}$  inherently includes some ionic interactions to a naturally occurring phase. In this case, basic distribution modelling can be done using the pH dependant  $K_{aw}$ ,  $K_{OC}$  and the organic carbon-air partitioning coefficient  $K_{OC,a}$ . For perfluoroalkylsulphonates, values for these terms are presented in Table 2.

*Table 2. Physiochemical properties needed to estimate environmental distribution*

Parameter	PFBS	PFHxS	PFOS	PFDS	References
log Kaw (neutral)	-2.6	-2.4	-1.7	-1.2	(Wang et al. 2011)
log Daw (pH 8)	-14.5	-13.8	-13.1	-12.0	Derived (Wang et al. 2011)
log Koc	2.2	2.6	3.0	3.4	PFBS (Kwadijk et al. 2012), PFOS (Zareitalablad , 2010), PFHxS and PFDS extrapolated (read-across)
log Koc,a	4.8	5.0	4.7	4.6	Calculated from the thermodynamic triangle: log Koc,a = log Koc - log Kaw

As evident from Table 2, the range in log Daw, log Kow and log Koc,a values are quite similar between these PFAS. The spread in log Koc,a is only from 4.7 (PFOS) to 5.0 (PFHexS). For log Daw, the values for all species are so negative, that this means volatilization is similarly negligible. The log Koc values spread from 2.2 (PFBS) to 3.4 (PFDS), which would imply PFDS, PFOS and PFHxS sorb than PFBS by factors of 16, 6 and 2.5 respectively. Thus, the difference between PFHxS and PFBS sorption to negligible is relatively minor compared to, e.g. heterogeneity of sorption phases in soil.

The Globo-POP model (Wania et al. 2007) has been established to model the global distribution neutral substances. In Figure 1 below, output from the Globo-POP model is used to illustrate the partitioning properties of substances that, globally, are predominantly in the air, water or soil phases, based on the following assumptions: the substance is non-degradable (which is appropriate for PFBS), 10 years of continuous emissions has occurred, emissions occur equally to soil, water, air (1/3<sup>rd</sup> each), and the global distribution of emissions is zonally distributed similarly to the human population. On this Figure, lines are overlaid that represented the physical chemical properties of PFBS, PFHxS, PFOS and PFDS (Table 2), though using Koc,a instead of Koa, and the pH dependence of the Daw.

As is indicated by this Figure, PFBS is tightly clustered along with PFHxS, PFOS and PFDS, to indicate they are primarily in the water phase.

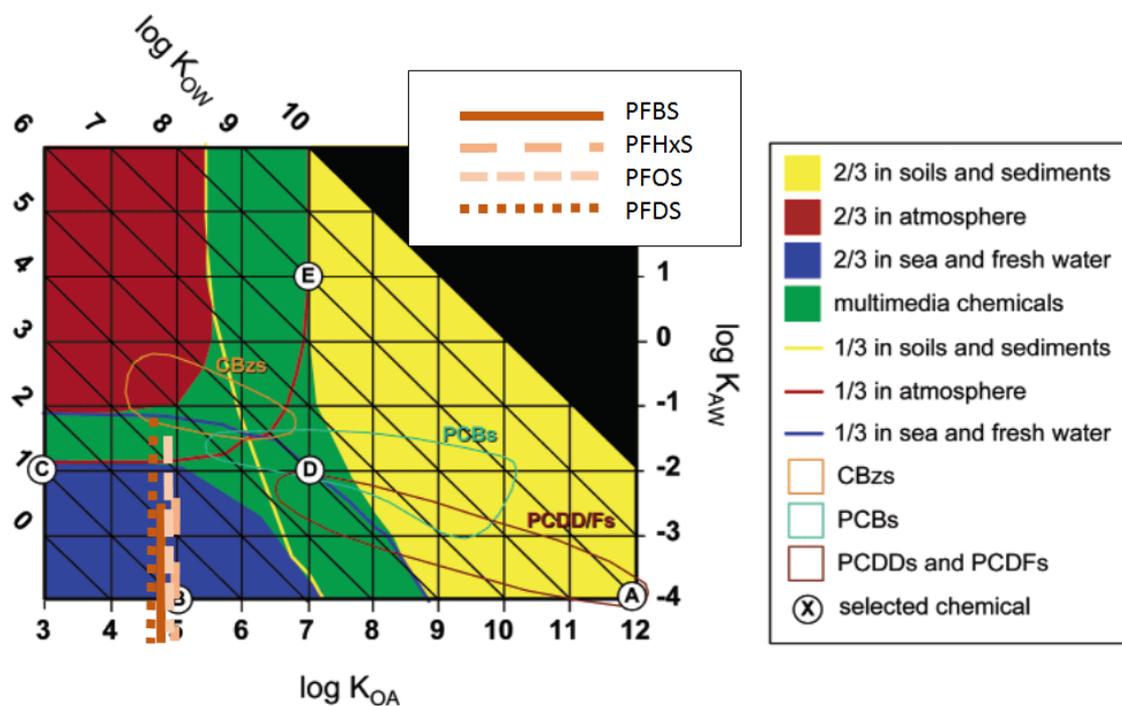


Figure 1. Global POP chemical space distribution for non-degradable substances being emitted into air-water-soil at equal levels for the 10 years, with a similar zonal distribution the human population. The location of PFBS, PFHxS, PFOS and PFDS is overlaid, using  $\log K_{oc}$  instead of  $\log K_{oa}$  and considering the pH dependence of  $\log K_{aw}$ . Note that at ambient pH, the  $\log K_{aw}$  is even lower than presented in this chart, and the substances would be strongly within the sea and freshwater media area of the chart. Other substances presented in this figure for comparison are CBzs (Chlorobenzenes), PCBs (polychlorinated biphenyls) and PCDDs and PCDFs (Dioxins). This Figure is modified and reprinted with permission from Wania (2003). Copyright 2003 American Chemical Society.

## 4.4 Monitoring Data

There are numerous studies reporting PFBS data in the environment; herein a compilation of some of this data from a dataset of 84 diverse peer-reviewed scientific research papers, thesis and reports is presented. No target environmental media was used in this search. Future work could expand this compilation, particularly as more data becomes available.

PFBS concentration data were sorted into the following media: air, rain, surface water, marine water, drinking water, ground water, soil, sediment, waste water treatment plants, landfills, marine biota, freshwater biota, terrestrial biota (non plants), terrestrial plants and humans. Further, marine biota and fresh water data for Arctic/Antarctic regions is presented separately, as several studies in this compilation were focused on such analysis. Further, some other studies were focussed near known PFBS sources (e.g. PFAS production facilities, airports, textile industries). Concentrations in these area should not be considered representative of typical environmental concentrations. Therefore, such data are marked, and in the case of fresh water, presented separately.

Blood samples have been analysed in Europa and China. PFBS was not detected in a 2009 German blood study (Yeung et al., 2013), though it was in an Italian study (max 0.36 and 4.26 ng/g for non-exposed and exposed populations in the Veneto region (Ingelidoo et al., 2018)), and with high frequency pregnant and primiparous mothers in Uppsala, Sweden (means from 0.03-0.08 ng/L, max 0.80 ng/L) (Gyllenhammar et al., (2015) and Glynn et al., (2012)). Shanghai cord blood samples from Shanghai contained a max of 0.46 ng/L (Wang et al., 2016). Near the PFAS production facility in Fuxin a max of 1.3 ng/L was reported (Bao et al., 2010). A study in Spain (Pérez et al., 2013) examined PFAS levels in 99 samples of autopsy tissues and found highest levels in the lung (17.8 ng/L) and kidney (8 ng/L).

Table 16. Concentrations of PFBS in human samples (ng/g ww)

Region	Location	Year	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Europe	Germany, Halle and Münster	1982-2009	nd			Blood plasma	(Yeung et al., 2013)
Europe	Italy, Veneto	2018	<LOQ	<LOQ - 4.26 (<LOQ)	257 (31 %)	Blood (exposed areas)	(Ingelidoo et al., 2018)
Europe	Italy, Veneto	2018	<LOQ	<LOQ - 0.36 (<LOQ)	250 (18 %)	Blood (non-exposed areas)	(Ingelidoo et al., 2018)
Europe	Spain, Tarragona	2008	0.9			Liver	(Pérez et al., 2013)
Europe	Spain, Tarragona	2008	3.2			Bone	(Pérez et al., 2013)
Europe	Spain, Tarragona	2008	<LOD			Brain	(Pérez et al., 2013)
Europe	Spain, Tarragona	2008	17.8			Lung	(Pérez et al., 2013)
Europe	Spain, Tarragona	2008	8			Kidney	(Pérez et al., 2013)
Europe	Sweden, Uppsala	1996-1999	0.03 ± 0.00	<MDL - 0.21 (0.02)	132 (77 %)	Blood serum pregnant mothers (1996-1999)	(Gyllenhammar et al., 2015)
Europe	Sweden, Uppsala	2008-2011	0.06 ± 0.01	<MDL - 0.80 (0.03)	134 (86 %)	Blood serum pregnant mothers (2008-2011)	(Gyllenhammar et al., 2015)
Europe	Sweden, Uppsala	1996-2010	0.08 ± 0.02	0.05 - 0.10 (0.09)	6 (100 %)	Blood serum primiparous mothers	(Glynn et al., 2012)
Asia	China, Shanghai	2011-2012	0.053	LOD - 0.46 (0.05)	686 (97 %)	Cord blood	(Wang et al., 2016)
Asia	China, Fuxin	2009	0.19 ± 0.22	0.01 - 1.30 (0.12)	120 (93 %)	Human blood	(Bao et al., 2010)

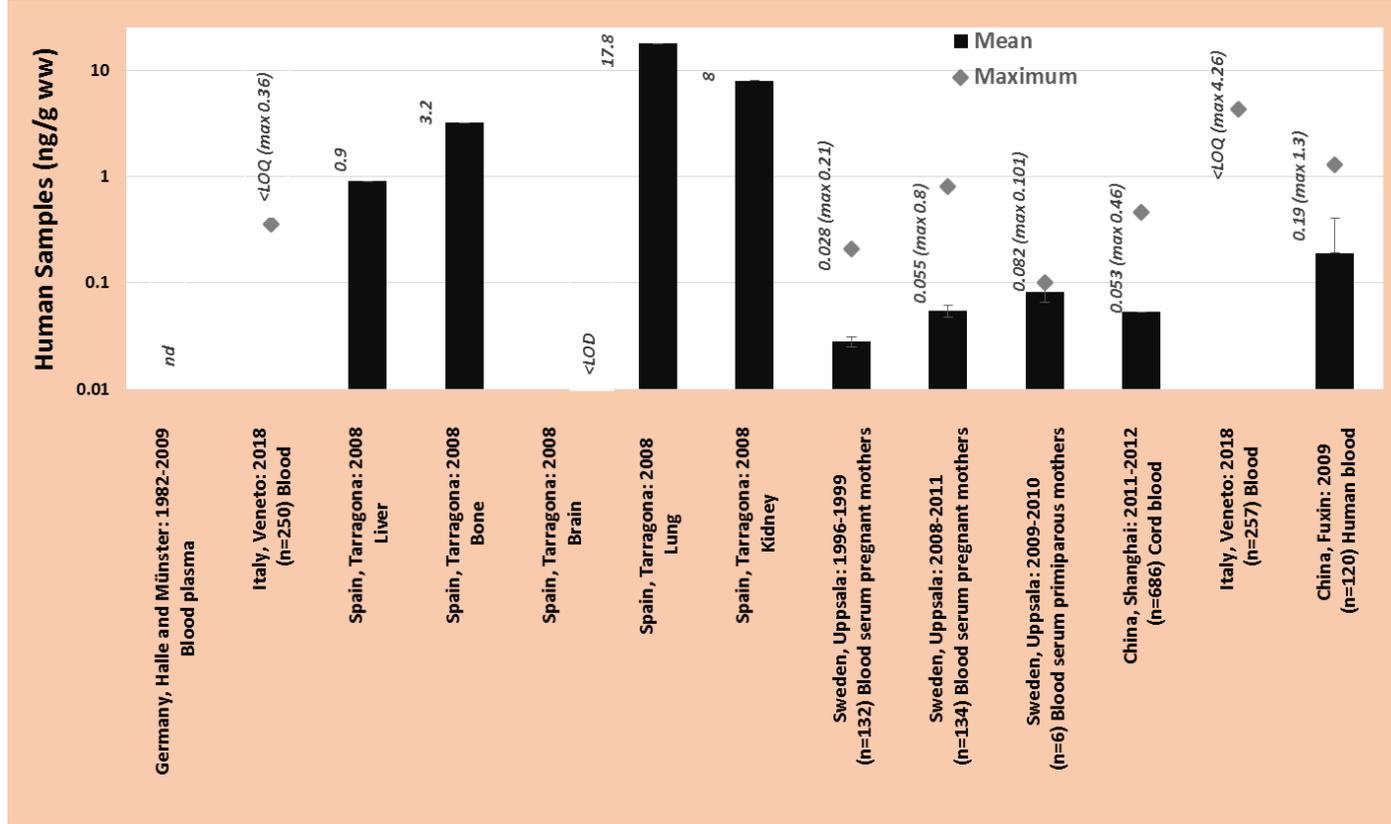


Figure 14. Concentrations of PFBS in human samples (ng/g ww)

PFBS has been reported in atmospheric samples at trace levels throughout the world, though mostly in rain. It has been detected in Arctic air in one study (Alert, Greenland at  $0.1 \pm 0.2 \text{ pg/m}^3$ ). The highest reported concentration in rain was in Hong Kong, at 1.54 ng/L. Due to tendency for PFBS to prefer water to air (based on the  $K_{aw}$  value), air emissions are likely prone to wet deposition, by partitioning with clouds and rain droplets (see section 4.2).

Table 4. Environmental concentrations of PFBS in air ( $\text{pg/m}^3$ ) and rain (ng/L)

Region	Location	Year	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Units	Reference
Arctic	Alert, Greenland (Air)	2006-2015	$0.1 \pm 0.2$	BDL - 1.5 (0.0)	169 (66 %)	$\text{pg/m}^3$	(Wong et al., 2018)
Arctic	Zeppelin, Svalbard (Air)	2006-2015	nd		383	$\text{pg/m}^3$	(Wong et al., 2018)
North America	Canada (Landfill Air)	2009	nd			$\text{pg/m}^3$	(Ahrens et al., 2011)
Europe	Finland (Rain)	2004	nd		2	ng/L	(Kallenborn et al., 2004)
Europe	Sweden (Rain)	2004	nd		4	ng/L	(Kallenborn et al., 2004)
Europe	Toulouse, France (Rain)	2008	<0.05			ng/L	(Kwok et al., 2010)
Asia	Hong Kong (Rain)	2007	1.54	<0.05 - 1.5		ng/L	(Kwok et al., 2010)
Asia	Kawaguchi, Japan (Rain)	2006-2008	0.24	<0.05 - 1.7		ng/L	(Kwok et al., 2010)
Asia	Patna, India (Rain)	2008	<0.05			ng/L	(Kwok et al., 2010)
Asia	Tsukuba, Japan (Rain)	2006-2008	0.16	<0.05 - 2.0		ng/L	(Kwok et al., 2010)
North America	Albany, USA (Rain)	2006-2007	<0.05			ng/L	(Kwok et al., 2010)
North America	Slingerlands, USA (Rain)	2006-2007	0.1	<0.05 - 0.6		ng/L	(Kwok et al., 2010)

BDL = below detection limit

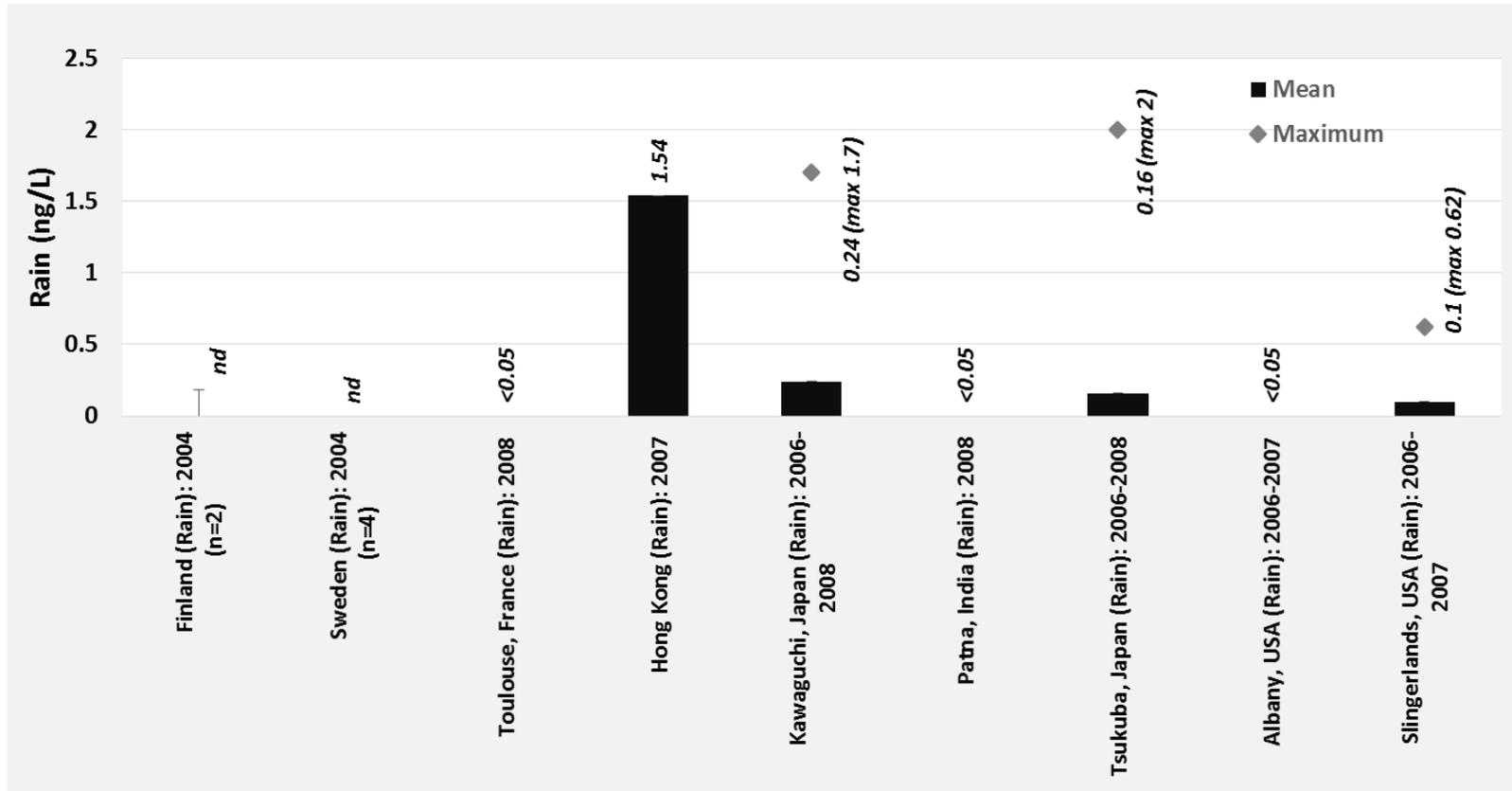


Figure 2. Environmental concentrations of PFBS in rain (ng/L).

#### 4.4.3.1 Arctic – marine

Prior to 2012, the majority of studies on arctic marine biota in this compilation did not report PFBS in Arctic Biota above detection limits. In more recent studies, it is starting to appear more frequently. A study on samples collected between 2012-2013 (Gebbinck et al. 2016b) quantified PFBS in the livers of polar bears and killer whales from Greenland, at concentrations of 0.03 and 0.01 ng/g ww respectively. Further, PFBS has also been reported in polar bear plasma from Svalbard in two separate studies, the first for samples collected between 2000-2014 having a mean concentration of 0.27 ng/g ww (Routti et al., 2017) though with no clear time trend, the second for samples collected in 2017 having a mean of 0.04 ng/g ww (Miljødirektoratet, 2018). It has also been reported in mink liver (mean 0.19 ng/g ww) and common gull liver (mean 0.03 ng/g ww).

Table 5. Environmental concentrations of PFBS in arctic biota (ng/g ww). See Appendix A1 for Latin names.

Region	Location	Date	Mean +/- SD	Min-Maks (Median)	n (det. Freq)	Remark <sup>a)</sup>	Reference
Arctic	Greenland	2012-2013	<0.002		10	Ringed seal liver	(Gebbinck et al., 2016b)
Arctic	Greenland	2012-2013	0.03 ± 0.01		8 (100 %)	Polar bear liver	(Gebbinck et al., 2016b)
Arctic	Greenland	2012-2013	0.01 ± 0.00		6 (66 %)	Killer whale liver	(Gebbinck et al., 2016b)
Arctic	Hornøya	1983	<0.009		5	Herring Gull egg	(Verreault et al., 2007)
Arctic	Hornøya	1993	<0.009		5	Herring Gull egg	(Verreault et al., 2007)
Arctic	Hornøya	2003	<0.009		5	Herring Gull egg	(Verreault et al., 2007)
Arctic	Nunavut, Canada	1972-2005	nd		184	Ringed Seal liver	(Butt et al., 2008)
Arctic	Røst	1983	<0.009		5	Herring Gull egg	(Verreault et al., 2007)
Arctic	Røst	1993	<0.009		5	Herring Gull egg	(Verreault et al., 2007)
Arctic	Røst	2003	<0.009		5	Herring Gull egg	(Verreault et al., 2007)
Arctic	Røst	2017	<0.06		5	European shag eggs	(Miljødirektoratet, 2018)

Arctic	Svalbard	1990-2010	<0.07			Ringed seal plasma	(Routti et al., 2016)
Arctic	Svalbard	2000-2014	0.27	0.08 - 0.69 (0.27)	70 (100 %)	Polar bear plasma	(Routti et al., 2017)
Arctic	Svalbard	2007	nd			Black guillemots liver	(Axelson et al., 2014)
Arctic	Svalbard	2007	nd			Glaucus gull liver	(Axelson et al., 2014)
Arctic	Svalbard	2016	nd			Ringed seal liver	(Schlabach et al., 2017)
Arctic	Svalbard	2016	nd			Polar bear whole blood	(Schlabach et al., 2017)
Arctic	Svalbard	2017	<0.05		10	Common eider eggs	(Miljødirektoratet, 2018)
Arctic	Svalbard	2017	<0.07		5	Kittiwake eggs	(Miljødirektoratet, 2018)
Arctic	Svalbard	2017	<0.08		5	Glaucus gull eggs	(Miljødirektoratet, 2018)
Arctic	Svalbard	2017	0.04 ± 0.02	0.02 - 0.08 (0.04)	10 (60 %)	Polar bear plasma	(Miljødirektoratet, 2018)
Arctic	Troms	2013-2014	0.19 ± 0.11	0.07 - 0.33 (0.19)	10 (100 %)	Mink liver	(Miljødirektoratet, 2018)
Arctic	Tromsøya	2017	0.03 ± 0.03	0.01 - 0.07 (0.02)	5 (80 %)	Common gull egg	(Miljødirektoratet, 2018)

a) See Appendix Table A1 for Latin Names. nd = not detected

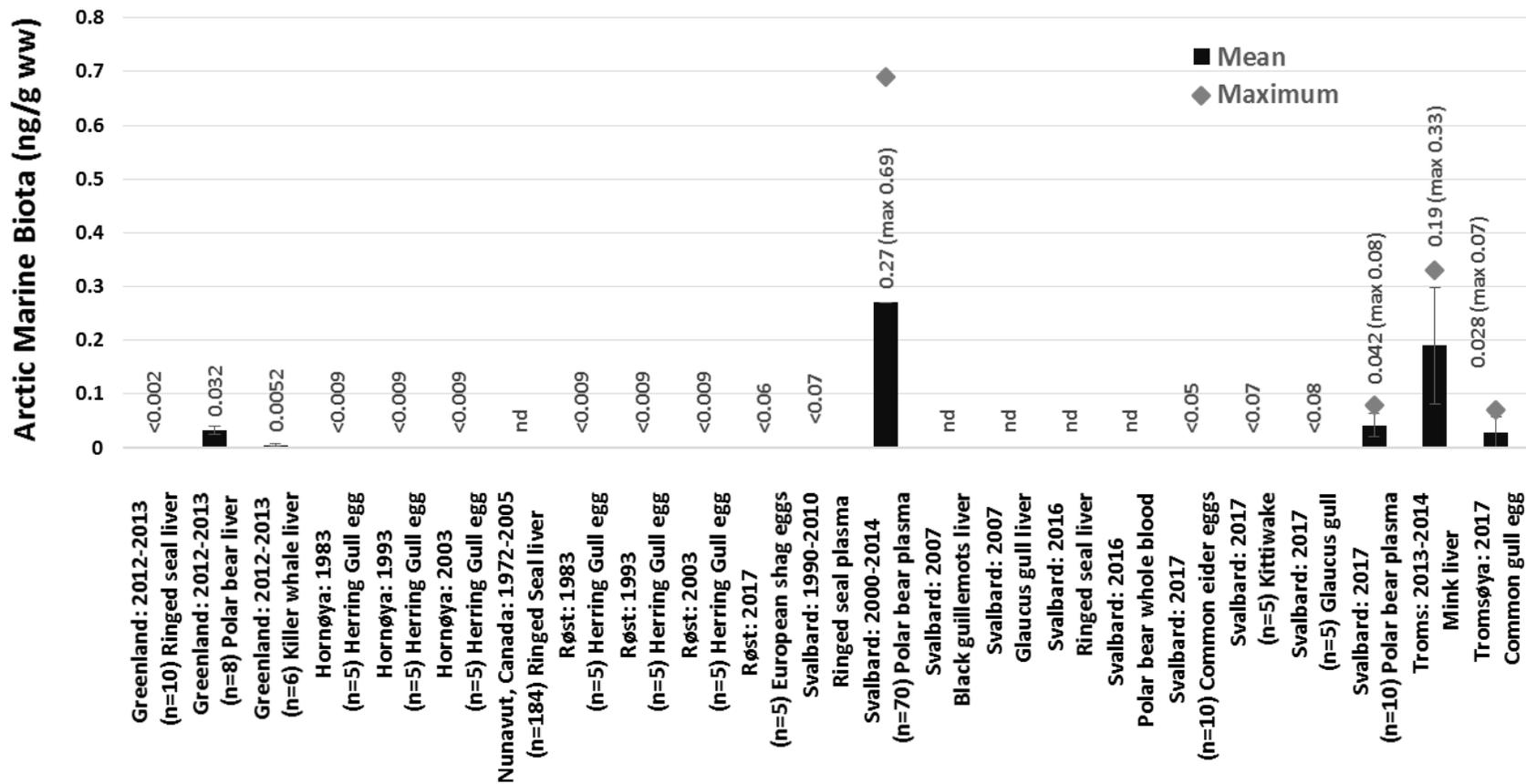


Figure 3. Environmental concentrations of PFBS in arctic marine biota (ng/g ww).

#### 4.4.3.2 Marine

In non-arctic areas, PFBS has been reported in several marine biota samples throughout the world. The largest concentration was found in shark liver (*Sphyrna tiburo* or *Rhizoprionodon terraenovae*) at a mean of 0.7 ng/g ww and max of 2.1 ng/g ww (Green et al., 2016). The largest concentration found for turtles was in green turtle plasma (*Chelonia mydas*), at a mean of 0.09 and a max of 0.85 ng/g ww (Keller et al., 2012).

Table 6. Environmental concentrations of PFBS in marine biota from other regions than the arctic (ng/g ww). See Appendix A1 for Latin names.

Region	Location	Date	Mean +/- SD	Min-Maks (Median)	n (det. Freq)	Remark	Reference
Europe	Baltic sea	2013-2014	0.002			Zooplankton	(Gebbinck et al., 2016a)
Europe	Baltic sea	2013-2014	0.01			Herring whole fish	(Gebbinck et al., 2016a)
Europe	Baltic sea	2013-2014	0.06			Sprat whole fish	(Gebbinck et al., 2016a)
Europe	Baltic sea	2013-2014	0.004 ± 0.000		(100 %)	Guillemot egg	(Gebbinck et al., 2016a)
Europe	Black Sea	1997-1998	nd			Harbor porpoise organs	(Van de Vijver et al., 2007)
Europe	Faroe Islands	1986-2013	<0.01			Pilot whale muscle	(Dassuncao et al., 2017)
Europe	Norway	2015	0.1	(0.10)	128	Cod liver	(Green et al., 2016)
Europe	Spain	2009	nd			Fish and shellfish (composite samples)	(Domingo et al., 2012)
North America	Minnesota/Mississippi R.	2007	nd			Bluegill, Black crappie & Pumpkinseed fillet	(Delinsky et al. 2010)
North America	USA, Georgia	2006	0.3	0.3		Shark soft tissue	(Kumar et al., 2009)
North America	USA, Georgia	2006	0.7	<0.1 - 2.10		Shark liver	(Kumar et al., 2009)
North America	USA, Georgia	2006	0.4	<0.1 - 0.80		Shark muscle	(Kumar et al., 2009)
North America	USA	2007	nd		7	Leatherback turtle plasma	(Keller et al., 2012)
North America	USA	2007	0.02 ± 0.04	<0.01 - 0.13 (0.00)	15 (20 %)	Loggerhead turtle plasma	(Keller et al., 2012)
North America	USA	2007	0.02 ± 0.02	<0.01 - 0.06 (0.02)	10 (30 %)	Kemp's ridley turtle plasma	(Keller et al., 2012)
North America	USA	2007	0.04 ± 0.06	<0.02 - 0.14 (0.01)	5 (40 %)	Hawksbill turtle plasma	(Keller et al., 2012)
North America	USA	2007	0.09 ± 0.27	<0.02 - 0.85 (0.00)	10 (20 %)	Green turtle plasma	(Keller et al., 2012)

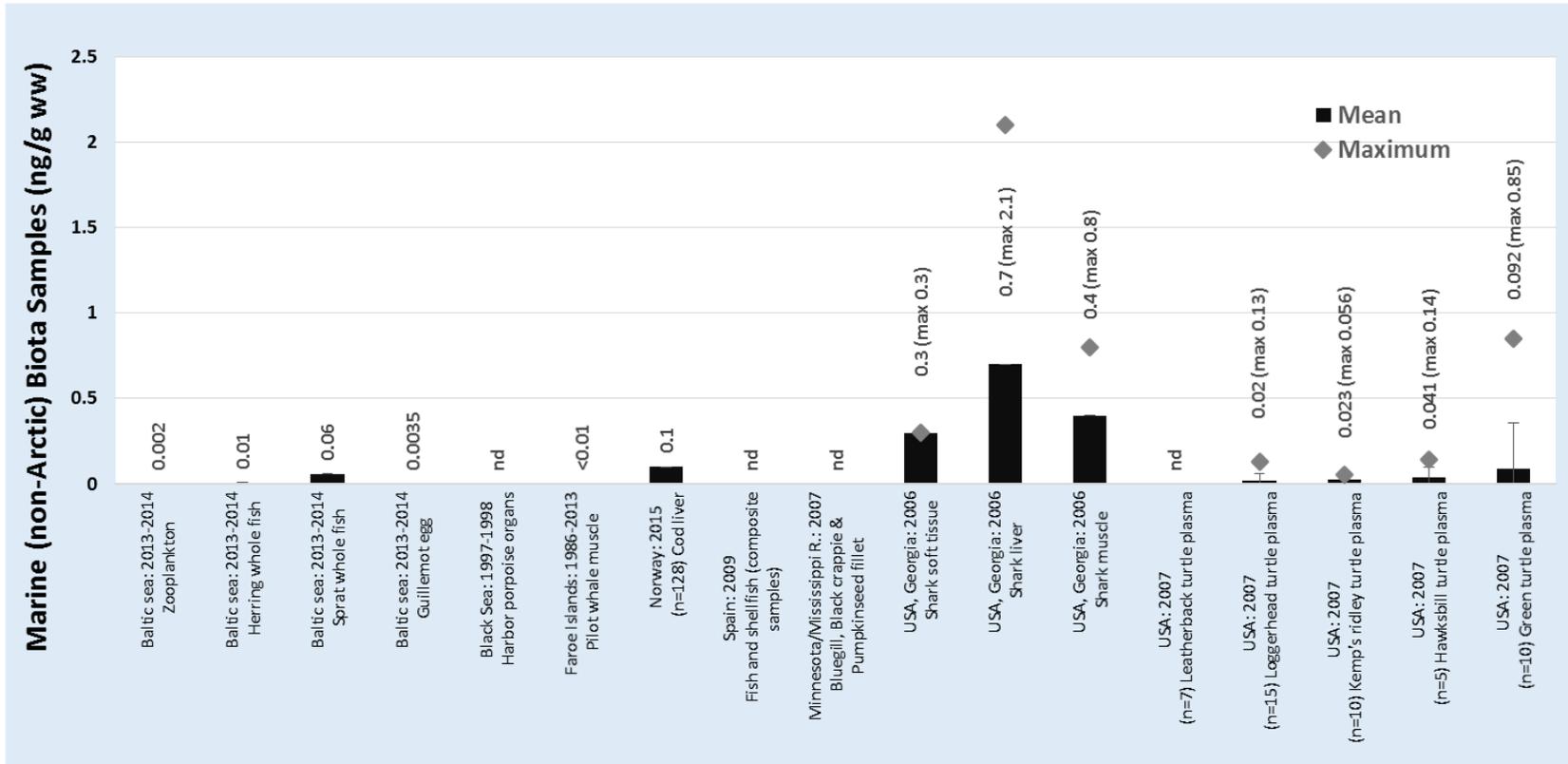


Figure 4. Environmental concentrations of PFBS in marine biota from other regions than the arctic (ng/g ww).

Measurements in freshwater biota were primarily from Taihu Lake, China (Fang et al. 2014) and a national survey of river basins in Vietnam (Lam et al. 2017). The highest concentration in Taihu Lake was associated with zooplankton (1.68 ng/g ww) and in Vietnam with Tilapia liver (1.34 ng/g ww).

Table 7. Environmental concentrations of PFBS in freshwater biota (ng/g ww). See Appendix A1 for Latin names.

Region	Location	Date	Mean +/- SD	Maks	n	Remark	Reference
Asia	China, Taihu Lake	2012	nd			Phytoplankton	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			Crucian muscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	0.08 ± 0.00			Lake saury muscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	0.10 ± 0.00			Carp muscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	0.54 ± 0.01			Mongolian culter muscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	0.24 ± 0.01			Mudfish muscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			Chinese bitterling muscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			Gobiesmuscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	1.68 ± 0.04			Zooplankton	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			Lake shrimp soft tissue	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			White shrimp soft tissue	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			Freshwater mussel soft tissue	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			Pearl mussel soft tissue	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			Minnow muscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	nd			Silver carp muscle	(Fang et al. 2014)
Asia	China, Taihu Lake	2012	1.20 ± 0.03			Whitebait muscle	(Fang et al. 2014)
Asia	Vietman	2013-2015	0.11 ± 0.54	1.34	149	Fish and shellfish tissue (average of 5 fish species, 2 crustaceans (paddle crab, giant prawn), 1 gastropod (golden apple snail), 1 bivalve (golden freshwater clam))	(Lam et al., 2017)

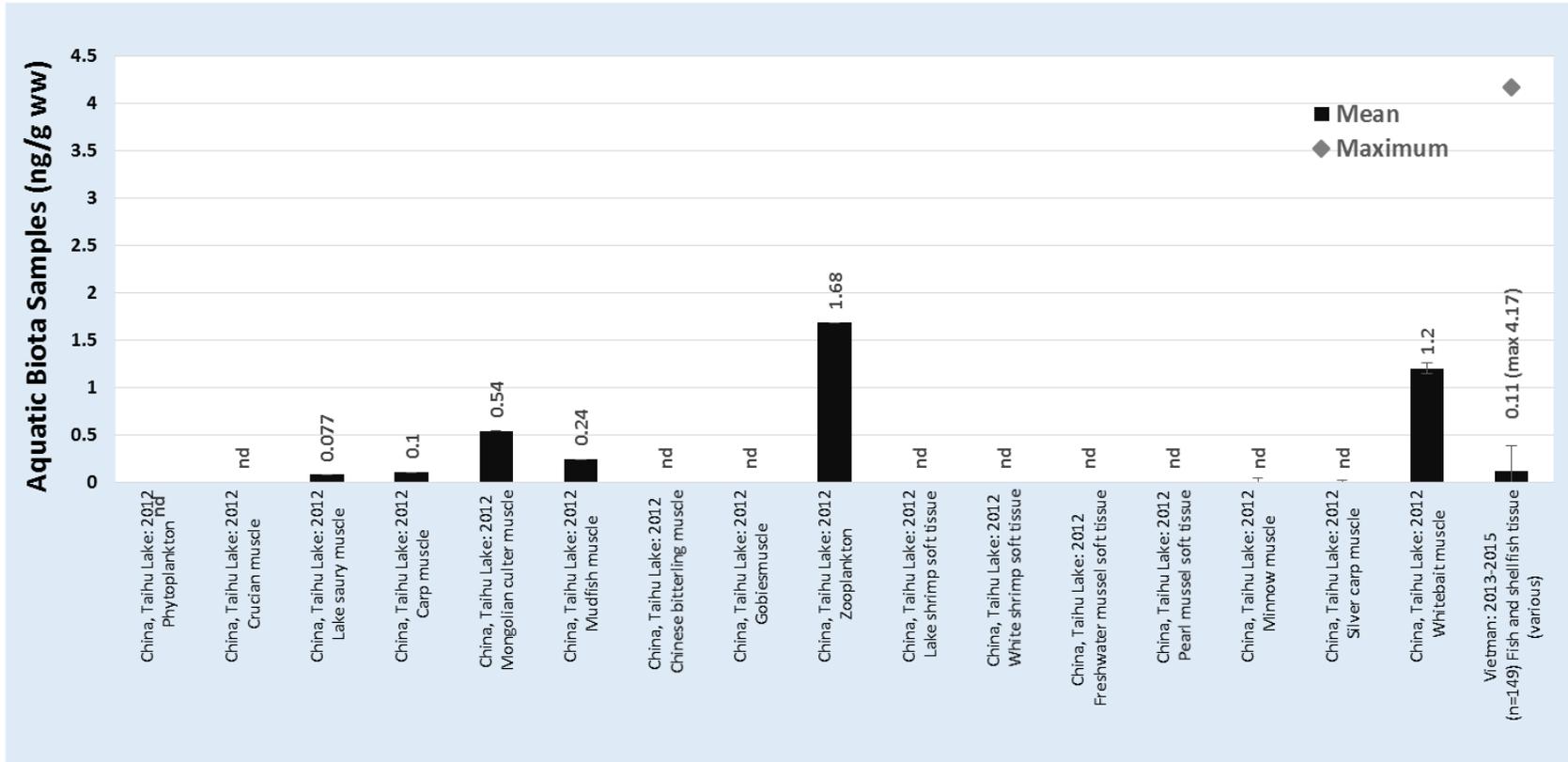


Figure 5. Environmental concentrations of PFBS in freshwater biota (ng/g ww).

PFBS has shown a high propensity to transfer and enrich in plants, due to its high mobility in plant xylem. Most of the data on this are from plants grown in PFAS contaminated soil that was unintentionally impacted through fertilizer impurities (Kowalczyk et al., 2013) or from soil augmented intentionally with PFAS-contaminated biosolid-fertilizer (Blain et al., 2014). This data indicates that plants may reach level as high as a 1 µg/g w (Kowalczyk et al., 2013). Hence, exposure to PFBS through plants grown in contaminated soil is an important pathway to consider in risk assessment regarding contaminated farmland.

Table 9. Environmental concentrations of PFBS in terrestrial plants (ng/g ww). See Appendix A1 for Latin names.

Region	Location	Year	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Europe	Germany	2013	68.40 ± 23.10	29.00 - 98.00	7	Grass silage (dw=0.41 ww)	(Kowalczyk et al., 2013)
Europe	Germany	2013	993.60 ± 224.40	843.00 - 1,419.00	7	Hay (dw=0.41 ww)	(Kowalczyk et al., 2013)
North America	USA, Greenhouse	2013	107.00 ± 29.18			Celery shoot industrial	(Blain et al., 2014)
North America	USA, Greenhouse	2013	164.20 ± 13.36			Radish root	(Blain et al., 2014)
North America	USA, Greenhouse	2013	34.40 ± 15.08			Tomato root	(Blain et al., 2014)
North America	USA, Greenhouse	2013	177.10 ± 21.78			Tomato shoot	(Blain et al., 2014)
North America	USA, Greenhouse	2013	43.00 ± 10.63			Pea root	(Blain et al., 2014)
North America	USA, Greenhouse	2013	200.10 ± 20.13			Pea shoot	(Blain et al., 2014)
North America	USA, Greenhouse	2013	4.50 ± 2.80			Celery shoot municipal	(Blain et al., 2014)
North America	USA, Greenhouse	2013	<0.07			Pea fruit control	(Blain et al., 2014)
North America	USA, Greenhouse	2013	16.20 ± 2.55			Pea fruit industrial	(Blain et al., 2014)
North America	USA, Greenhouse	2013	<0.07			Pea fruit municipal	(Blain et al., 2014)
North America	USA, Greenhouse	2013	22.40 ± 2.74			Radish root control	(Blain et al., 2014)
North America	USA, Greenhouse	2013	61.90 ± 19.35			Radish root industrial	(Blain et al., 2014)
North America	USA, Greenhouse	2013	23.90 ± 2.10			Radish root municipal	(Blain et al., 2014)
North America	USA, Greenhouse	2013	122.60 ± 23.86			Celery root	(Blain et al., 2014)

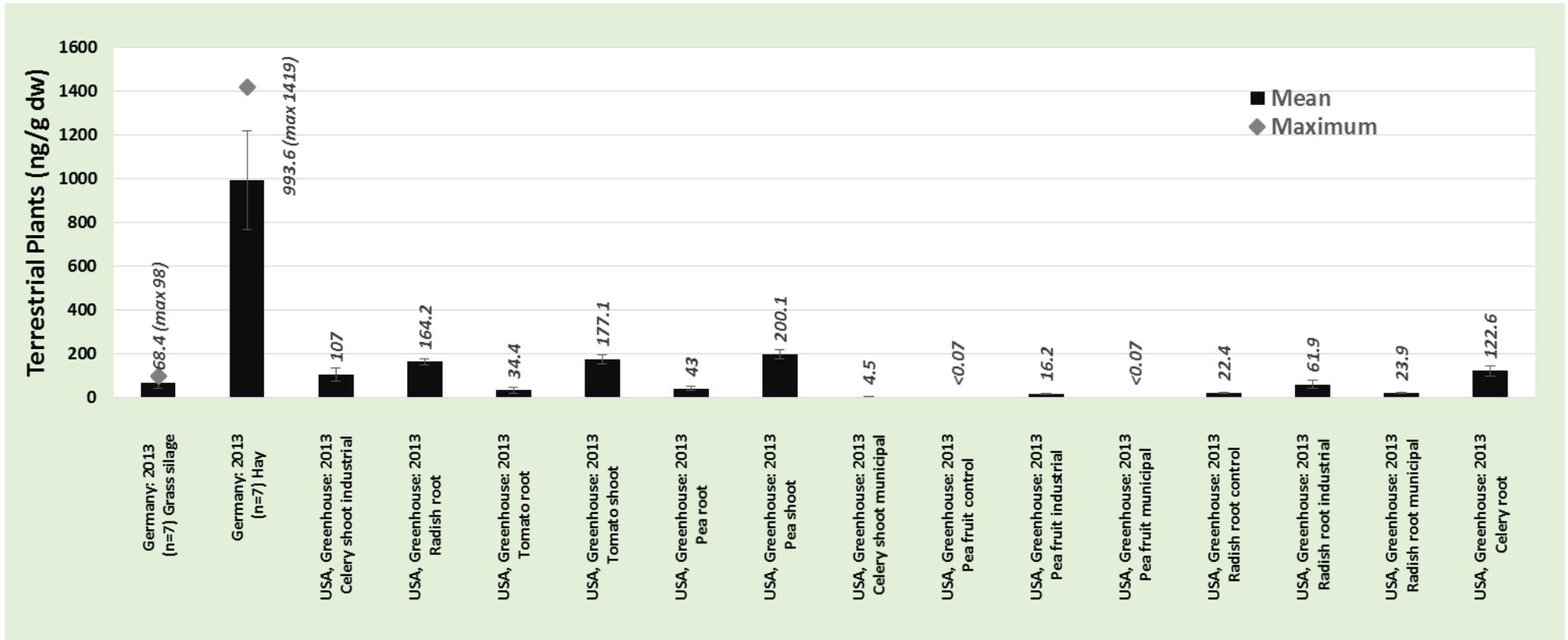


Figure 7. Environmental concentrations of PFBS in terrestrial plants (ng/g dw).

Measurements in terrestrial biota were available from a study on cows eating contaminated hay grown mentioned in the previous section for 28 days, resulting in kidney mean  $1.00 \pm 0.30$  ng/g ww (Kowalczyk et al., 2013). A Norwegian study on earthworms reported a mean of 0.75 ng/g ww (Miljødirektoratet, 2016).

Table 8. Environmental concentrations of PFBS in freshwater biota (ng/g ww). See Appendix A1 for Latin names.

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Europe	Germany	2013	$0.30 \pm 0.30$		3 (66 %)	Cow liver (After 28 days feeding PFAS contaminated hay)	(Kowalczyk et al., 2013)
Europe	Germany	2013	$1.00 \pm 0.30$		3 (100 %)	Cow kidney (After 28 days feeding PFAS contaminated hay)	(Kowalczyk et al., 2013)
Europe	Germany	2013	nd		3	Cow muscle tissue (After 28 days feeding PFAS contaminated hay)	(Kowalczyk et al., 2013)
Europe	Germany	2013	$0.02 \pm 0.04$		3 (100 %)	Cow milk (After 28 days feeding PFAS contaminated hay)	(Kowalczyk et al., 2013)
Europe	Norway	2015	0.75	0.13 - 1.10 (0.13)	6 (83 %)	Earthworms	(Miljødirektoratet, 2016)

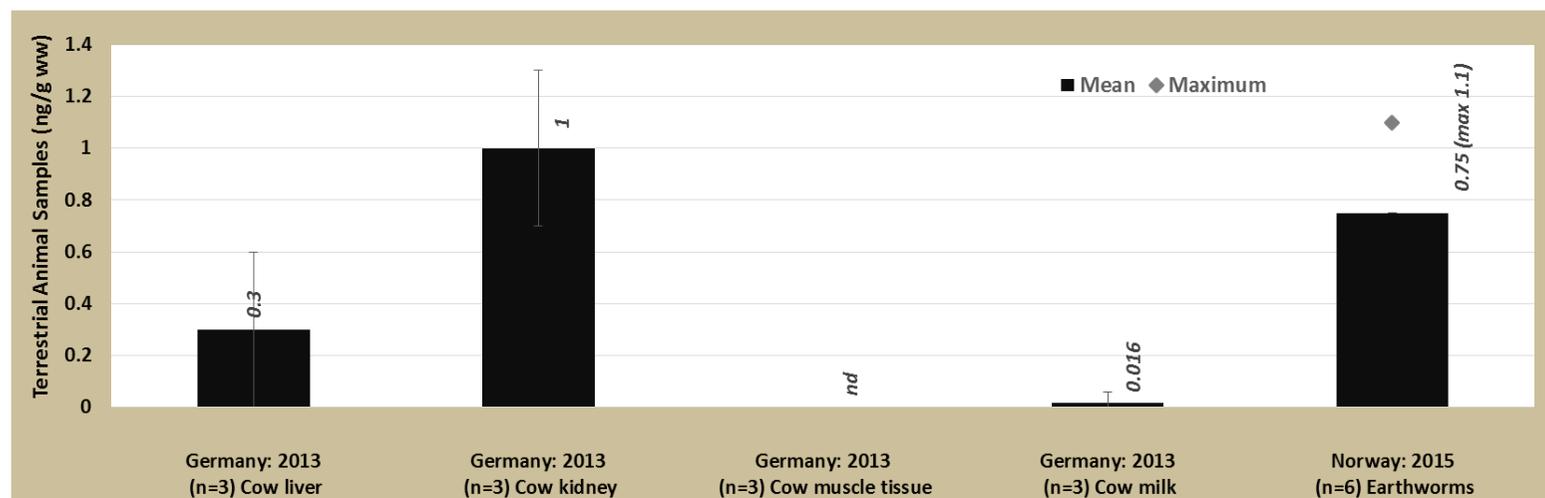


Figure 6. Environmental concentrations of PFBS in terrestrial biota (ng/g ww).

PFBS has been reported in marine water throughout the world. Seven studies have detected PFBS in arctic marine water, with the highest value at 0.11 ng/L (Kallenborn et al., 2004). Two studies have reported PFBS in antarctic marine water, with a maximum at 0.10 ng/L (Cai et al., 2011). The highest European concentration were off the coast of Denmark at 1.09 ng/L (Kallenborn et al., 2004) and the highest in Asia was from the South China Sea both at 1.48 ng/L (Kwok et al., 2015).

Table 10. Environmental concentrations of PFBS in marine water samples (ng/L).

Region	Location	Year	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Arctic	Arctic Ocean	2010	0.03 ± 0.03	<0.017 - 0.08 (<0.017)	13 (38 %)		(Cai et al., 2011)
Arctic	Central Arctic	2012	0.01 ± 0.01	0.04			(Yeung et al., 2017)
Arctic	Faroe Islands	2004		0.05 - 0.11			(Kallenborn et al., 2004)
Arctic	Iceland	2004		0.05 - 0.08			(Kallenborn et al., 2004)
Arctic	North Atlantic	2009-2010	nd	0.045	62		(Zhao et al., 2012)
Arctic	Northwest Pacific Ocean	2010	0.02 ± 0.03	<0.017 - 0.10 (<0.017)	9 (33 %)		(Cai et al., 2011)
Arctic	Russian Arctic Baydaratskaya Bay	2007	0.0132				(Saez et al., 2008)
Antarctic	Antarctica	2007	0.0029				(Wei et al., 2007)
Antarctic	South Atlantic	2009-2010	nd	nd-0.013	39		(Zhao et al., 2012)
International	Mid-Atlantic	2009-2010	nd	nd-0.017	20		(Zhao et al., 2012)
Europe	Baltic sea, Kattegat	2013	0.32	0.06 - 0.57	18 (65 %)		(Nguyen et al., 2017)
Europe	Denmark	2004	0.8	0.30 - 1.09	4		(Kallenborn et al., 2004)
Europe	Farao Islands	2004	0.1	0.05 - 0.20	4		(Kallenborn et al., 2004)
Europe	Finland	2004	0.07	<LOQ - 0.93	3		(Kallenborn et al., 2004)
Europe	Iceland	2004	0.06	0.05 - 0.08	4		(Kallenborn et al., 2004)
Europe	Western Mediterranean Sea	2014	0.01 ± 0.01	nd - 0.02 (0.02)	0.012 (0 %)		(Brumovsky et al. 2016)
Asia	China	2013	0.66	0.32 - 1.46 (0.49)	(100 %)	(July)	(Chen et al., 2016)
Asia	China	2013	nd	<MLQ - 0.24 (<MLQ)	(19 %)	(November)	(Chen et al., 2016)
Asia	Pacific Ocean	2007	0.02 ± 0.00		19 (16 %)		(Wei et al., 2007)
Asia	Pacific Ocean	2007	0.07 ± 0.01				(Wei et al., 2007)
Asia	South China Sea	2012-2013	0.63 ± 0.43	0.25 - 1.48 (0.45)	17 (100 %)		(Kwok et al., 2015)

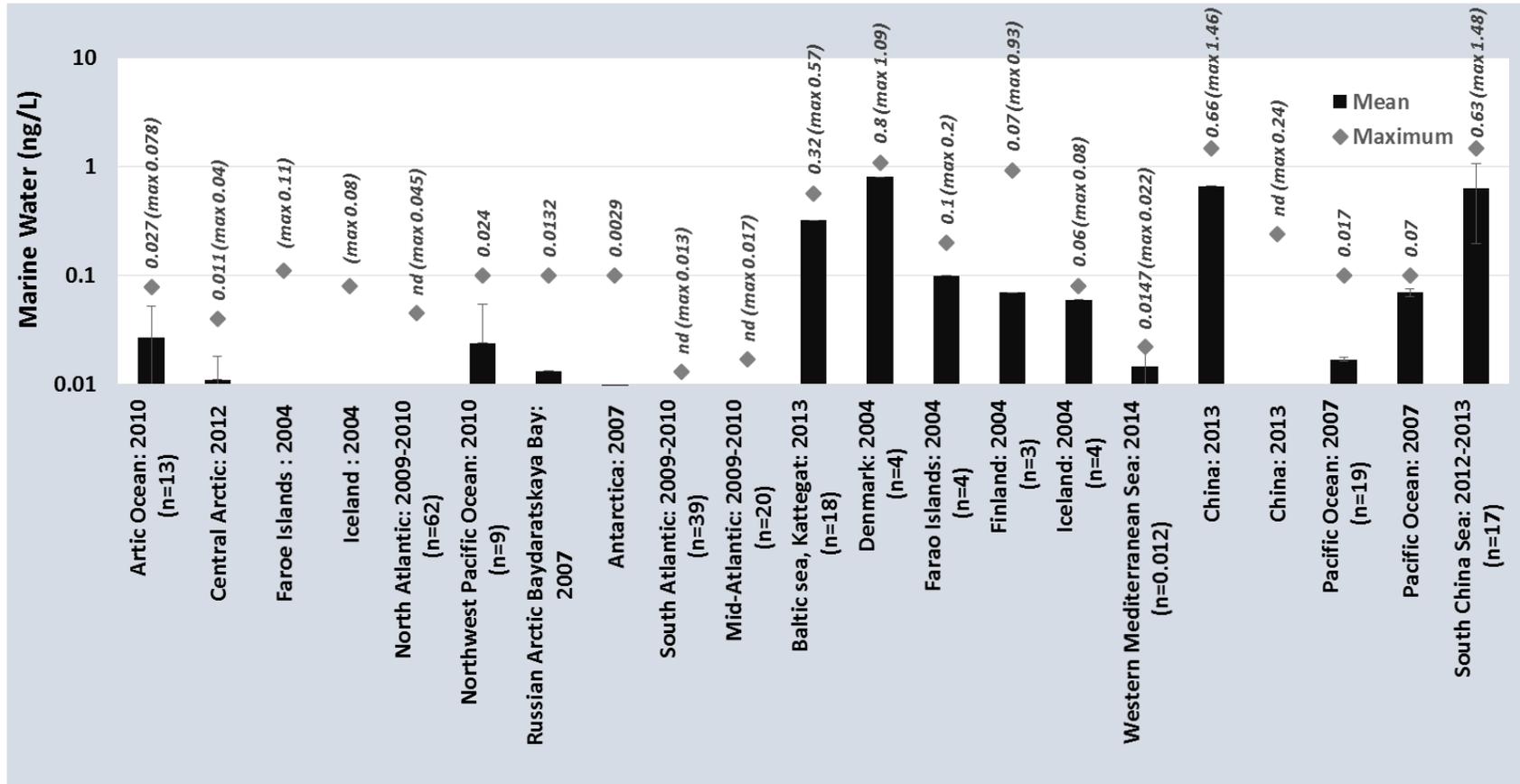


Figure 8. Environmental concentrations of PFBS in marine water samples (ng/L).

### 4.4.5.1 Arctic fresh water, snow and ice

PFBS has been frequently detected in fresh water, snow and ice samples throughout the Arctic and Antarctic. The largest concentration from this review was measured at 4.90 ng/L (Lescord et al., 2015), but this was considered to be due to pollution from a local airport. Elsewhere concentrations typically ranged between 0.02-0.2 ng/L, which is in the low end of the range observed for rain in non-Arctic areas (Section 4.4.1), though one sample from northern Sweden contained 2.15 ng/L (Codling et al., 2014).

Table 11. Environmental concentrations of PFBS in Arctic fresh water, snow and ice samples (ng/L).

Region	Location	Year	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Arctic	Arctic Ocean (Snow/Ice)	2010	0.17 ± 0.42	<0.017 - 1.50 (0.02)	12 (50 %)	Snow/Ice	(Cai et al., 2011)
Arctic	Canada	2007 - 2008		0.01 - 0.02	11		(Veillette et al., 2012)
Arctic	Canada	2010 -2011	0.07 ± 0.01		5		(Lescord et al., 2015)
Arctic	Canada	2010-2011	4.90 ± 1.00		5	Lake (local pollution)	(Lescord et al., 2015)
Arctic	Greenland	2015	0.0068			Ice cap (19 cm = 2015)	(Pickard et al., 2018)
Arctic	Greenland	2015	0.0042			Ice cap (134 cm = 2013 )	(Pickard et al., 2018)
Arctic	Northern Sweden	2009	0.099	nd - 2.16	24	Snow/Ice	(Codling et al., 2014)
Arctic	Svalbard	2015	0.023		23	Lake Linnévatnet,	(Skaar, 2016)
Arctic	Svalbard	2015	0.022		2	melt water	(Skaar, 2016)
Arctic	Svalbard	2015	0.022		2	River	(Skaar, 2016)
Arctic	Svalbard	2015	0.024		2	Snow/Ice	(Skaar, 2016)
Antarctic	Antarctica (Lake)	2011	0.038	<0.0083 - 0.05	4	Lake (King George Island)	(Cai et al., 2012)
Antarctic	Antarctica	2011	0.017	<0.0083 - 0.02	4	Snow/Ice (King George Island)	(Cai et al., 2012)

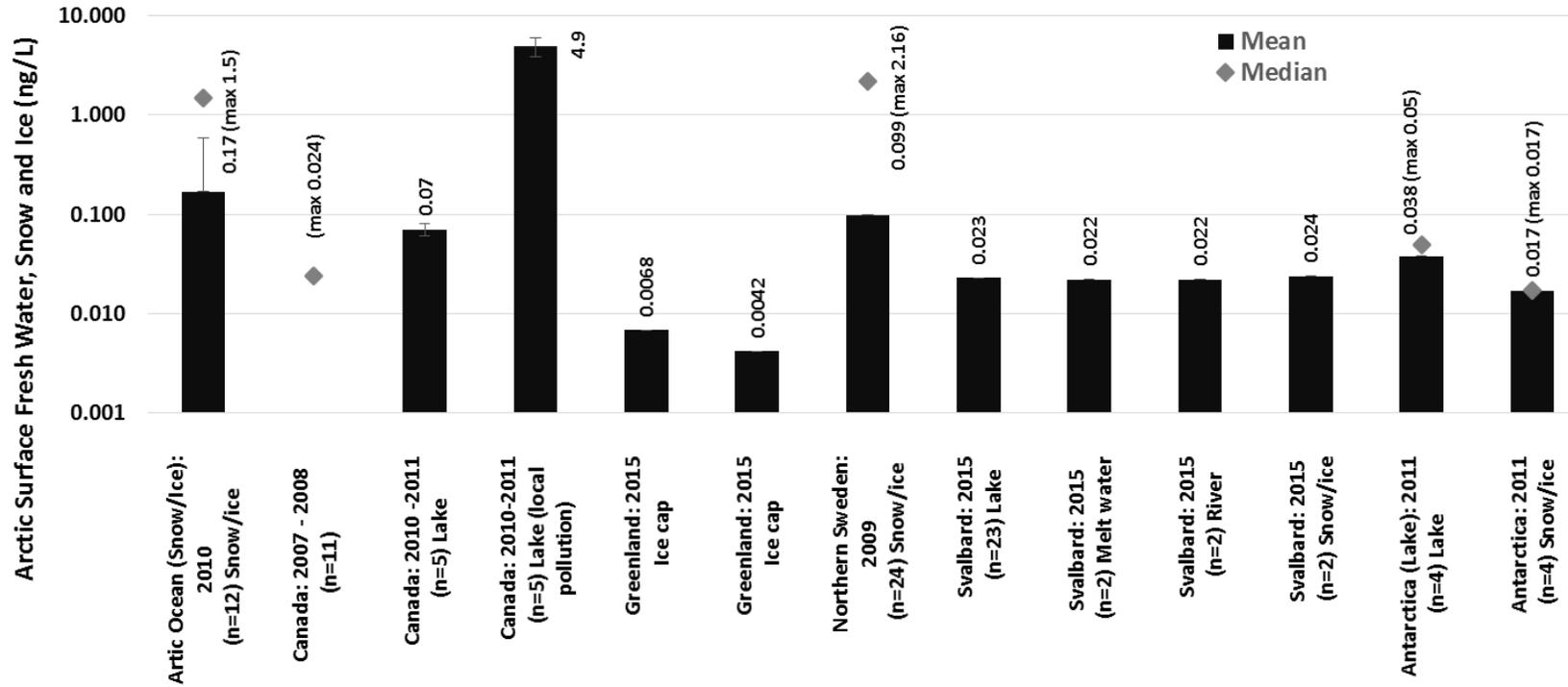


Figure 9. Environmental concentrations of PFBS in Arctic fresh water, snow and ice samples (ng/L). Note the logarithmic scale on the y-axis.

#### 4.4.5.2 Surface fresh water near source zones

Surface water has been measured near PFAS production facilities in the Netherlands (Gebbinck et al., 2017), China (Wang et al., 2016b), (Bao et al., 2010), (Zhou et al., 2013), electronic production facility wastewaters in Tawian (Lin et al., 2014), Aqueous Film-Forming Foam (AFFF) contaminated areas in Canada, as well as mixed industrial areas that include fluorochemical plants in Italy (Valsecchi et al. (2015) and (Castiglioni et al. (2015)). The highest concentrations were found Tangxu Lake, near a PFAS production facility, where concentrations reached up to 5.3 µg/L (Zhou et al., 2013). In Europe the highest concentration was 1.7 µg/L from the Fratta Garzone river in Italy which receives water from textile industry and a fluorochemical plant (Valsecchi et al., 2015).

Table 12. Environmental concentrations of PFBS in surface water near PFAS production facilities or known hotspots (ng/L)

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Europe	Italy (Bormida, Tanaro)	2010-2013	6.8 ± 5.5	<LOD - 17.0 (5.9)	33 (80 %)	River basin survey	(Valsecchi et al., 2015)
Europe	Italy (Brenta, Fratta-Gorzzone)	2010-2013	878.0 ± 764.0	56.0 - 1,665.7 (894.2)	4 (100 %)	River basin survey	(Valsecchi et al., 2015)
Europe	Italy	2010-2013	11	0.0 - 66.0 (2.0)	(74 %)	Industrialized river	(Castiglioni et al., 2015)
Europe	Netherlands	2016	20.3 ± 3.7	12.0 - 27.0	18 (100 %)	River	(Gebbinck et al., 2017)
Asia	China, Daling River	2014	1090	nd - 3,780.0 (668.0)		River	(Wang et al., 2016b)
Asia	China, Fuxin	2009	320	7.8 - 445.0 (353.0)		River	(Bao et al., 2010)
Asia	China, Tangxun Lake	2013	4950	4,600.0 - 5,300.0	2	WWTP	(Zhou et al., 2013)
Asia	China, Tangxun	2013	3720	2,240.0 - 4,520.0		Lake	(Zhou et al., 2013)
Asia	Taiwan	2013	0.3 ± 0.2		3	Upstream WWTP	(Lin et al., 2014)
Asia	Taiwan	2013	329.0 ± 16.0		3	WWTP	(Lin et al., 2014)
Asia	Taiwan	2013	392.0 ± 6.0		3	Downstream WWTP	(Lin et al., 2014)
Asia	Taiwan	2013	282.0 ± 9.0		3	Downstream WWTP	(Lin et al., 2014)
Asia	Taiwan	2013	262.0 ± 4.4		3	Downstream WWTP	(Lin et al., 2014)
North America	Canada	2012-2016	6.4 ± 4.5	0.8 - 13.0 (4.4)	14 (100 %)	AFFF source	(D'Agostino and Mabury et al., 2017)

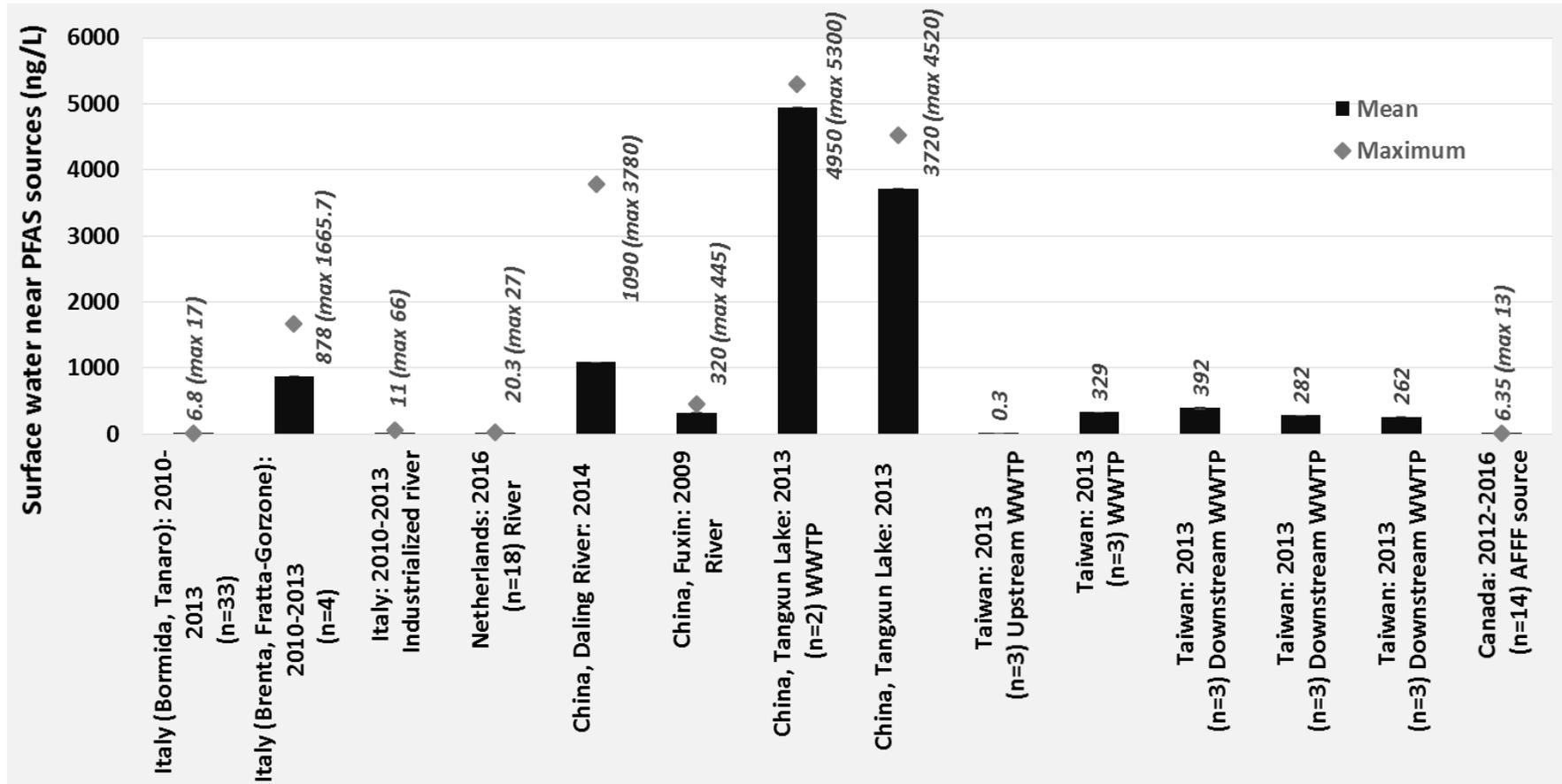


Figure 10. Environmental concentrations of PFBS in surface water near PFAS production facilities or known hotspots (ng/L)

#### 4.4.5.3 Surface fresh water (excluding Arctic and near source zones)

Most PFBS data in the peer-reviewed literature is for surface fresh water. It has been found in surface fresh waters throughout Europe, Asia and North America, where it has been reported over a wide range of concentrations. The highest PFBS concentration of 1450 ng/L, reported in the Möhne river in Germany (Skutlarek et al., 2006), was attributed to the use of contaminated fertilizer in an agricultural area. The ubiquity of PFBS in water samples shows that it is highly mobile and well distributed in the freshwater environment, even apart from source zones.

Table 13. Environmental concentrations of PFBS in surface fresh water samples (ng/L).

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Europe	Baltic sea	2013-2014	0.10 ± 0.00		(100 %)		(Gebblink et al., 2016a)
Europe	Elbe River	2014	2.3	0.80 - 3.60 (2.40)	(100 %)		(Heydebreck et al. 2015)
Europe	France	2009		5	(1 %)		(Boiteaux et al., 2012)
Europe	France	2012		<0.02 - 29.00	(65 %)		(Munos et al., 2015)
Europe	Germany Bad Godesberg	2008-2009	<0.01	<0.01 - 0.00 (<0.01)			(Wilhelm et al., 2010)
Europe	Germany Bimmen-lobith	2008-2009		0.00 - 0.08 (0.02)	(89 %)		(Wilhelm et al., 2010)
Europe	Germany Düsseldorf-Flehe	2008-2009		0.00 - 0.10 (0.03)	(91 %)		(Wilhelm et al., 2010)
Europe	Germany Moehne river	2008-2009		0.02 - 0.03 (0.02)	35 (100 %)		(Wilhelm et al., 2010)
Europe	Germany Ruhr River 0-100 km	2008-2009	0.023	0.00 - 0.09 (0.02)	(11 %)		(Wilhelm et al., 2010)
Europe	Germany Ruhr River 100-200 km	2008-2009	0.01	<0.01 - 0.02 (<0.01)	(81 %)		(Wilhelm et al., 2010)
Europe	Germany WkSt Rhein-Nord Kleve	2008-2009		0.00 - 0.06 (0.03)	(92 %)		(Wilhelm et al., 2010)
Europe	Germany WkSt Süd/Bad Honnef	2008-2009	<0.01	<0.01 - 0.03 (<0.01)	(7 %)		(Wilhelm et al., 2010)
Europe	Germany, Moehne river	2006	319	<LOD - 1,450 (83)	12		(Skutlarek et al., 2006)

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Europe	Germany, Rhine river	2006	14.3	<LOD - 46.00 (12.50)	38		(Skutlarek et al., 2006)
Europe	Germany, Rhine River	2016	21.9	0.46 - 146.00	20 (100 %)		(Pan et al., 2018)
Europe	Germany, Rhine watershed	2008		<0.08 - 181.00			(Möller et al., 2010)
Europe	Germany, Ruhr river	2006	16.7	<LOD - 71.00 (13.00)	27		(Skutlarek et al., 2006)
Europe	Germany	2007	6.3	3.40 - 17.70 (5.40)			(Ahrens et al., 2009a)
Europe	Italy (river basin survey)	2010-2013	8.90 ± 8.90	<LOD - 31.40 (5.60)	104 (74 %)		(Valsecchi et al., 2015)
Europe	North Sea, Baltic Sea and Norwegian Sea	2009		6.51			(Ahrens et al., 2010)
Europe	Norway	2004	nd		5	Lake	(Kallenborn et al., 2004)
Europe	Norway	2004	42.8	5.64 - 112.00	6	Lake	(Kallenborn et al., 2004)
Europe	Rhine River	2013	15.6	1.40 - 40.00 (15.00)	(100 %)		(Heydebreck et al. 2015)
Europe	Spain	2009	1.22 ± 1.55	n.d. - 5.50	12 (17 %)		(Pico et al., 2012)
Europe	Spain	2009	1.33 ± 3.01	<0.10 - 10.10 (0.20)	30 (57 %)		(Domingo et al., 2012)
Europe	SW along River Elbe	2007	2.2	0.00 - 3.40 (2.30)	30 (100 %)		(Ahrens et al., 2009b)
Europe	Sweden, Mälaren Lake	2016	1.43	0.75 - 1.92	10 (100 %)		(Pan et al., 2018)
Europe	Sweden	2015	0.24 ± 0.10	0.11 - 0.35 (0.23)	4 (100 %)	River	(Tröger et al., 2018)
Europe	Sweden	2015	0.54 ± 0.46	0.19 - 1.20 (0.39)	2 (100 %)	Lake	(Tröger et al., 2018)
Europe	Swedish rivers	2013	9.5	0.03 - 19.00	40 (59 %)		(Nguyen et al., 2017)
Europe	Switzerland, Glatt river	2007	4.3	2.30 - 7.70 (2.80)	3		(Huset et al., 2008)
Europe	UK, Thames River	2016	5.06	3.26 - 6.75	6 (100 %)		(Pan et al., 2018)
Europe	Xiaoqing River	2014	nd				(Heydebreck et al. 2015)
Asia	China, Chao Lake	2016	15.4	1.50 - 81.50	13 (100 %)		(Pan et al., 2018)
Asia	China, Huai River	2016	0.83	0.52 - 1.59	9 (100 %)		(Pan et al., 2018)
Asia	China, Liao River	2016	0.94	0.43 - 2.16	6 (100 %)		(Pan et al., 2018)

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Asia	China, Pearl River	2016	4.49	0.21 - 21.50	13 (100 %)		(Pan et al., 2018)
Asia	China, Shuangtaizi Estuary	2013	4.7	0.95 - 12.60 (4.45)	21 (100 %)		(Shao et al., 2006)
Asia	China, Tai Lake	2016	2.02	0.17 - 4.85	15 (100 %)		(Pan et al., 2018)
Asia	China, Taihu Lake	2012	3.76 ± 0.72				(Fang et al. 2014)
Asia	China, Yangtze River	2016	1.84	0.22 - 4.68	35 (100 %)		(Pan et al., 2018)
Asia	China, Yellow River	2016	0.99	0.07 - 2.23	15 (100 %)		(Pan et al., 2018)
Asia	Hong Kong	2008-2010	6.83 ± 2.40	2.18 - 8.69 (7.30)	12 (100 %)		(Loi et al., 2011)
Asia	Korea, Han River	2016	2.27	1.34 - 3.17	6 (100 %)		(Pan et al., 2018)
Asia	South Korea, Shihwa Industrial zone	2004	2.5	4.27			(Rostkowski et al., 2006)
Asia	Vietman	2013-2015		0.10 - 8.28 (4.19)			(Lam et al., 2017)
North America	Canada	2012-2016	2.52 ± 1.04	1.40 - 4.00 (2.50)	5 (100 %)	Urban	(D'Agostino and Mabury et al., 2017)
North America	Canada	2012-2016	0.78 ± 0.90	0.00 - 1.70 (0.70)	4 (50 %)	Rural	(D'Agostino and Mabury et al., 2017)
North America	NJ, Delaware River	2016	2.19	0.52 - 4.20	12 (100 %)		(Pan et al., 2018)

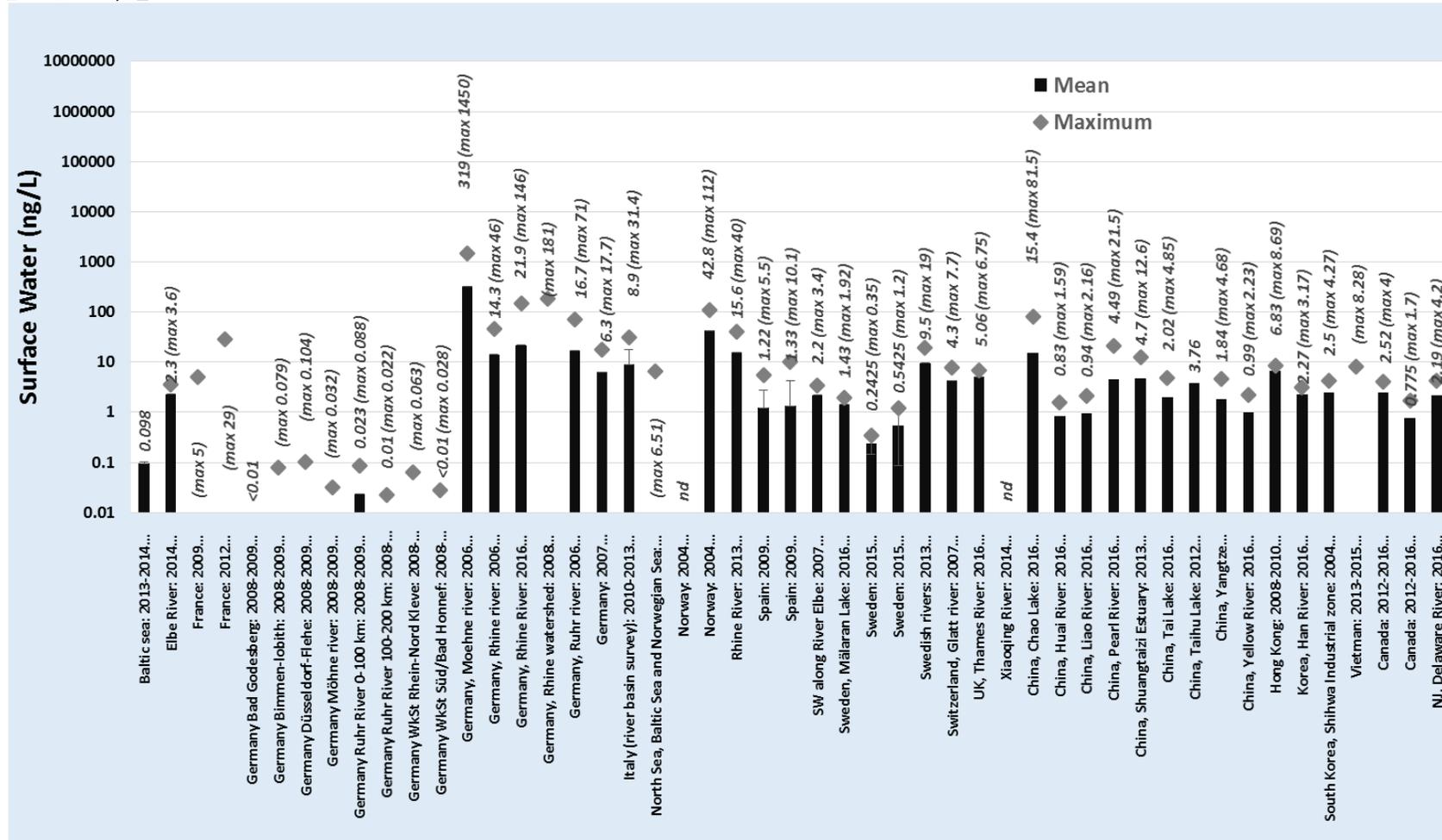


Figure 11. Environmental concentrations of PFBS in surface fresh water samples in non-Arctic areas (ng/L).

Groundwater data was available near two PFAS production facilities in China (Wang et al., 2018; Bao et al. 2010). Both were substantially contaminated with PFBS (max 870 ng/L). Away from PFAS sources, there is currently little data available. A European survey from 2008 found PFBS in 15% of samples, with max 25 ng/L and mean 0.3 ng/L (Loos et al., 2010). A French study found up to 9 ng/L, but it was only in 4% of tested samples (Boiteaux et al., 2012). A Vietnam GW survey did not find PFBS (Lam et al., 2017).

Table 14. Environmental concentrations of PFBS in groundwater (ng/L)

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Europe	Europe - 26 countries	2008	0.3	25	164 (15 %)	GW	(Loos et al., 2010)
Europe	France	2009		9	(4 %)	GW	(Boiteaux et al., 2012)
Asia	Vietman	2013-2015	<0.3			GW	(Lam et al., 2017)
Asia	China, Daling River	2014	375	865	4	Source zone: GW	(Wang et al., 2016b)
Asia	China, Fuxin	2009	235	1.2 - 872.0 (34.4)		Source zone: GW	(Bao et al., 2010)

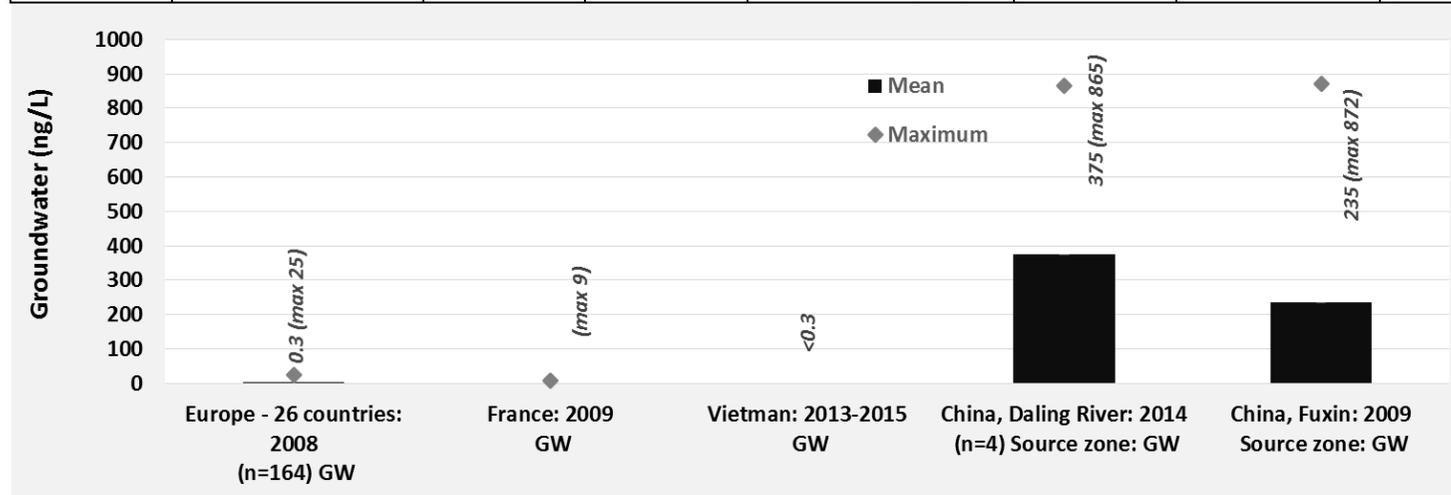


Figure 12. Environmental concentrations of PFBS in groundwater (ng/L)

Drinking water samples, including finished water, bottled water, and treatment steps, have been analysed for PFBS in areas near and far removed from PFAS source zones. PFBS appears ubiquitous in drinking water, both from the tap and from bottles. In regions away from established PFAS source areas, substantial drinking water contamination can occur, with a France max of 15 ng/L (Schwanz et al., 2016), German max of 26 ng/L (Wilhelm et al., 2010), Italy max of 45 ng/L (IRSA-CNR, 2013), Spain max of 69 ng/L (Ericson et al., 2009), China max of 18 ng/L (Mak et al., 2009), and Brazil max of 16 ng/L (Schwanz et al., 2016). These concentrations even exceed those of some known source zones, such as 19.0 ng/L near a PFAS production facility in the Netherlands (Gebbinck et al., 2017), and 0.6 ng/L for drinking water near the PFAS production area of Fuxin, China (Bao et al., 2010). The highest concentration, however, was near a source zone, at 97.8 ng/L, along the Daling River, China (Wang et al., 2016b). This indicates that PFBS, like other PFAS, persists through drinking water production, and therefore currently is ubiquitously present in global drinking water (Kaboré et al., 2018).

Table 15. Environmental concentrations of PFBS in drinking water (ng/L)

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
International	Global	2015	0.1	1.6	38 (47 %)	Bottled water (Canada, Burkina Faso, Chile, Ivory Coast, France, Japan, Mexico, Norway, USA)	(Kaboré et al., 2018)
International	Global	2015	0.24	0.0 - 1.1 (0.2)	59 (88 %)	Tap water (Canada, Burkina Faso, Chile, Ivory Coast, France, Japan, Mexico, Norway, USA)	(Kaboré et al., 2018)
Europe	France	2015	3.2	1.3 - 6.7 (2.9)	(32 %)	Bottled water	(Schwanz et al., 2016)
Europe	France	2015	6.8	2.0 - 15.0 (6.5)	(62 %)	Drinking water	(Schwanz et al., 2016)
Europe	Germany	2008-2009		<0.01 - 0.0 (<0.01)	70 (3 %)	Drinking water	(Wilhelm et al., 2010)
Europe	Germany, Ruhr river	2006	12.2	<LOD - 26.0 (13.5)	37	Drinking water	(Skutlarek et al., 2006)
Europe	Italy	2010-2012	6.7 ± 11.3	<0.5 - 45.0 (1.8)	46 (63 %)	Drinking water	(IRSA-CNR, 2013)
Europe	Netherlands	2008	24.0 ± 10.0	10.0 - 47.0	6	Infiltrated river water	(Eschauzier et al., 2010)

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Europe	Netherlands	2008	2.4 ± 4.9	0.5 - 18.0	6	Infiltrated rainwater	(Eschauzier et al., 2010)
Europe	Spain	2009	4.5 ± 14.5	<0.07 - 69.4 (0.4)		Drinking water	(Ericson et al., 2009)
Europe	Spain	2015	nd			Bottled water	(Schwanz et al., 2016)
Europe	Spain	2015	11	2.8 - 24.0 (11.0)	(31 %)	Drinking water	(Schwanz et al., 2016)
Europe	Sweden	2015	0.8 ± 0.3	0.3 - 1.3 (0.7)	11 (92 %)	Various parts of DW treatment production	(Tröger et al., 2018)
Asia	China, Shuangtaizi Estuary	2013	5.42	1.0 - 13.8 (4.4)	21 (100 %)	Bottled water	(Shao et al., 2006)
Asia	China	2008-2010		0.0 - 18.0 (2.8)	70 (74 %)	Drinking water	(Mak et al., 2009)
North America	New Jersey	2009-2010	nd	6	30 (10 %)	Raw water	(Post et al., 2013)
South America	Brazil	2015	3.4	3.1 - 3.6 (3.5)	(50 %)	Bottled water	(Schwanz et al., 2016)
South America	Brazil	2015	4.4	0.5 - 16.0 (1.3)	(90 %)	Drinking water	(Schwanz et al., 2016)
Europe	Netherlands	2016	4.94	0.5 - 19.0	6 (100 %)	Source zone: Drinking water	(Gebbinck et al., 2017)
Asia	China, Daling River	2014	25.4	97.8	4	Source zone: Drinking water	(Wang et al., 2016b)
Asia	China, Fuxin	2009	0.47	0.2 - 0.7 (0.5)		Source zone: Raw water	(Bao et al., 2010)
Asia	China, Fuxin	2009	0.54	<0.1 - 0.6 (0.5)		Source zone: Finished water	(Bao et al., 2010)
Asia	China, Fuxin	2009	0.54	<0.1 - 0.6 (0.5)		Source zone: Drinking water	(Bao et al., 2010)

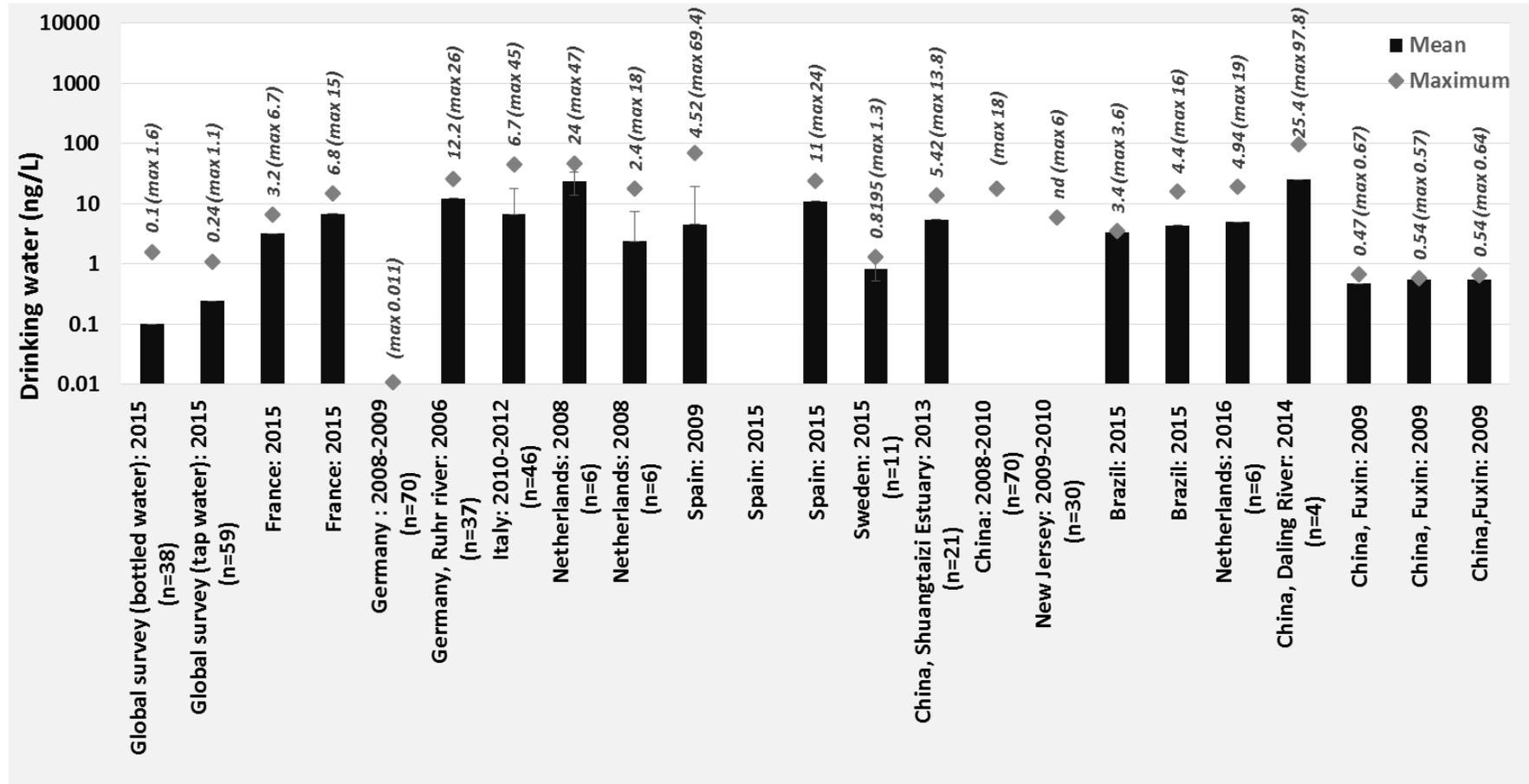


Figure 13. . Environmental concentrations of PFBS in drinking water (ng/L)

Only one study of PFBS in soil could be found, which reported only 10% frequency of detection and a max of 0.003 ng/g dw (Miljødirektoratet, 2016). A study on Arctic sediments in 2003, however, was able to quantify PFBS in surface sediments, at a max of 0.1 ng/g dw, which is an indicator of long range transport. There is in general a lack of soil and sediment data. Based on the log K<sub>oc</sub> of 2.2 (units L/kg<sub>organic carbon</sub> Table 1), it would be anticipated under equilibrium conditions that the concentrations in soil/sediment with 1% organic carbon in ng/g would be 0.16% of water concentrations in ng/L ( $c_{\text{sediment}} \text{ (ng/g)} = K_{oc} * c_{\text{water}} * 0.01 \text{ organic carbon} * 0.001 \text{ kg/g} = 0.0016 c_{\text{water}} \text{ (ng/L)}$ ).

Table 17. Environmental concentrations of PFBS in soil and sediment samples (ng/g dw)

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Arctic	Canada Resolute Lake	2003		nd - 0.1		0-3 cm cores	(Stock et al., 2007)
Arctic	Canada Char Lake	2003	<1.1			0-3 cm cores	(Stock et al., 2007)
Arctic	Canada Amituk Lake	2003		0.0 - 0.1		0-3 cm cores	(Stock et al., 2007)
Europe	Baltic sea (sediment)	2013-2014	0.0002 ± 0.0001		(75 %)		(Gebbink et al., 2016a)
Europe	Norway (soil)	2015	<LOD	<LOD - 0.003 (<LOD)	10 (10 %)		(Miljødirektoratet, 2016)
Asia	China (sediment)	2013	0.06	0.0 - 0.2 (0.1)	(100 %)	Surface sediments (July)	(Chen et al., 2016)
Asia	China (sediment)	2013	0.06	0.1 - 0.1 (0.1)	(100 %)	Surface sediments (November)	(Chen et al., 2016)
Asia	Hong Kong (sediment)	2008-2010	<0.026				(Loi et al., 2011)
North America	Canada (sediment)	2012-2016	nd			Urban	(D'Agostino and Mabury et al., 2017)

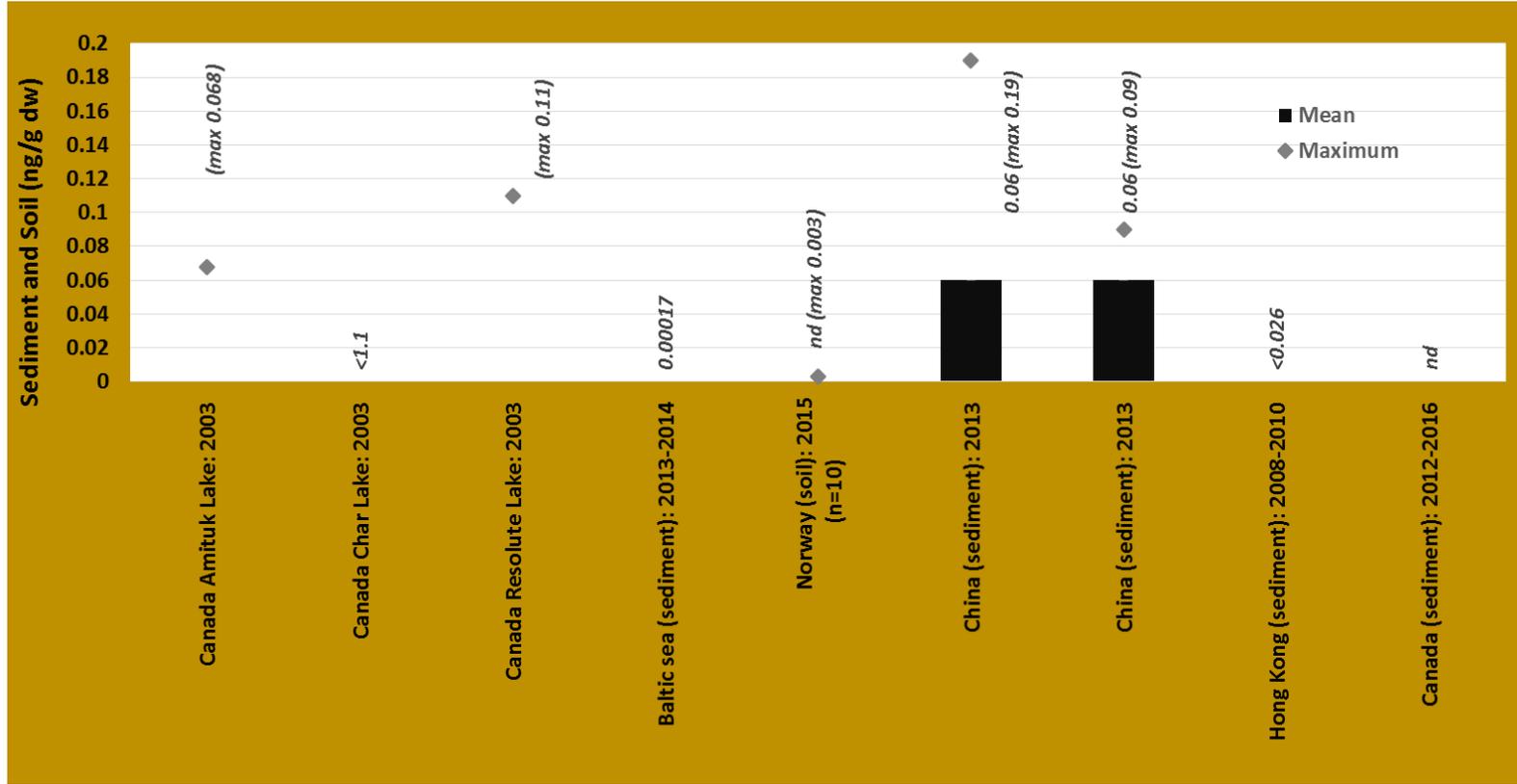


Figure 15. Environmental concentrations of PFBS in soil and sediment samples (ng/g dw)

#### 4.4.7 Waste Water and Leachate

PFBS is also commonly found in WWTP and Leachate effluent. In general, concentrations in landfill effluent are higher, with a max of 3410 ng/L, (Lang et al. 2017), compared to the maximum identified WWTP effluent sample of 26 ng/L (Ahrens et al., 2009b). This indicates that landfills can be environmental hotspots for PFBS emissions. By comparison, the highest concentration in surface water near a PFAS production facility was 5300 ng/L (Zhou et al., 2013).

Table 18. Environmental concentrations of PFBS in waste water and leachate samples (ng/L)

Region	Location	Date	Mean +/- SD	Min-Maks(Median)	n (det. Freq)	Remark	Reference
Arctic	Faroe Islands	2004	0.2			WWTP	(Kallenborn et al., 2004)
Europe	Finland	2004	64.6	<LOQ - 68.00	3	Landfill	(Kallenborn et al., 2004)
Europe	Finland	2004	2.9	2.61 - 3.09	3	WWTP	(Kallenborn et al., 2004)
Europe	Germany	2009		<0.39 - 1,356.00	20	Landfill	(Busch et al., 2010)
Europe	Norway	2004	1.64	1.00 - 2.60	3	WWTP	(Kallenborn et al., 2004)
Europe	Sweden	2012-2015	1.9	3.7		WWTP	(Eriksson et al., 2017)
Europe	WWTP along River Elbe	2007	8.23	0.00 - 25.90 (5.10)	9 (100 %)	WWTP (9 wwtp, 18 samples)	(Ahrens et al., 2009b)
North America	San Francisco	2009	6.00 ± 6.50			WWTP	(Houtz et al., 2016)
North America	San Francisco	2014	2.70 ± 1.50			WWTP	(Houtz et al., 2016)
North America	USA (three temperate zones)	2013-2014	231.00 ± 577.33	3.44 - 3,410.00 (41.05)	87 (100 %)	Landfill (Ref organizes data based on climate zone and age)	(Lang et al. 2017)

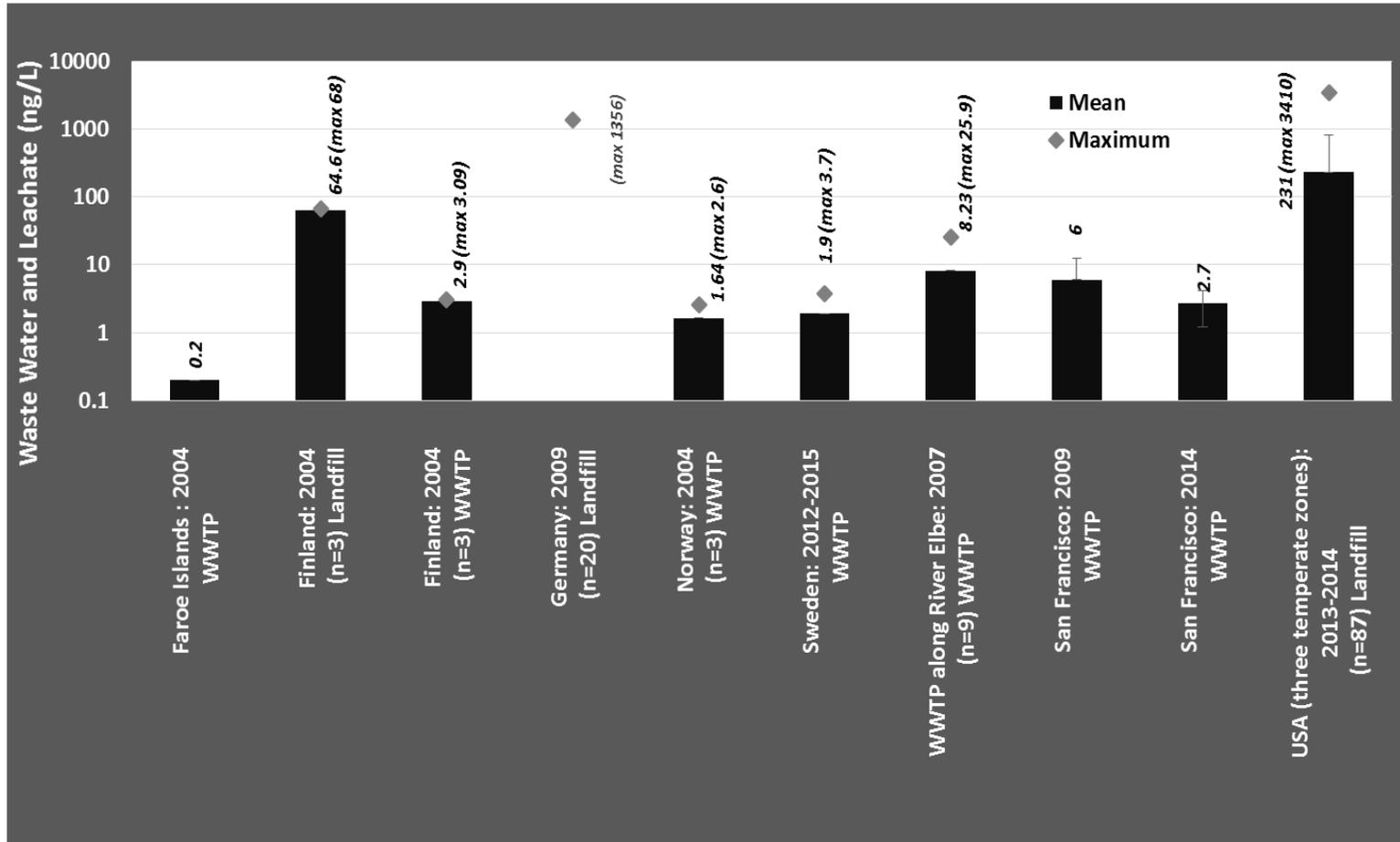


Figure 16. Environmental concentrations of PFBS in waste water and leachate samples (ng/L).

## 4.5 Summary and Discussion of environmental distribution

The chemical properties of PFBS indicated that it is anticipated to be mainly present in aquatic media in the environment. In particular the high water solubility (miscible), extremely low  $K_{ow}/D_{aw}$  (indicating negligible partitioning to air), and the log  $K_{oc}$  value of 2.2 (implying that in soil containing 1% organic carbon the concentration per L water is similar to per kg soil), all collectively indicate PFBS will predominantly be transported by water. In the case of continuous or increasing emissions, PFBS will likely accumulate in water bodies, globally.

These expectations based on physical-chemical properties are largely supported by the literature review of monitoring data. PFBS was ubiquitously reported in oceanic/marine water samples, surface fresh water samples, and drinking water samples. It was noticeably less present in soil, sediment and air samples; however, there are noticeably fewer data these media compared to aquatic and biological media.

The affinity of PFBS for the water phase is also evident by the general trace concentrations being observed in many (though not all) aquatic biota samples. Trace concentrations were observed for the majority of marine, freshwater and terrestrial biota. For vegetation and plants there were relatively elevated concentrations. This is likely accounted for by PFBS mobility in water-soil systems, along with uptake through plant xylem.

## 4.6 Comparison with other PFAS

It is relevant to put this monitoring data in context with other regulated PFAS. In all of the studies included in this review of monitoring data, data for these and other PFAS have also been reported. However, comparing the concentrations on a study-by-study basis is complicated by the temporal changes in emission levels. Therefore, the data in these monitoring studies are first considered on the basis of temporal trends.

### 4.6.1 Temporal trends

PFBS was largely introduced into the market as a replacement chemical for PFOS (Olsen et al., 2009). It is anticipated, therefore, that as PFOS use has declined, that PFBS emissions have increased. Corresponding to this, as is presented in this section, several studies have reported that PFBS concentrations are increasing with time, and, unlike previously, several other recent studies have reported PFBS to be the dominating PFAS present in their monitoring study.

*Human blood.* Glynn et al. (2012) reported that over a time series from 1996-2010, PFOS in blood could be seen to be decreasing over time, but replacement substances like PFBS and PFHxS increased by 11% and 8.3% per year, respectively.

*Biota.* The first known measurement of PFBS in biota dates back to 2005, in a study on harbor Seals (van de Vijver et al., 2005). PFBS was rarely reported in Arctic marine

biota in samples prior to 2012, but is more common in more recent samples, particularly in polar bears (Section 4.4.2.1). Further indication that PFBS may be rising while PFOS levels are sinking is a time series observed in dolphin livers in the South China Sea, which reported the ratio of PFBS/PFOS concentrations in the liver has increased from 2002 to 2014 (Lam et al., 2016).

*Water.* The emergence of PFBS in the environment is particularly noticeable in water monitoring studies. In a global survey of surface water from 2016, both PFBS and PFOS were detected in all samples, however, PFBS was significantly higher in concentration, with the median PFBS/PFOS ratio being 3.9 (Pan et al. 2018). A recent survey of surface water in Northern Europe, with sampling in 2013, found PFBS to be the dominating PFAS, contributing 21% of the sum PFAS (Nguyen et al. 2012). Similarly, a survey of European and Chinese rivers from 2013-2014 found PFBS to be the dominating PFAS (average 15.6 ng/L), with PFOA (4.8 ng/L) and PFPeA (4.7 ng/L) in second and third place (Heydebreck et al., 2015). In the South China Sea, PFBS was one of the major PFAS analysed, contributing 21% of the total concentrations, along with PFOA (~26%) and PFOS (~20%). In the Bohai Sea, PFBS was the third most abundant PFAS, after PFOA and PFHexA (Chen et al. 2016). A study in Chinese rivers in 2012 found PFBS to be the third largest contributor (Pan et al. 2014).

*Drinking water.* A study on drinking water from Brazil, France and Spain (Schwanz et al. 2016) reported that PFBS was one of the most frequently detected PFAS at 27.2% of samples, along with PFOS (100%), PFHpA (51.3%) and PFOA (23.0%). A global survey found similar results, with PFBS being the third most frequently detected PFAS in bottled water (47%) and tap water (88%) (Kabore et al. 2018).

*Source zones.* Increasing emissions of PFBS are noticed at source areas as well. Near a PFAS production facility in the Netherlands, PFBS was the dominating PFAS in both river samples (12-27 ng/L) and drinking water (0.5-19 ng/L) (Gebink et al. 2017). Near the PFAS production facility at Tangxun Lake, China, the two most dominating PFAS in water were PFBA and PFBS, at means of 4770 and 3660 ng/L, respectively

*WWTP and Landfills.* In a recent survey of WWTP in Sweden, PFBS, PFOS, and PFHxS had similar concentrations (1.9 ng/L, 1.9 ng/L, and 1.5 ng/L, respectively) (Eriksson et al. 2016). In San Francisco in 2014, PFBS was not the most dominating, but was emitted on average 2.7 ng/L, whereas PFOS and PFHxS were at 13 and 4.8 ng/L respectively.

Hence the most recent data collectively gives an indication that PFBS is one of the PFAS that is becoming the most commonly emitted, and is increasing in various environmental media, though in water in particular. If PFBS emission continue to increase, it follows that concentration in water samples and other environmental media would increase.

## 4.6.2 Maximum Concentrations

As an approximate indicator of the extent of PFBS contamination in different environmental media compared to other PFAS substances, maximum PFBS concentrations reported in this compilation are compared with those in previous compilations that were used to form the basis of regulations. These compilations include:

- 1) **PFOS (2004)**: Swedish Chemicals Agency and Swedish EPA (2004). PERFLUOROOCTANE SULFONATE (PFOS): Dossier prepared in support for a nomination of PFOS to the UN-ECE LRTAP Protocol and the Stockholm Convention.
- 2) **PFOA (2013)**: BAuA (2013). Annex XV Dossier. Proposal for identification of a substance as a CMR1a or 1b, PBT, vPvB or a substance of an equivalent level of concern. Substance Name(s): Pentadecafluorooctanoic Acid (PFOA). EC Number(s): 206-397-9. CAS Number(s): 335-67-1
- 3) **PFDA (2016)**: Swedish Chemicals Agency and German Environment Agency (2016). Annex XV Dossier. Proposal for identification of a substance as a CMR1a or 1b, PBT, vPvB or a substance of an equivalent level of concern. Substance Name(s): Nonadecafluorodecanoic acid (PFDA) and its sodium and ammonium salts.
- 4) **PFHxS (2018)**: UNEP (2018). Perfluorohexane sulfonic acid (CAS No: 355-46-4, PFHxS), its salts and PFHxS-related compounds. ADDITIONAL INFORMATION. Prepared by the intersessional working group on PFHxS, its salts and PFHxS-related compounds. Persistent Organic Pollutants Review Committee. September 2018.

One caveat with this comparison is that neither the PFBS compilation in this report considers all published literature reports, and many of the compilations cited in the above references may be similarly incomplete (or outdated). This comparison of maximum concentrations is therefore just considered a qualitative comparison, and is not a quantitative presentation of actual maximum concentrations. This comparison for aquatic media is presented in Table 19 and for arctic biota in Table 20.

Table 19. Comparison of maximum concentrations of PFBS, PFHxS, PFOS, PFOA and PFDA in various compilations for aquatic media (ng/L).

Sample type	PFBS	PFHxS	PFOS	PFOA	PFDA
Marine water	1.48	5.6	0.056	-	-
Arctic water	2.15	24	-	0.21	19
Fresh water	1457	978.5	138	-	0.85
Drinking water	97.8	1770 (second max: 36)	63	-	-
WWTP effluent	26	5689	5290	1050	35
Landfill leachate	3410	16000	-	-	55.1
Refs	<i>This report</i>	<i>PFHxS (2018)</i>	<i>PFOS (2004)</i>	<i>PFOA (2013)</i>	<i>PFDA (2016)</i>

As evident from Table 19, the maximum concentration for PFBS in freshwater (1457 ng/L) is highest amongst the considered PFAS compilations, followed by PFHxS at 978.5 ng/L. PFBS had the second highest maximum concentration for drinking water (97.8 ng/L), due to the maximum for PFHexS being 1770 ng/L. However, this is an outlier as the second highest value for PFHxS was 35 ng/L. There were several drinking water samples of PFBS containing more than 35 ng/L in this compilation, so another metric could have said PFBS is the more contaminating in drinking water than PFHxS. The maximum arctic fresh water concentration for PFAS at 2.15 ng/L is larger than PFOA (0.21 ng/L), but not as large as maximum values for PFHxS (24 ng/L) and PFDA (19 ng/L). The maximum concentration in non-Arctic marine water for PFBS at 1.48 ng/L have been report is larger than PFOS (0.056 ng/L) but not PFHxS (5.6 ng/L). PFBS can therefore be considered to be reaching or to have reached concentrations in aquatic media that are similar or higher than those previously observed for regulated PFAS substances, during the time they were becoming regulated.

Table 20. Comparison of maximum concentrations of PFBS, PFHxS, PFOS, PFOA and PFDA in various compilations for arctic biota (ng/g ww).

Sample type	PFBS	PFHexS	PFOS	PFOA	PFDA
Polar Bear Liver	0.04	> 500	4000	36	103
Glaucus Gull Eggs	<0.08	1.23			
Mink Liver	0.33	4			
Ringed seal liver	<0.002	nd - 3	1.01		2.5
<i>Refs</i>	<i>This report</i>	<i>PFHxS (2018)</i>	<i>PFOS (2004)</i>	<i>PFOA (2013)</i>	<i>PFDA (2016)</i>

As evident from Table 20, though PFBS is appearing in arctic biota, it is currently at much smaller concentrations than observed for other PFAS (for which the data for the same media is available). For instance, for polar bear liver, the current maximum concentration for PFBS is 0.04 ng/L, which is less than the maximum observed for PFOS (4000 ng/L), PFHxS (>500 ng/L), PFOA (36 ng/L) and PFDA (ng/L).

It is concluded from this quick, qualitative comparison that in the short term PFBS has the potential to contaminate water resources more so than PFHexS, PFOS, PFOA and PFDA has. Over the short term in arctic biota, it is unlikely PFBS will reach the same levels as PFHexS, PFOS and PFOA attained in previous studies.

## 5 Data indicating potential for long-range transport

PFOS and PFHxS have been shown to contaminate the Arctic through long-range transport. It can be expected simply based on read-across from the physicochemical properties that PFBS should also contaminate the Arctic. For extremely persistent substances, the two key critical parameters to predict long range transport is the Kaw and the Koa (Meyer and Wania, 2007); though, as discussed in section 2 for ionic substances like PFAS, one should use the Daw rather than Kaw, and Koc,a rather than

Koa (Armitage et al. 2009). Recalling from Table 2, the log K<sub>oc</sub> values for PFBS (4.8) is very similar to PFHxS (5.0) and PFOS (4.7). The log D<sub>aw</sub> values at pH 8 for PFBS (-14.5) are considered extremely low, similar to PFHxS (-13.8) and PFOS (-13.1), such that volatilization from water to air for all substances is negligible. Therefore this combination of physical-chemical properties implies that PFBS will reach and accumulate in the Arctic under steady state emissions, similar to PFOS and PFHxS.

Supporting this expectation is the large number of measurements that have found PFBS in the Arctic and Antarctic regions, where it is commonly found in Arctic biota and Antarctic water samples (Section 4.4.5.1 and 4.6.2). The major difference with PFBS regarding the arctic presence of PFBS compared to PFHxS and PFOS is that PFBS is less present in Arctic (Section 4.4.2.1 and 4.2.6), where it is only found in a few samples with considerable levels. This is related to the lower anticipated bioaccumulation potential of PFBS compared to longer chain PFAS, as described in pharmacokinetic studies (Olsen et al. 2009) and in Section 6.

The ubiquitous presence water samples in general (Sections 4.4.4 to 4.4.5) is an additional indicator of PFBS being able to undergo long range transport via the water phase. It was found in all marine (oceanic) samples, both near shore and far at sea (Section 4.4.4). It is also found in remote freshwater environments and even groundwater (4.4.5.3 and 4.4.5.4). PFBS' ubiquitous presence in drinking water and bottled water, at locations near and far from PFBS sources, is another indicator for long range transport. To reach drinking water, PFBS has to first be transported from the point of emission to the source of the drinking water (raw water), and then it would have to survive drinking water production. Though not all of the drinking water treatment preparation steps were considered individually in section Section 4.4.5.5, collectively they would include some kind of filtration (e.g. bank filtration, sand filtration), and in many cases involve more advanced filtration (e.g. activated carbon) or oxidation processes (like ozonation). Studies of PFAS during drinking water production have indicated conventional methods are not effective at PFAS removal (Rahman et al. 2014); thereby, PFAS removal from drinking water requires dedicated (and costly) setups.

## 6 Bioaccumulation - Field Data

The presence of PFBS in biota was presented in Section 4.4.2, and in humans in 4.4.5. It appears that PFBS can be quantified in several biological matrices. The concentrations in these matrices, however, are in general less than observed for longer chain PFAS substances, like PFHxS and PFOS, as discussed in section 4.6.2.

There have been several studies that indicate that PFBS is rapidly excreted after introduction, for instance in rats (Olsen et al., 2009b) and cows (Kowalczyk et al., 2013); in humans half-lives in blood/plasma up to 46 days have been measured (Olsen et al, 2009). However, if animals and humans are continuously exposed to increasing environmental concentrations of PFBS, the excretion pathway is less relevant, as biota would reach some equilibrium with the exposure concentrations.

The enrichment of PFBS in plants is more substantial than accumulation in animals. This is indicated by the relatively high concentrations of PFBS reported in plants grown on PFAS contaminated soil, compared to other biota. This is relevant for exposure considerations, as it indicates that humans and animals can be exposed to PFBS both through drinking water and vegetation in PFAS contaminated areas, particularly farmland.

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## Appendix

Table A1. Latin names of biota presented in this report

Common Name	Latin Name
Black crappie	<i>Pomoxis nigromaculatus</i>
Black guillemot	<i>Cepphus grylle</i>
Bluegill	<i>Lepomis Macrochirus</i>
Carp	<i>Cyprinus carpio</i>
Catfish	<i>Siluriformes</i>
Celery	<i>Apium graveolens var. Dulce</i>
Chinese bitterling	<i>Rhodeus sinensis Gunther</i>
Cod	<i>Gadus morhua</i>
Common eider	<i>Somateria mollissima</i>
Common gull	<i>Larus vanus</i>
Cow	<i>Bos taurus</i>
Crucian	<i>Carassius cuvieri</i>
Earthworms	<i>Lumbricidae</i>
European shag	<i>Phalacrocorax aristotelis</i>
Freshwater mussel	<i>Lamellibranchia</i>
Glaucus gull	<i>Rissa tridactyla</i>
Gobies	<i>Ctenogobius giurinus</i>
Green turtle	<i>Chelonia mydas</i>
Guillemot	<i>Uria aalge</i>
Harbor porpoise	<i>Phocoena phocoena</i>
Hawksbill turtle	<i>Eretmochelys imbreicata</i>
Herring	<i>Clupea harengus membras</i>
Herring Gull	<i>Larus argentatus</i>
Kemp's ridley turtle	<i>Lepidochelys kempii</i>
Killer whale	<i>Orcinus orca</i>
Kittiwake	<i>Larus hyperboreus</i>
Lake saury	<i>Coilia mystus</i>
Lake shrimp	<i>Macrobrachium nipponense</i>
Leatherback turtle	<i>Dermochelys coriacea</i>
Loggerhead turtle	<i>Caretta caretta</i>
Mink	<i>Neovison vison</i>
Minnow	<i>Hemiculter leucisculus</i>
Mongolian culter	<i>Culter mongolicus</i>
Mudfish	<i>Oriental weatherfish</i>
Pea	<i>Pisum sativum var. Macrocarpon</i>
Pearl mussel	<i>Lamellibranchia</i>
Pilot whale	<i>Globicephala melas</i>
Polar bear	<i>Ursus maritimus</i>

<b>Common Name</b>	<b>Latin Name</b>
Pumpkinseed	<i>Lepomis gibbosus</i>
Radish	<i>Raphanus sativus</i>
Ringed Seal	<i>Pusa hispida</i>
Shark	<i>Sphyrna tiburo or Rhizoprionodon terraenovae</i>
Silver carp	<i>Hypophtha Imichthys molitrix</i>
Sprat	<i>Sprattus sprattus</i>
Tilapia	<i>Tilapia</i>
Tomato	<i>Lycopersicon lycopersicum</i>
White shrimp soft tissue	<i>Exopalaemon</i>
Whitebait muscle	<i>Reganisalanx brachyrostralis</i>



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