Norwegian University of Life Sciences
Faculty of Veterinary Medicine and Biosciences
Department of Chemistry, Biotechnology and
Food Science

Master Thesis 2016
60 credits

Occurrence of Selected Poly- and Perfluoroalkyl Substances (PFAS) in Arctic Freshwater: *a Case Study from Svalbard*

Forekomst av utvalgte poly- og perfluoralkylforbindelser (PFAS) i Arktisk ferskvann: *en studie fra Svalbard*

Jøran Solnes Skaar

Preface

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This master thesis in Chemistry was written at the Department of Chemistry, Biotechnology and Food Sciences (IKBM) at the Norwegian University of Life Sciences (NMBU) in Ås, Norway, and the Department of Arctic Technology at the University Centre in Svalbard, Longyearbyen, Svalbard.

Keywords: Perfluoroalkyl substances (PFAS), Arctic, Svalbard, Lake, Freshwater

Norwegian University of Life Sciences

Department of Chemistry, Biotechnology and Food Sciences.

The University Centre in Svalbard, Department of Arctic Technology

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Ås, 11.04.2016

Acknowledgements

I would like to thank supervisor Professor Roland Kallenborn for giving me the opportunity to work with this exciting subject, which included fieldwork in beautiful Arctic landscapes and analysis using advanced instrumentation. In addition, thank you for the encouraging words and advice during my work.

Morover, I am hugely grateful to everyone else for their contributions. I would like to thank you all:

My co-supervisors Associate Professor Tone Normann Asp and Professor Jan Ludvig Lyche for their support, input and for letting me use laboratories and instrumentation at the Department of Food Safety and Infection Biology (MatInf).

Erik Magnus Ræder for method development and instrument training at the Department of Food Safety and Infection Biology (MatInf).

Stig Magnus Lunde, Lutz Ahrens, Jelena Rakovic and Siri Axelson for fieldwork cooperation. In addition, methodical advice from Lutz Ahrens and laboratory collaboration with Stig Magnus Lunde.

Tatiana Drotikova and Jessica Bosch for facilitating the UNIS laboratory in short and hectic working periods. In addition, for sample collection in March 2014 by Jessica Bosch.

The University Centre in Svalbard (UNIS) for letting me use laboratory facilities, and a special thanks to the Logistics department for fieldwork advice and logistical assistance.

The laboratory at Statoil Kollsnes processing plant for letting me use the laboratory and selected instrumentation for water analysis.

This study was funded by the following projects; FluoroImpact (Svalbard Environmental Protection Fund: 14/103), Internal support UNIS project SvalPOP and the Arctic monitoring and assessment program (AMAP).

Abstract

Polyfluoroalkyl and perfluoroalkyl substances (PFASs) is a diverse group of fluorine-containing organic compounds containing the perfluoro moiety within its structure and different functional groups. PFASs have been found ubiquitously in the aquatic environment, even at remote locations such as the Arctic. A recent study found high concentrations of short-chain PFASs in muscle and liver of Arctic Char *(Salvelinus alpinus)* from Lake Linnévatnet. All PFASs are very persistent, long-chain PFASs tend to bioaccumulate in the food web and several adverse effects have been observed for some compounds. Two major transport pathways of PFASs to the Arctic have been suggested; direct oceanic transport of ionic PFASs and long-range atmospheric transport and oxidation of neutral precursor compounds.

In this study, samples of lake water were collected in March 2014, April 2015 and June 2015 from Lake Linnévatnet in Svalbard. In addition, snow, meltwater and river water was collected in June 2015. As a reference for local pollution, samples were collected downstream a firefighting training site (FFTS) at Svalbard Airport in November 2014 and June 2015. Samples were extracted by weak anion-exchange (WAX) solid phase extraction (SPE) and analysed for 18 target PFASs by liquid chromatography coupled with tandem mass spectroscopy (HPLC-(-)ESI-MS/MS).

The limits of quantification (LOQs) in a two-liter water sample ranged from 0.006 ng L^{-1} for perfluorohexane sulfonate (PFHxS) to 0.68 ng L^{-1} for perfluorobutanoic acid (PFBA). A contamination issue later identified was the reason for the high LOQ for PFBA. Procedural recoveries were good for the ionic PFASs, with mean absolute recoveries in the range of 76 to 106 % for native PFCAs, PFSAs and 6:2 FTSA in sample matrix, and 66 to 94 % for their internal standards. Low recoveries obtained for the neutral PFASs excluded them for further analysis. Mean between-laboratory difference of parallel samples collected in June 2015 used to assess reproducibility showed a difference below 30 % for most compounds, except PFBA, PFHxA and PFUnDA, which was comparable to reproducibility reported in a recent inter-laboratory comparison.

Sum PFASs in Lake Linnévatnet was in the range of 4.7 – 5.1 ng L^{-1} in March 2014, 1.6 – 8.3 ng L^{-1} in April 2015 and 0.49 – 1.7 ng L^{-1} in June 2015. Higher ΣPFAS in the winter indicated a seasonality in concentrations. Samples were categorized in five distinct groups based on their composition profiles using principal component analysis (PCA). Linear regression in addition to congener ratios was used to identify patterns, and used to discuss possible source origins. The short-chain perfluoroalkyl carboxylic acid PFBA was the dominating compound in lake water, meltwater and river water, contributing approx. 50 percent of the total PFAS concentration. Samples from March 2014 where dominated by the long-chain perfluorooctanoic acid (PFOA) and perfluorononanoic acid (PFNA) was the dominating compound in snow. Runoff downstream FFTS had high total PFAS concentrations during melt in June, where perfluorooctane sulfonate (PFOS) was dominating, and with no runoff in November the total PFAS concentrations were lower and dominated by perfluoroheptanoic acid (PFPeA) and perfluorohexanoic acid (PFHxA). Ratios between PFOA/PFNA in surface water samples were similar as reported elsewhere in the Arctic, which indicated long-range atmospheric transport as the main source. Significant linear correlation between PFBA, PFOA and PFNA indicated a common transport route.

Norsk sammendrag

Polyfluoralkyl og perfluoralkyl forbindelser (PFAS) er en mangfoldig gruppe av fluorholdige organiske forbindelser som inneholder perfluor-gruppen som en del av strukturen samt ulike funksjonelle grupper. PFASer finnes omtrent over alt i det akvatiske miljøet, også i villmarkspregede områder langt fra lokale kilder som i Arktis. I en nylig studie ble høye konsentrasjoner av kortkjedete PFASer funnet i muskel og lever hos Røye *(Salvelinus alpinus)* fra Linnévatnet. Alle PFASer er veldig persistent mot nedbrytning, langkjedete er kjent for å bioakkumulere og flere negative helseeffekter har blitt registrert for noen av forbindelsene. Hovedsakelig to transportmekanismer til Arktis har blitt foreslått, direkte transport av ioniske PFAS via havstrømmer og marine aerosoler og transport forløperforbindelser gjennom atmosfæren som oksideres til perfluorerte syrer.

I denne studien ble det tatt prøver av innsjøvann fra Linnévatnet på Svalbard i mars 2014 og april 2015, i juni 2015 ble det i tillegg tatt snø-, elv- og smeltevannsprøver. Som en referanse for lokal forurensning, ble det tatt prøver nedstrøms et brannøvingsfelt ved Svalbard lufthavn i november 2014 og juni 2015. Prøvene ble ekstrahert ved hjelp av fastfaseekstraksjon (SPE) med en svak anion-bytter som sorbent (WAX) og analysert for 18 ulike PFAS forbindelser ved hjelp av væskekromatografi og tandem massespektroskopi (HPLC-(-)ESI-MS/MS).

Kvantifiseringsgrensen i en to liter vannprøve var mellom 0.006 ng L^{-1} for PFHxS til 0.68 ng L^{-1} for PFBA. En kontaminasjonskilde som senere ble oppdaget var grunn til den høye kvantifiseringsgrensen for PFBA. Metodens gjenvinningstall var gode for ioniske PFAS, med absolutt gjenvinning fra 76 til 106 % PFCAer, PFSAer og 6:2 FTSA tilsatt i prøvematrix, og 66 til 94 % for internstandardene. På grunn av lave gjenvinningstall ble de nøytrale PFASene ekskludert fra videre analyse. Gjennomsnittlig forskjell mellom resultater fra to ulike laboratorier for parallellprøver tatt i juni ble brukt for å undersøke reproduserbarhet. Gjennomsnittlig forskjell var mindre enn 30 % for de fleste komponenter, med unntak av PFBA, PFHxA og PFUnDA. Dette var sammenlignbart med reproduserbarhet rapportert i nylige sammenlignende laboratorieprøvinger.

Sum PFASs i Linnévatnet var mellom 4,7 til 5,1 ng L^{-1} i mars 2014, 1,6 til 8,3 ng L^{-1} i april 2015 og 0,49 til 1,7 ng L^{-1} i juni 2015. Høyere ΣPFAS observert om vinteren kan indikere sesongvariasjoner i konsentrasjonene. Prøvene ble kategorisert i fem ulike grupper etter deres komposisjonsmønster ved bruk av prinsipalkomponentanalyse (PCA). Lineær regresjon og forhold mellom komponenter ble brukt til å identifisere mønster, som ble brukt til å diskutere mulige kilder. Den kortkjedete perfluorkarboksylsyren PFBA dominerte innsjø-, elv og smeltevannsprøver, hvor den bidro ca. 50 % av total PFAS konsentrasjon. Prøvene fra mars 2014 var dominert av langkjedete perfluorkarboksylsyrer som PFOA, og PFNA dominerte i snøprøver. Avrenning fra brannøvingsfeltet ved flyplassen i juni inneholdte høye konsentrasjoner av total PFAS, hvor PFOS dominerte. I november var konsentrasjonene lavere, og kortkjedete PFPeA og PFHxA dominerte. Forholdet mellom PFOA/PFNA i prøver av overflatevann var tilsvarende det som tidligere er rapportert fra andre steder i Arktis, som indikerte at langtransport i atmosfæren trolig er hovedkilden. Signifikant lineær korrelasjon mellom PFBA, PFOA og PFNA indikerte en felles transportrute for disse.

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Abbreviations

AFFF	Aqueous film forming foams (firefighting foams)
AJS ESI	Agilent jet stream electrospray ionization
Br-PFOS	Branched isomers of PFOS.
FASA	Perfluoroalkyl sulfonamides
FASE	Perfluoroalkyl sulfonamidoethanols
FFTS	Firefighting training site
FTIR	Fourier transform infrared spectroscopy
FTOH	Fluorotelomer alcohol
HPLC	High performance liquid chromatography
IDL	Instrument detection limit
ISTD	Internal standard (for quantification of target compounds)
LC	Liquid Chromatography
LOQ	Limit of quantification
LRAT	Long-range atmospheric transport
m.a.s.l	Meters above sea level (terrain altitude)
m/z	Mass/charge ratio
MDL	method detection limit
MeOH	Methanol (CH_3OH)
MRM	Multiple reaction monitoring (specific m/z selected in first quadrupole, collided in collision cell, specific m/z selected in second quadrupole).
MS	Mass spectrometry
MS/MS	tandem mass spectrometry
NA	Not available/analysed
ND	Not detected
ng	Nanogram (10^{-9} gram)
NH_4OAc	Ammonium acetate (CH_3COONH_4)
NMBU	Norwegian University of Life Sciences
PCB	Polychlorinated biphenyls.
PE	polyethylene (LD – low density, HD – high density)
PFAA	Perfluoroalkyl acids (include PFCAs and PFSAs)
PFAM	Perfluoroalkyl amides
PFAS	Poly- and perfluoroalkyl substances
PFC	Perfluorocarbons, aliphatic compounds exclusively containing Fluor and Carbon.
PFCA	perfluoroalkyl carboxylic acids/carboxylates
PFSA	Perfluoroalkyl sulfonic acids/sulfonates
Pg	Picogram (10^{-12} gram)
POCIS	Polar Organic Chemical Integrative Samplers
POP	Persistent organic pollutants
PP	Polypropylene
QqQ	Triple quadrupole mass spectrometer (Q is a DC/RF mass filter, q is a RF only quadrupole/hexapole/octapole used as a collision cell)
ROS	Reactive oxygen species
RSTD	Recovery standard (to determine recovery of ISTD)
SLU	Swedish University of Agricultural Sciences
SIP	Sorbent-impregnated polyurethane foam disk
SPE	Solid-phase extraction
UNIS	The University Centre in Svalbard
UPLC	Ultra-high Performance Liquid Chromatography
WAX	Weak anion-exchange resin

1 Introduction

1.1 Terminology of studied PFASs

Polyfluoroalkyl and perfluoroalkyl substances (PFASs) is a diverse group of fluorine-containing organic compounds found ubiquitously in the aquatic environment. Most environmental studies on PFASs have been published in the last decade, and several different acronyms and terminologies have been used. Buck et al. made an effort to harmonize existing terminology and acronyms for polymeric and non-polymeric PFASs (Buck et al. 2011). Terminology by Buck et al. is as far as possible used in this study.

Polyfluoroalkyl and perfluoroalkyl substances (PFASs) as a compound class is defined as compounds containing the perfluoro moiety (C_nF_{2n+1}) within its structure. PFCs have been used in many previous studies as an acronym for these substances. This term however should be avoided since PFCs also refer to perfluorocarbons, exclusively containing carbon and fluorine, known for their potential as greenhouse gases (Buck et al. 2011).

Table 1.1. Target analytes in this study.

Analyte	Acronym	CAS#	Formula
PFCAs			
Perfluorobutanoic acid	PFBA	375-22-4	$F(CF_2)_3COOH$
Perfluoropentanoic acid	PFPeA	2706-90-3	$F(CF_2)_4COOH$
Perfluorohexanoic acid	PFHxA	307-24-4	$F(CF_2)_5COOH$
Perfluoroheptanoic acid	PFHpA	375-85-9	$F(CF_2)_6COOH$
Perfluorooctanoic acid	PFOA	335-67-1	$F(CF_2)_7COOH$
Perfluorononanoic acid	PFNA	375-95-1	$F(CF_2)_8COOH$
Perfluorodecanoic acid	PFDA	335-76-2	$F(CF_2)_9COOH$
Perfluoroundecanoic acid	PFUnDA	2058-94-8	$F(CF_2)_{10}COOH$
Perfluorododecanoic acid	PFDoDA	307-55-1	$F(CF_2)_{11}COOH$
PFSAs			
Perfluorobutanoic sulfonate	PFBS	29420-49-3 (potassium salt)	$F(CF_2)_4SO_3^- K^+$
Perfluorohexanoic sulfonate	PFHxS	3871-99-6 (potassium salt)	$F(CF_2)_6SO_3^- K^+$
Perfluorooctanoic sulfonate	PFOS	1763-23-1 (sodium salt)	$F(CF_2)_8SO_3^- Na^+$
FTSAs			
6:2 Fluorotelomer sulfonate	6:2 FTSA	27619-97-2	$F(CF_2)_6(CH_2)_2SO_3^- Na^+$
FASAs			
Perfluorooctane sulfonamide	FOSA	754-91-6	$F(CF_2)_8SO_3NH_2$
N-methyl-perfluorooctane sulfonamide	MeFOSA	31506-32-8	$F(CF_2)_8SO_3NHCH_3$
N-ethyl-perfluorooctane sulfonamide	EtFOSA	4151-50-2	$F(CF_2)_8SO_3NHCH_2CH_3$
FASEs			
N-methyl perfluorooctane sulfonamidoethanol	MeFOSE	24448-09-7	$F(CF_2)_8SO_3NH(CH_3)CH_2CH_2OH$
N-ethyl perfluorooctane sulfonamidoethanol	EtFOSE	1691-99-2	$F(CF_2)_8SO_3NH(CH_2CH_3)CH_2CH_2OH$

Perfluoroalkyl substances are aliphatic compounds of which all hydrogens attached to carbon atoms, except those connected to a functional group, are replaced by fluorine (Buck et al. 2011). PFOS ($F[CF_2]_8SO_3H$) is an example of a perfluoroalkyl substance. Polyfluoroalkyl substances are defined as aliphatic compounds where all fluorine connected to at least one, but not all carbons, are replaced by fluorine (Buck et al. 2011). 6:2 FTSA ($F[CF_2]_6CH_2CH_2SO_3H$) is an example of a polyfluoroalkyl substance. *Perfluoroalkyl carboxylic acids* (PFCAs) and *perfluoroalkyl sulfonic acids*, sometimes referred to as the common term *perfluoroalkyl acids* (PFAAs), are for convenience referred to as acids in this study, even if they are likely to be highly or completely ionized in environmental matrices (Buck et al. 2011). Long chain PFASs are defined as PFSA with six or more perfluorocarbons ($F[CF_2]_nSO_3H$, $n \geq 6$) or PFCAs with seven or more perfluorocarbons

($F[CF_2]_nCO_2H$, $n \geq 7$) (Butt et al. 2010). Acronyms of PFAS-classes discussed in this paper are described in *Table 1.2*.

For this study 18 PFASs were selected as target analytes *(Table 1.1*. Target analytes in this study. *)*, chosen for their environmental relevance in aquatic samples (Ahrens et al. 2010) and based on findings in a previous study of PFASs in Arctic char *(Salvelinus alpinus)* at the same site (Garsjø 2013).

Table 1.2. Selected PFAS compound groups discussed in this study.
n = number of perfluorocarbons. Table adapted from Buck et al. (2011)

	Compound group	Acronym	$F(CF_2)_nR$, where R=	ECF / Telomer	Uses
Perfluoroalkyl acids (PFAAs). n = 3, ..., 17	Perfluoroalkyl carboxylic acids	PFCA	-COOH	E/T	Surfactants
	-carboxylates		$-COO^-$	E/T	
	Perfluoroalkyl sulfonic acids	PFSA	$-SO_3H$	E	Surfactants
	-sulfonates		$-SO_3^-$	E	
	Perfluoroalkyl fluorides	PASF	$-SO_2F$	E	Major raw material for surfactants and surface protection products.
	Perfluoroalkyl fluorids	PAF	-COF	E	Raw material for PFOA by ECF process, surfactants and surface protection products.
	Perfluoroalkyl iodides (Telomer A)	PFAI	-I	T	Raw material for surfactants and surface protection products.
	Perfluoroalkyl aldehydes and aldehyde hydrates	PFAL $PFAL*H_2O$	$-CHO$ / $-CH(OH)_2$	T	Intermediate environmental transformation product.
Perfluoroalkyl sulfonamido substances n = 4,..., 8	Perfluoro sulfonamides	FASA	$-SO_2NH_2$	E	Major raw material for surfactants and surface protection products.
	N-alkyl perfluoroalkyl sulfonamides	FASA	$-SO_2NH(R')$ $R' = C_mH_{2m+1}$ (m= 1,2,4)	E/T	Major raw material for surfactants and surface protection products.
	N-alkyl perfluoroalkyl sulfonamidoethanols	FASE	$-SO_2NH(R')CH_2CH_2OH$ $R' = C_mH_{2m+1}$ (m= 0,1,2,4)	E/T	Major raw material for surfactants and surface protection products.
	N-alkyl perfluoroalkyl sulfonamido acetic acids	FASAA	$-SO_2NH(R')CH_2COOH$ $R' = C_mH_{2m+1}$ (m= 0,1,2,4)	E/T	Intermediate environmental transformation product.
	Perfluoroalkyl amides	FAMs	$-CO_2NHR'$	E	Unintentionally produced as byproducts of the ECF-process. (Jackson et al. 2013)
Fluorotelomer substances n = 4, 6, 8, . . . , 18	Fluorotelomer iodides (Telomer B)	n:2 FTI	$-CH_2CH_2I$	T	Raw material for surfactants and surface protection products.
	Fluorotelomer olefines	n:2 FTO	$-CH=CH_2$	T	Raw material for surfactants and surface protection products.
	Fluorotelomer alcohols	n:2 FTOH	$-CH_2CH_2OH$	T	Major raw material for surfactants and surface protection products.
	Fluorotelomer aldehyes	n:2 FTAL	$-CH_2CH_2CHO$	T	Intermediate environmental transformation product.
	Fluorotelomer carboxylic acids	n:2 FTCA	$-CH_2COOH$	T	Intermediate environmental transformation product.
	Fluorotelomer unsaturated acids	n:2 FTUCA	$-CF=CHCOOH$	T	Intermediate environmental transformation product.
	Fluorotelomer sulfonic acids	n:2 FTSA	$-CH_2CH_2SO_3H$	T	Surfactant and environmental transformation product.

1.2 Physico-chemical properties and synthesis of PFASs

The physico-chemical properties of PFASs differs in many ways from the classic legacy-POPs; PFAAs found in the environment have low vapor pressures and high water solubility, in the order of a few to several thousand mg L^{-1} (Taniyasu et al. 2013b). PFCAs and PFSAs are usually found as anionic species at environmental pH-values in aqueous matrices because of their strong acidic properties. Cheng et al. (2009) estimated pK_a-values for perfluorooctane sulfonic acid (PFOS) and Perfluorooctanoic acid (PFOA) to be <1, Rayne et al. (2009) estimated pK_a-values for C_1-C_8 PFSAs to be in the range of -5.3 to -9.0 (Cheng et al., 2009; Rayne et al., 2009). According to Rayne et al., less than 10^{-9} % of PFSAs will exist as molecular species in a lake with a pH-value of 6.5 at these pK_a-levels. A study by Burns et al. determined $pK_a = 3.8 \pm 0.1$ for PFOA at environmentally relevant concentrations, suggesting a considerable amount exists as the protonated PFOA (Burns et al. 2008).

The high persistence of PFASs is due to shielding of carbon by the fluorine atoms in the perfluoroalkyl moiety along with the strong bonding between carbon and fluorine (approx. 460 kJ mol^{-1}), the strongest in organic chemistry, making PFASs very persistent to thermal and chemical attack (Kissa 2001).

One of major uses for PFAS has been as surfactants. Surfactant compounds combine molecules with a lyophobic (solvent-insoluble) and a lyophilic (solvent-soluble) part in order to reduce the surface tension between two liquids or between a liquid and a solid, and are used for several applications (Kissa 2001). The high electronegativity of fluorine in the perfluoroalkyl moiety makes it amphiphobic, meaning that it is *both* hydrophobic and lipophobic (Moody & Field 2000; Renner 2006). In fluoro-surfactants, this property combined with a hydrophilic (in aqueous medium) or a hydrophobic (in hydrocarbon or fluorocarbon medium) functional group further lowers the surface tension compared to non-fluoro surfactants, making fluoro-surfactants superior at much lower concentrations (Kissa 2001).

This amphiphobic property of the perfluorocarbon moiety has also been widely utilized in surface protecting coatings of material surfaces in order to make them repellent towards water, lipids and soil (Kissa 2001).

PFASs as a chemical group is almost exclusively of anthropogenic origin, but trifluoroacetic acid (TFA) also have natural sources (Frank et al. 2002). PFASs have been manufactured by two major synthesis routes; electrochemical fluorination (ECF) and the fluorotelomer process (Butt et al. 2010). *Figure 1.1* illustrates characteristics, starting materials, intermediates and typical products of the two processes.

Manufacture of PFCAs by the ECF process first began in 1947 and perfluorooctane sulfonyl fluoride (POSF) based production by mainly the 3M Company from the 1950s (Butt et al. 2010; Prevedouros et al. 2006). Briefly, the manufacture by the ECF process is done by electrolysis at voltages less than 8 volts of organic raw material (i.e. alkanecarbonyl- or alkanesulfonyl chlorides) immersed in anhydrous hydrofluoric acid (HF), where all hydrogen except some at functional groups are replaced by fluorine (Kissa 2001). Hydrogen gas is generated at the cathode, and fluorination takes place at the anode. Because of the free-radical nature of the reaction, carbon-carbon bonds are broken and rearranged, yielding a complex mixture of linear and branched isomers, shorter chain homologues and by-products (Buck et al. 2011). Commercial technical mixtures of PFOS consisted of approx. 70 % of the linear isomer and 30 % branched, of these eleven of the major isomers has been separated and elucidated by ^{19}F NMR (Arsenault et al. 2008).

Equation 1.1. Simplified reaction for ECF manufacture of PAF- and PASF-based raw material (Kissa 2001).

$$C_nH_{n+1}COCl + {}_{(2n+2)}HF \rightarrow C_nF_{n+1}COF + HCl + by-products$$

$$C_nH_{n+1}SO_2Cl + {}_{(2n+2)}HF \rightarrow C_nF_{n+1}SO_2F + HCl + by-products$$

Manufacture by fluorotelomer-based synthesis was developed by DuPont Company in the 1970s, and is today the major manufacture route for PFASs (Kissa 2001; Prevedouros et al. 2006). A perfluoroalkyl iodide (often pentafluoroethyl iodide) is reacted with tetrafluoro ethylene to form a perfluoroalkyl iodide (PFAI, referred to as Telomer A). Telomer A, also referred to as a "telogen", is reacted further with ethene, referred to as a "taxogen", to form a n:2 fluorotelomer iodide (Telomer B). Telomer B is used as a raw material for fluorotelomer-based surfactants, surface treatment and polymers (Buck et al. 2011). Fluorotelomer substances are named using X:Y numbering, e. g. 8:2 FTOH, where X is the number of perfluorocarbons and Y is the number of non-fluorinated carbons (Buck et al. 2011; Wang et al. 2014).

Equation 1.2. Simplified schematics of telomerization process (Kissa 2001).

$$A)\ F(CF_2)_2I\ (Telogen, "Telomer\ A") + \frac{(n-2)}{2} CF_2 = CF_2(Taxogen) \rightarrow F(CF_2)_nI\ ("Telomer\ B")$$

$$B)\ F(CF_2)_nI\ +\ CH_2 = CH_2\ \rightarrow\ F(CF_2)_nCH_2CH_2I \xrightarrow{hydrolysis} F(CF_2)_nCH_2CH_2OH$$

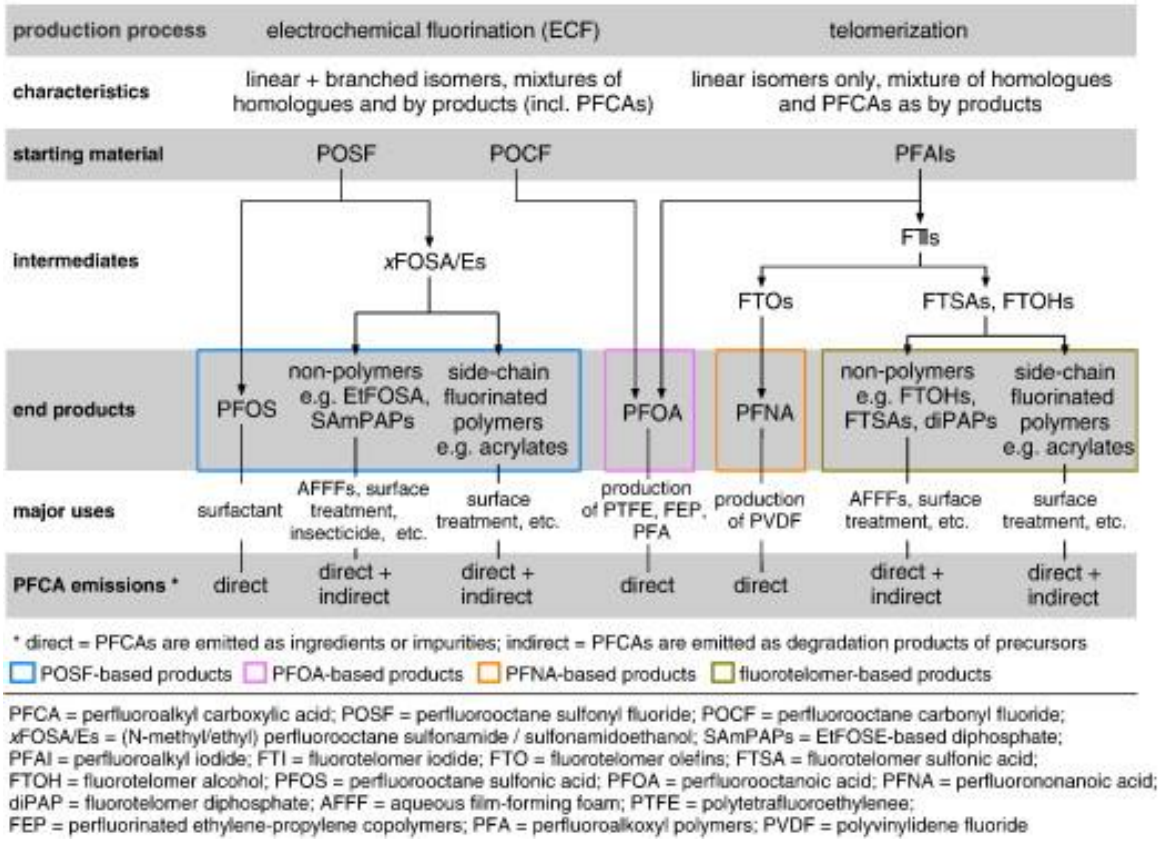

Figure 1.1. Schematic of different synthesis routes for PFASs.
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1.3 Environmental relevance

PFASs are found ubiquitously in the environment in matrices such as air, water, food, wildlife and humans, including in remote regions such as the Arctic (Ahrens 2011; Giesy & Kannan 2001; Jahnke et al. 2007; Taniyasu et al. 2005; Yamashita et al. 2004; Yamashita et al. 2005). In the Arctic food web for instance, levels of PFOS in Polar bears (*Ursus maritimus*) have been reported to be the highest of any species studied, with concentration levels similar to those reported for PCBs (Dietz et al. 2008). As a consequence, adverse effects such as reduced size of reproductive organs, reduction of bone mineral density, and disruption of endocrine and immune system have been observed (Dietz et al. 2008).

In contrast to the traditional POPs, PFASs does not bioaccumulate in lipid tissue because of their relatively high water solubility. Instead they bind to proteins in blood serum, and accumulate in blood-rich organs such as the liver, kidney and bile secretions. The longer chain PFASs have the highest potential for bioaccumulation (Butt et al. 2010; Dietz et al. 2008). Some PFASs have a very slow elimination rate from the human body, PFOA half-lives for serum/plasma elimination between 2.3 and 8.5 years have been reported (Post et al. 2012).

Several adverse effects of PFASs have been reported. Liver toxicity, disruption of the immune and endocrine systems and lipid metabolism, adverse neurobehavioral effects, neonatal toxicity, tumors in multiple organ systems (Lau et al. 2007; Post et al. 2012). Wielsøe et al studied the effects on endpoints related to oxidative stress and DNA damage in HepG2 cells. Effects of seven PFASs ubiquitously found in human blood and tissue (PFHxA, PFOS, PFOA, PFNA, PFDA, PFUnDA and PFDoDA) were studied. They found a dose dependent increase in in DNA strand breaks for PFHxA, PFOS, PFOA and PFNA, and increased ROS generation for all PFASs except PFDoDA. The carbon chain length did not seem to affect potential for oxidative stress, DNA damage or ROS generation for the PFSAs. For the PFCAs the chain length was found to some degree affect potency, with the highest effect for shortest carbon chains (Wielsøe et al. 2015).

In 2005 PFOS was classified as an animal carcinogen by the US EPA, and PFOA was classified as a likely carcinogen in 2006 (USEPA 2014).

Because of their high persistence in the environment, their ability to bioaccumulate, adverse health effects for human and wildlife and presence in remote regions indicating long-range transport, some PFASs have been and are being subject for increasing regulation. In Europe the use of PFOS was restricted from December 2007, with remaining permitted uses to be phased out by 2011 (EU 2006). In 2009 PFOS, its salts and PFOSF was listed to the Stockholm convention on Persistent Organic Pollutants annex. B after evidence for its persistence, tendencies for bio-accumulation, potential for long-range environmental transport and adverse effects on human and wildlife had been provided (UNEP 2009). Measures to restrict the production and use must be taken by participating parties. However, several acceptable applications are stated, i.e. in aviation hydraulic fluids. PFOA, its salts and PFOA-related compounds was recently proposed to be listed under the Stockholm convention (UNEP 2015).

After some long-chain PFASs have been regulated, they are being replaced with short-chain PFASs with similar structures, or compounds with fluorinated segments joined by ether linkages (Scheringer et al. 2014). Short-chain PFASs are assumed to be less bioaccumulative, however still persistent in the environment or have persistent degradation products. Because of this similar persistence, substitution of long-chain PFASs towards short chain PFASs will not reduce the amounts in the environment. Also, because some short-chain PFAS are less effective, larger quantities are required to provide the same performance. Not much information is available to the public about chemical structures, properties, use and toxicological profiles for the new fluorinated alternatives. Recently in the Madrid statement (Blum et al. 2015) and the Helsingør statement (Scheringer et al. 2014), several scientists and professionals have been stating their concern about this development.

1.4 Sources, LRAT and transformation of precursor PFASs

As a chemical group of high economic value, PFASs have been widely used for decades, and still are, in both industrial and consumer products (Renner 2006). They are predominantly used in surface treatment as water- and soil repellant (i.e. paper, textiles, leather, carpets and food contact material), in the fluoropolymer production, metal plating, fire-fighting foams, polishes and paints and other consumer materials (Renner 2006; Wang et al. 2013; Young et al. 2007).

One example of large volume use of PFASs is in aqueous film-forming foams (AFFF) used to extinguish hydrocarbon fires at airports, military bases, petroleum production sites among others (Moody & Field, 2000; Place & Field, 2012). Place and Field elucidated the structure of fluorochemicals in different AFFF cocentrates used by the US military, and found ten different classes of fluorochemicals, including anionic, cationic and zwitterionic surfactants with chains of 4 to 12 perfluorocarbons attached (Place & Field 2012). Emissions from use of AFFF at these sites after training and accidental spills have been known to leak into groundwater (Moody & Field, 2000). AFFF produced by 3M Company have contained several different compositions of PFAS throughout the last five decades. Between 1960 to early 1970s it contained mostly PFCAs, and PFSAs between 1970s until 2001 when 3M ceased production of POSF-based products (perfluorooctane sulfonfluoride) because of their tendency to bioaccumulate/magnify and their adverse effects (Place & Field, 2012). After the phase-out of POSF/PFOS based compounds and regulations on longer-chain PFCAs (3M 2000), the industry have changed to alternative poly- and perfluorinated compounds, many of which are still unknown to the public (Wang et al. , 2013).

Estimated historic POSF emissions in the period between 1972 and 2002 are in the range of 6800 to 45250 metric tons, the majority to the aquatic environment and a small amount into the air (Ahrens 2011; Paul et al. 2009). For C_4 – C_{14} PFCAs the historic emission estimates the time period 1951 to 2015 are between 2610 and 21400 metric tons (Wang et al. 2014). Emissions for PFOS and PFOA are assumed to be reduced because the voluntary phase-out of POSF based products in 2002 (3M 2000) and international and regional regulations (EU 2006; Scheringer et al. 2014; UNEP 2009), and decline in biota concentrations have been recorded at some locations (Butt et al. 2007).

Due to their high persistence and virtually no degradation, the final fate of PFAAs are burial in environmental sinks, which are defined as compartments with a long resident time. For PFASs sediment burial and transport to deep oceans have been identified as major sinks (Prevedouros et al. 2006). Sorption of PFAAs to sediment were found in a laboratory study to increase with sediment organic content, number of perfluoroalkyl moieties, the presence of the SO_3^- moiety, increasing aqueous Ca^{2+} and decreasing pH (Higgins & Luthy 2006). A similar conclusions was drawn from a field study (Ahrens et al. 2009b).

Despite the low vapor pressures and high water solubility of PFCAs and PFSA, they have been found in remote regions where no significant local sources exists (Shoeib et al., 2006; Xie et al., 2015). Several studies has suggested that they are transported through the atmosphere as the neutral more volatile precursor PFASs such as fluorotelomer alcohols (FTOHs), fluoro sulfonamidoethanols (FASEs) and fluoro sulfonamides (FASAs) (Shoeib et al. , 2006; Styler et al. , 2013; Taniyasu et al. , 2013; Xie et al. , 2015). The non-fluorinated part of the molecule of these precursor compounds can be degraded through photochemical-oxidation or microbial transformation to more persistent PFCAs and PFSAs respectively (D'Eon et al. , 2006; Shoeib et al. , 2006; Styler et al. , 2013). Direct transport of PFAAs to remote regions by oceanic currents and sea-spray aerosols is another suggested pathway; Prevedouros et al. estimated an oceanic transport to the Arctic of 2 – 12 tons/year for PFOA (Ahrens 2011; Armitage et al. 2009; Prevedouros et al. 2006). A study of an Arctic ice-cap found no correlation between PFAA concentration and sodium content, suggesting LRAT and transformation of semi-volatile precursors to be the primary source (Young et al. 2007).

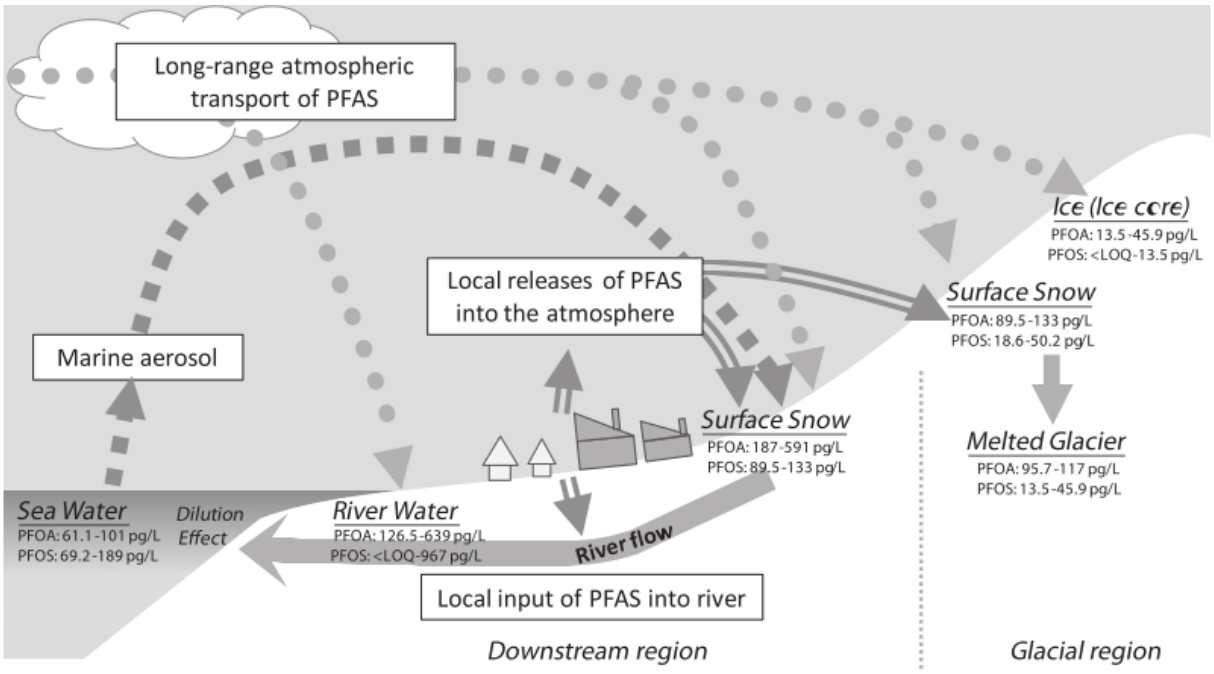


Figure 1.2. Schematics for suggested local and long-range transport of PFASs to the Arctic. Reprinted from (Kwok et al. 2013), with permission from Elsevier.

Long-range atmospheric transported precursor PFAS can oxidize through hydroxyl radicals in the atmosphere in the gas-phase or on atmospheric particles, or on ground surfaces such as snow and ice to PFCAs and PFSAs (D'Eon et al. 2006; Ellis et al. 2004; Styler et al. 2013; Taniyasu et al. 2013b). Aerobic microbial transformation in the aqueous environment have been described for FTOHs (Dinglasan et al. 2004).

Styler et al. (2013) examined reactions of 6:2 FTOH on environmental surfaces of Mauritanian sand and Icelandic volcanic ash containing iron and titanium (Styler et al. 2013). Reaction products and intermediates were identified by gas-phase FTIR and by LC-MS/MS. They found that these surfaces catalyzed the photochemical reaction with OH-radicals, and that PFCAs where created though aldehyde, unsaturated aldehyde and unsaturated carboxylic acid intermediates *(Figure 1.3A)*. PFCAs are known to be recalcitrant for OH-radical reactions, and therefore remain on the particle surfaces. The catalytic properties of some particle surfaces might be an answer to why the majority of FTOHs have been found in the gas-phase compared to the particle-phase, which earlier have been explained by the volatility of FTOHs (Cai et al. 2012a; Styler et al. 2013). Styler et al. suggested that aerosols of natural mineral dust and coal fly ash can be enriched by surface-sorbed PFCAs, and potentially be a source of long-range transported PFCAs to remote regions such as the Arctic (Styler et al. 2013).

Similarly, perfluoroalkyl sulfonamides and sulfonamidoethanols (FASAs and FASEs) can undergo degradation to the more persistent PFCAs and PFSAs in the environment. D'Eon et al. (2006) examined experimentally the degradation of N-methyl perfluorobutane sulfonamidoethanol (MeFBSE). They studied gas-phase reactions to measure reaction rates with OH-radicals and measured reaction products by online FT-IR and offline GC-MS and LC-MS/MS. They found that MeFBSE was readily oxidized at the alcohol moiety, surprisingly at the same rate as n-propanol. The reaction products included the more persistent N-methyl perfluorobutane sulfonamide (MeFBSA), perfluorobutane sulfonic acid (PFBS), and short-chain PFCAs, PFBA being the major product *(Figure 1.3B)*.

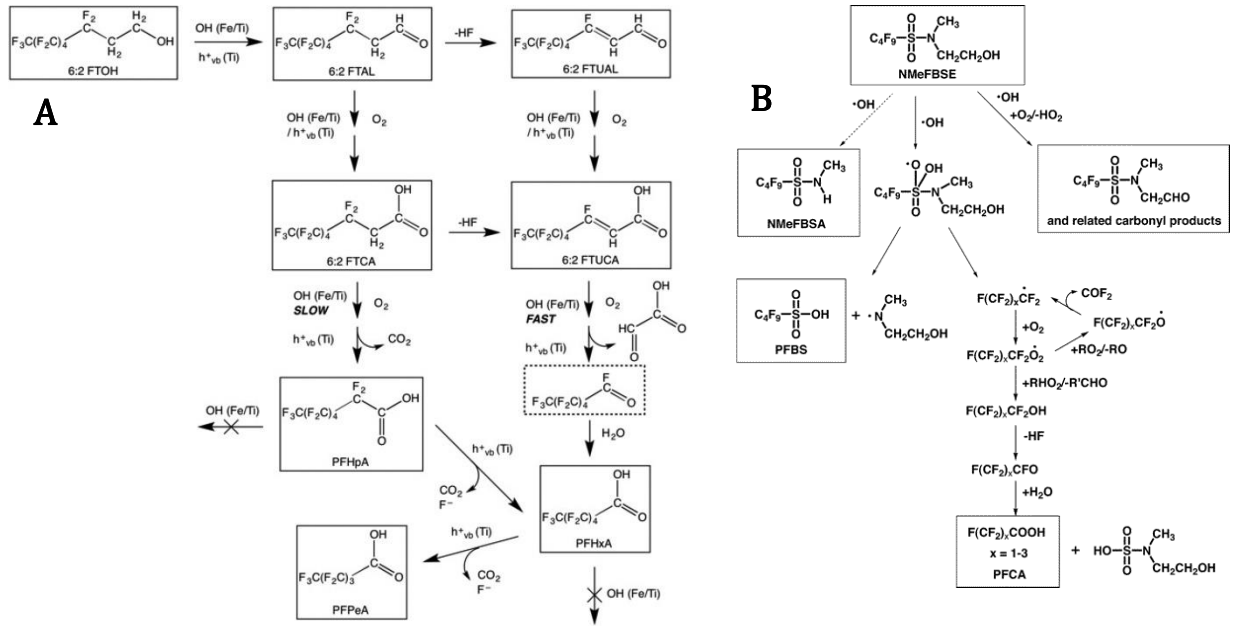


Figure 1.3. Proposed reaction mechanisms for photolytic oxidation of precursor PFASs FTOH and FASE yielding short-chain PFAAs. A) 6:2 FTOH on Fe/Ti containing particles (Styler et al. 2013) and B) MeFBSE in atmosphere gas-phase by hydroxyl radicals (D'Eon et al. 2006). Reprinted with permission from (Styler et al. 2013) and (D'Eon et al. 2006). Copyright 2006 and 2013 American Chemical Society.

Jackson et al. (2013) suggested another pathway for transport and transformation to PFCAs by oxidation of perfluorinated amides (FAMs), which were unintentionally produced as byproducts of the ECF-process. FAMs are predicted to be more volatile than similar FASAs, and should volatilize readily to the atmosphere. They examined the chlorine/hydroxyl oxidation of N-ethyl perfluorobutane amide (EtFBA), and found PFCAs were generated through N-dealkylation and elimination of two carbonyl compounds. Jackson et al. predicted similar reaction kinetics for the eight carbon FAMs since length of the perfluoroalkyl chain was assumed not to affect reaction rate with hydroxyl radical (Ellis et al. 2003; Jackson et al. 2013). Therefore eight-carbon based FAMs, could have historically been a source of PFOA and shorter chain PFCAs (Jackson et al. 2013).

D'Eon et al. estimated the atmospheric lifetime by OH reaction MeFBSE to be approx. 2 days, and the N-dealkylation product MeFBSA more than 20 days which illustrates the importance of considering potential degradation products of the parent compound (D'Eon et al. 2006). Atmospheric lifetime by OH reaction for FTOHs have been estimated to be approx. 20 days (Ellis et al. 2003), a lifetime of more than 50 days have been indicated (Xie et al. 2015). Since the length of the perfluorocarbon-chain does not affect the reaction rate, these atmospheric lifetimes are transferable to the longer-chain FTOHs, FASEs and FASAs, which are still present in Arctic atmosphere (Cai et al. 2012a; Ellis et al. 2003; Gawor et al. 2014; Jackson et al. 2013; Xie et al. 2015). Seasonal and geographic variation in OH-radical concentrations will affect reaction rates, OH radicals almost disappear in the Arctic polar night and the annual average concentrations at Arctic latitudes are approx. an order of magnitude lower than equatorial regions (Patra et al. 2014). Given an average global wind speed of 4 m s^{-1} and an atmospheric resident time of 20 days, travel distance will be approx. 7000 km (Ellis et al. 2003), which is sufficient to reach the Arctic from most industrialized regions on the northern hemisphere.

Neutral precursor PFASs have been found in Arctic and Antarctic atmosphere at levels ranging from low picogram to several hundred picograms per cubic meter, where FTOHs are the most abundant PFAS-group. 8:2 FTOH being the most abundant of the FTOHs, MeFBSE/MeFOSE the most abundant of the FASEs and MeFBSA the most abundant of the FASAs (Cai et al. 2012a; Del Vento et al. 2012; Shoeib et al. 2006; Xie et

al. 2015). The presence of these compounds in the atmosphere at high latitudes indicate a high potential for long-range atmospheric transport from source regions.

In 2009 near the Western Antarctic Peninsula, Del Vento et al. found an increase in MeFBSA and MeFBSE concentrations in air approx. 10-fold higher than previous measurements in 2007, while FTOHs and FOSAs where in the same range as previous measurements, these observations might reflect the increased use of short-chain PFASs (Del Vento et al. 2012).

Because of their relatively high water solubility and low Henry's law constant, PFCAs and PFSAs are unlikely to travel long distances in the atmosphere, but will readily be deposited to the ground by wet precipitation (Cai et al. 2012a). Due to its high surface area and enhanced surface sorption under subzero temperatures, snow has a high efficiency for scavenging both particle and vapor phase substances from the atmosphere (Xie et al. 2015). Evidence of perfluorinated acids (PFAAs) deposited on snow in the Arctic and Antarctic regions have been found (Cai et al. 2012a; Cai et al. 2012b; Codling et al. 2014; Kwok et al. 2013; Taniyasu et al. 2013b; Young et al. 2007).

Xie et al. conducted a sampling campaign in 2011 and 2012 to analyze the levels of neutral PFASs in the atmosphere and snow in Ny-Ålesund, Svalbard (Xie et al. 2015). They analysed 12 neutral PFASs in high-volume air-samples and in snow. Based on their results, they calculated the fluxes of these compounds from atmosphere to snow. They found that FTOHs (6:2-, 8:2-, 10:2- and 12:2 FTOH) and FTAs (6:2- and 8:2 FTA, fluorotelomer acrylates) had positive fluxes, meaning they had a strong potential for re-volatilization rapidly after deposition. The FASEs (MeFOSE, EtFOSE and MeFBSE) had all negative fluxes in the sampling period, indication net. deposition, while the FASAs (MeFOSA, EtFOSA and MeFBSA) were varying between negative and positive fluxes depending on temperature (Xie et al. 2015).

Taniyasu et al. (2013) found evidence that ionic PFASs were scavenged from the atmosphere by wet deposition. They measured the fluxes of ΣPFAS, and found they were at the highest in the first 1 mm of precipitation (Taniyasu et al. 2013b). Occurrence of ionic PFASs in wet precipitation implies wet deposition is an effective scavenger and a major pathway from the atmospheric to the hydrospheric compartment (Taniyasu et al. 2013b). They also suggests that snow on the ground can cold-trap contaminants, where photochemical reactions is likely taking place on the snow/ice surface due to the observed change of PFASs composition in aged compared to fresh snow (Taniyasu et al. 2013b). Similarly, in Northern Sweden, Codling et al. found changing PFASs composition profile through different stages of melt in a snowpack (Codling et al. 2014).

1.5 Aim of study

In a 2013 master thesis, Garsjø examined levels of selected PFASs in muscle and liver of Arctic char (*Salvelinus alpinus*) from Lake Linnévatnet, and found that PFBA, PFHxA and PFUnDA had the highest detection frequency, and found PFBA to be most abundant (Garsjø 2013). Short-chain PFASs include PFCAs with seven or less perfluorocarbons, PFSAs with six or less perfluorocarbons and their precursors (Scheringer et al. 2014). Short-chain PFASs are more hydrophilic, and less bioaccumulative, and is likely to be in equilibrium between the fish tissues and water. My working hypothesis was thus based on the above conclusions: short-chain PFASs are expected to be present in the water of Lake Linnévatnet in high concentrations.

The aim of this study was to examine the spatial distribution and the composition profiles of perfluoroalkyl and polyfluoroalkyl substances (PFASs) in freshwater, with emphasis on short-chain PFASs, in Lake Linnévatnet (Nordenskiöld Land, Spitsbergen) in Svalbard by measuring the concentration at different locations at different times in the lake. This was done by collecting water and snow samples at different locations in and around the lake in March 2014, April 2015 and June 2015. Water samples were also collected at a known locally polluted site near Svalbard airport Longyearbyen in November 2014 and June 2015. Samples were extracted by solid phase extraction (SPE) and analysed by liquid chromatography coupled with negative electrospray tandem mass spectrometry (HPLC-(-)ESI-MS/MS).

2 Materials and methods

2.1 Description of study sites and sample collection

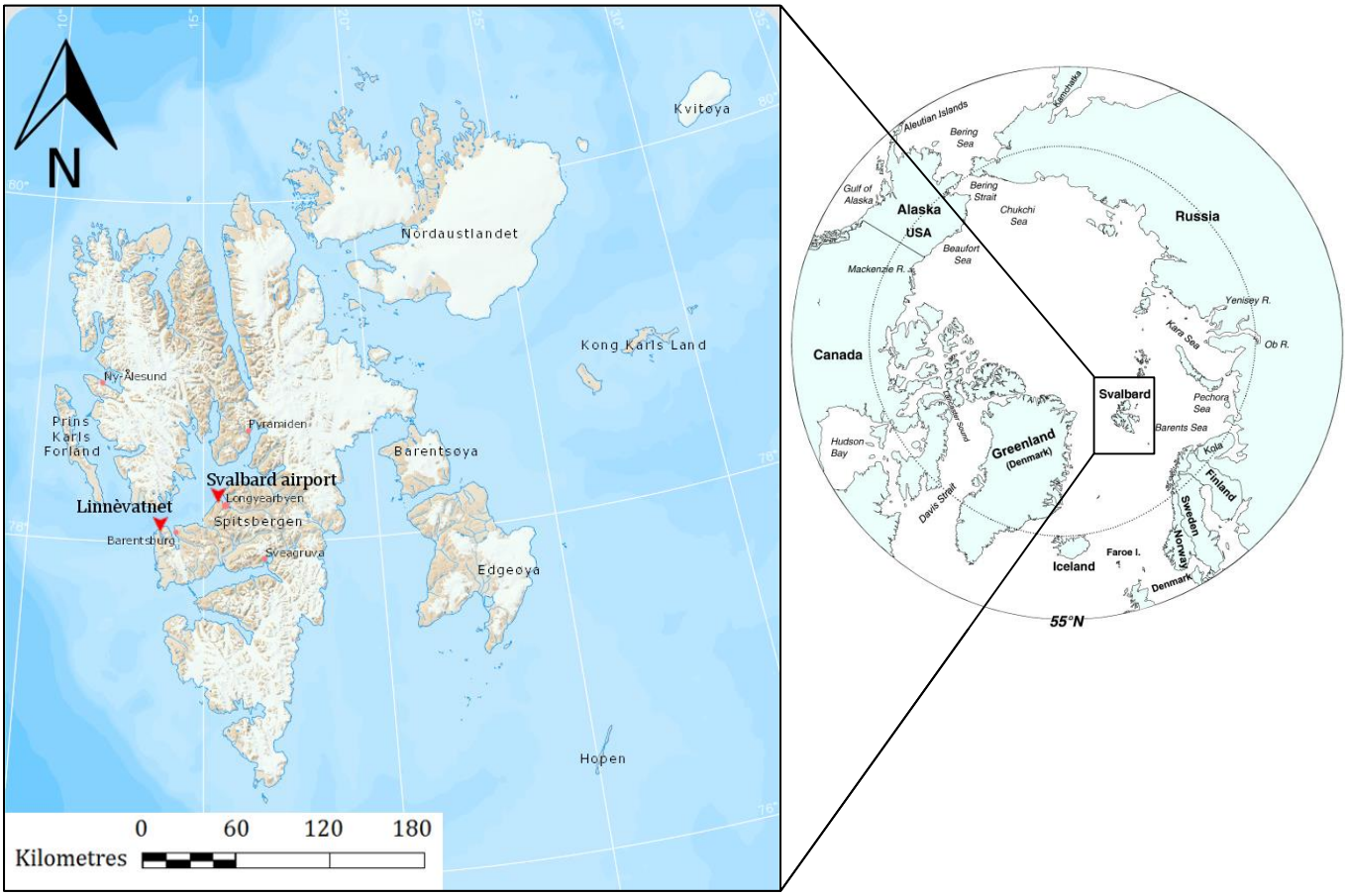


Figure 2.1. Overview of Svalbard and the study sites.
Svalbard map adapted from Topo Svalbard (NPI 2015). Circumpolar map reprinted from (Butt et al. 2010), with permission from Elsevier.

Lake Linnévatnet (78°03'N; 13°48E) is located in the region Nordenskiöld Land at the west-coast of Spitsbergen, the largest island in the Svalbard archipelago. Isfjord Radio is located 3 to 7 km in linear distance NW of the lake and is used as a tourist hotel parts of the year, it also hosts the nearest meteorological station to the sample sites around Lake Linnévatnet. In the winter season, Isfjord Radio is accessed by snowmobile, of which the track passes though the catchment and across the ice of Lake Linnévatnet. The nearest settlement is Barentsburg, approx. 10 km in a linear distance east, and Longyearbyen, the largest settlement on Svalbard, is located approx. 50 km NE.

The surface area of the lake is 4.7 km^2, making it the second largest lake on Svalbard. The catchment area is 36. 1 km^2 (Svendsen et al. 1989) and include the glacier Linnèbreen, several minor cirque glaciers and mountains with an altitude up to 781 m.a.s.l. The main inflow is in the south-end of the lake from the valley Linnèdalen, and the outflow is in the north-end connecting the lake to the sea by a river of approx. 2 km in length. The surface of the lake is typically ice-covered in the period between October and mid-July, with a maximum ice-thickness of approx. 1.5 – 2 m (Bøyum & Kjensmo 1978; Svenning et al. 2007). The lake is classified as a cold monomictic lake, meaning it is isothermal and isochemical, and maintains a temperature below 4 °C throughout the year (Bøyum & Kjensmo 1978). The lake is extremely well mixed in the ice-free

periods because of its location well exposed to southerly and northerly winds, and also the inflow of cold glacial meltwater containing fine sediment provide good mixing (Bøyum & Kjensmo 1978).

Table 2.1. Physical measures of Lake Linnévatnet and its catchment.

Lake surface area, km^2	4.6	a.
Lake surface altitude, m.a.s.l.	12	b.
Average lake depth, m	18.6	a.
Maximum lake depth, m	37	a.
Lake volume, m^3 x 10^6	85.8	a.
Catchment area, km^2	36.1	b.
Glaciated area in catchment, km^2	3.1	c.

a. (Bøyum & Kjensmo 1978)
b. (Svendsen et al. 1989)
c. Recent maps, Topo Svalbard (NPI 2015)

Annual mean temperature at Isfjord radio (1961 – 1990, normal defined by the Norwegian Meteorological Institute) was -5.1 °C, mean summer temperatures (June, July, August and September) was 2.8 °C. The mean annual precipitation was 480 mm (normal 1960 – 1990), were mean summer precipitation (June, July, August and September) was 175 mm (eKlima 2015). The predominate wind direction at Isfjord Radio is from northeast *(Figure 2.2)*.

The planetary atmospheric boundary layer (PBL) in Kongsfjorden, western Spitsbergen, was estimated to approx. 500 m.a.s.l. in summer and 1000 m.a.s.l. in winter (Esau & Repina 2012). If similar conditions apply, Lake Linnévatnet and the majority of its catchment are located below the PBL and are possibly susceptible for local- and regional source contamination.

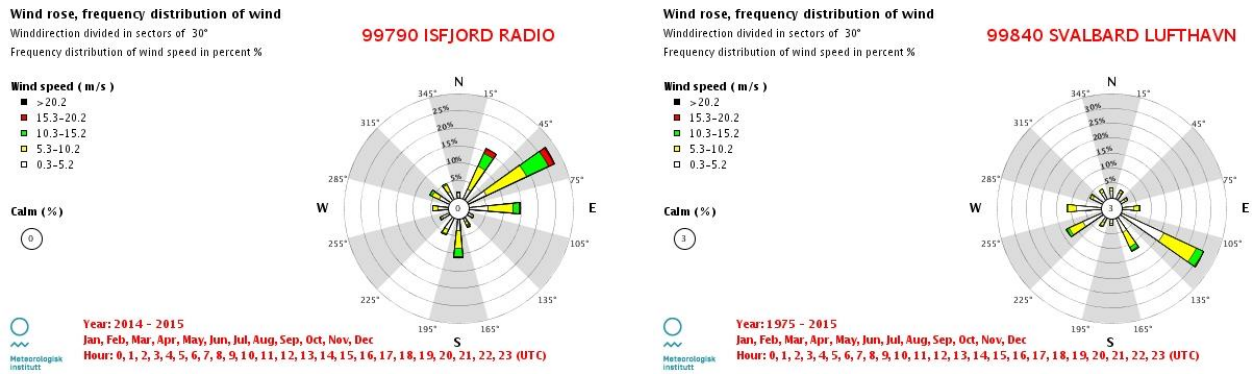


Figure 2.2. Wind rose, showing frequency distribution of wind speed and direction at Isfjord Radio and Svalbard Airport (eKlima 2015).

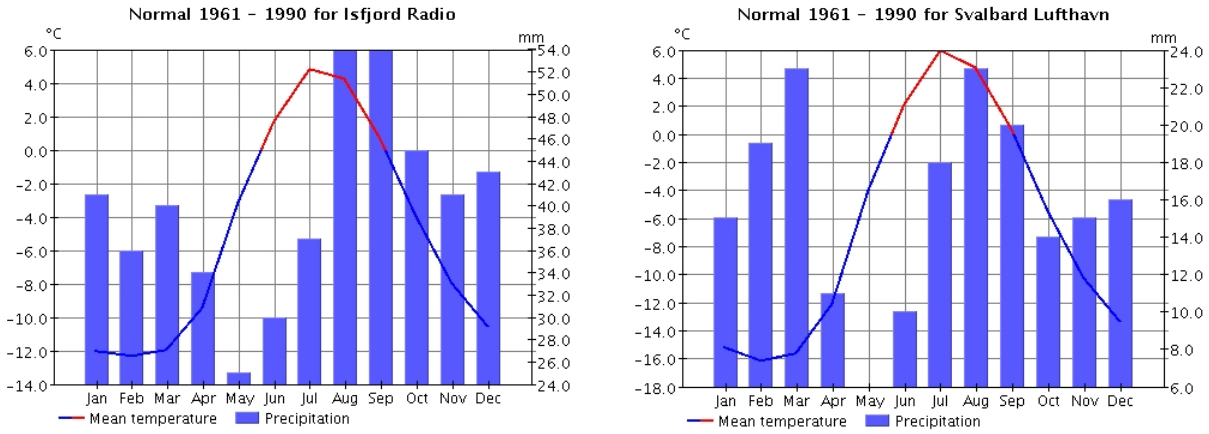


Figure 2.3. Mean monthly temperature and precipitation. Isfjord radio (left) and Svalbard Airport (right) (eKlima 2015).

As a reference site for a known local point source of PFAS-contamination, a small stream downstream a firefighting-training site near Svalbard Airport, Longyearbyen (78°14' 15°32'E) was chosen. Reports from the airport operator Avinor (unpublished) show high levels of PFASs, PFOS being the dominant, in soil and water at different locations near the FFTS in present and previous use. Due to no winter run-off, samples of seawater close to the shore where the stream flow into the fjord was collected in November 2014. Normal temperature and precipitation at Svalbard airport is provided in *Figure 2.3*, the predominant wind direction is from southeast *(Figure 2.2).*

Meteorological data from individual sampling dates is provided in *Table 2.2*. A simplified description of the sample sites is provided in *Table 2.3* and *Figure 2.4*. The complete sample protocol describing each individual sample is available in *Table E.1* in the appendix.

Table 2.2. Meteorological data for the sampling dates at the nearest meteorological station.

Date	Met. Station	Temperature (diurnal mean and range) [°C]	Wind speed (mean and range) [m s^{-1}]	Wind dir. (06 UTC) [deg.]	Atm. P at sea level [hPa]	Precipitation [mm]
22.03.2014	SVALBARD LUFTHAVN*	-15.2 (-17.8 – -12.3)	3.9 (1.1 – 6.6)	122	992.0	0
14.11.2014	SVALBARD LUFTHAVN	-8.8 (-12.1 – -7.6)	4.0 (0.6 -9.7)	132	1030.1	0,3
18.04.2015	ISFJORD RADIO	-2.7 (-3.7 – -1.4)	2.8 (0.5 – 7.2)	252	998.6	0
05.06.2015	SVALBARD LUFTHAVN	3.0 (1.7 –4.7)	2.8 (1.4 – 4.7)	275	999.1	0
13.06.2015	ISFJORD RADIO	3.2 (2.4 – 4.3)	13.5 (10.6 – 19.0)	49	995.4	0,1
14.06.2015	ISFJORD RADIO	4.1 (2.2 – 6.0)	10.1 (5.4 – 14.6)	38	1000.5	0
15.06.2015	ISFJORD RADIO	4.7 (3.2 – 6.8)	6.6 (1.3 – 10.4)	23	1009.7	0,1
16.06.2015	ISFJORD RADIO	4.0 (3.5 – 7.3)	3.8 (1.8 – 5.0)	204	1010.1	0

* Meteorological data from Isfjord radio was not available at 22. 03. 2014, Svalbard lufthavn was chosen as the closest alterative.

Table 2.3. Description of the sample sites.

Site identity	Description	Matrix	n	Position (Lat. /long. dd°mm'ss. s")	Lake depth [m]
I	River, main lake inlet	Freshwater	1	N78°01'42.5" E13°51'42.5"	
O	River, lake outlet	Freshwater	1	N78°03'59.9" E13°46'48.7"	
L1	Lake, south	Freshwater	6	N78°02'03.1" E13°51'16.3"	12
L2	Lake, middle/south	Freshwater	5	N78°02'23.2" E13°49'38.9"	32
L3	Lake, middle/north	Freshwater	6	N78°02'52.9" E13°48'05.3"	35
L4	Lake, north	Freshwater	6	N78°03'36.0" E13°46'20.6"	27
L5	Lake, north (only March 2014)	Freshwater	2	N78°03'28.6" E13°47'00.6"	
S1	Snow patch	Snow	1	N78°01'53.5" E13°47'34.6"	
S2	Snow patch	Snow	1	N78°02'24.0" E13°52'05.4"	
M1	Meltwater stream	Freshwater	1	N78°01'59.0" E13°47'51.0"	
M2	Meltwater stream	Freshwater	1	N78°02'19.8" E13°51'42.3"	
A1	Runoff stream from airport FFTS.	Saltwater/ freshwater*	6	N78°14'26.2" E15°32'13.0"	

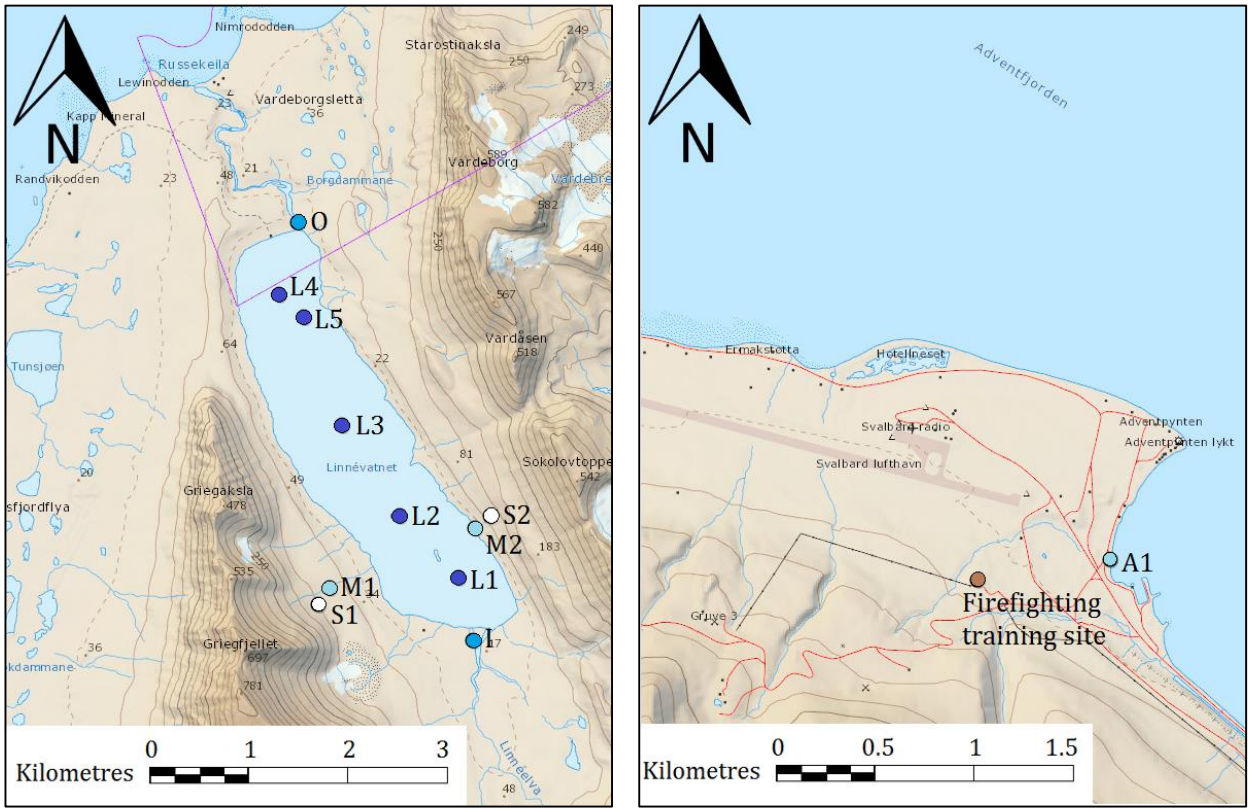


Figure 2.4. Maps of sampling sites at lake Linnévatnet (left) and Svalbard airport (right). Adapted from Topo Svalbard (NPI 2015).

Figure 2.5. Lake Linnévatnet during sampling in June 2015.

2.1.1 Lake samples

In the April 2015 sampling campaign, appropriate sample location were selected at least 100 meters from existing snowmobile or ski tracks. For the June 2015 sampling campaign, the former sampling locations were re-used. Surface snow was removed by an aluminum snow-shovel from the ice where holes were to be drilled. Six to eight holes were drilled by a motorized ice-drill with an 150 or 200 mm auger bit in a rectangle large enough for the sediment grab sampler to be lowered. An ice-saw was used to cut the ice between the holes. An aluminum snow shovel and a polypropylene/stainless steel sieve was used to remove floating ice and snow from the water.

Water samples were collected before sediment samples to avoid contamination from the sediments. Nitrile gloves with wool-liners inside to stay warm were used during sampling. Field blanks were left open during sampling at each location. The pre-cleaned sample bottles were rinsed with $^1/_3$ to ½ of the bottle volume of sample three times, before the bottles were lowered by hand at 5 to 20 cm below the surface and filled. The surface water layer was avoided. Samples collected during the April 2015 campaign were filled directly in pre-cleaned bottles without being rinsed with sample. The cap of the field blank was closed after all three replica at each site was collected. Unique sample identities were noted both on the sample bottles and in the sampling protocol along with sampling time, exact position and other information such weather conditions, ice thickness and lake depth. Lake depth was measured by the immersed depth of the sediment sampler with a 65 cm ice-axe as a reference, this measurement was only done in the June 2015 campaign.

In June 2015 parallel samples were taken at L1 – L4, S1 – S2 and M1 – M2, at L1 – L4 also sediment samples were collected (Rakovic et al. in prep.). These samples were analyzed separately at SLU, and results were used for an inter-laboratory comparison to assess the reproducibility of the method (see section 3.6).

2.1.2 Rivers and meltwater streams

For river samples, appropriate sampling points were chosen at approximately 50 to 150 meters from the inlet and outlet of the lake. The river was assumed to be well mixed since the river regularly had parts with turbulent stream. Sample locations for meltwater streams were selected below the sampled snow-patches to collect run-off water.

Pre-cleaned sample bottles were rinsed three times with sample and filled with sample as described above for lake samples.

2.1.3 Snow

Surface snow was collected by a pre-cleaned aluminum snow shovel in a 25-liter polypropylene barrel, pre-cleaned with methanol, enough in water equivalent to rinse and fill desired sample bottles. The snow was left to melt over night at room temperature, before being transferred to pre-cleaned 2-liter polypropylene bottles. The sample bottles were rinsed with sample as described above for lake samples, before the bottles were filled.

2.1.4 Sample transportation and storage

In April, sample bottles were transported in aluminum boxes by snowmobile directly from Lake Linnévatnet to UNIS. In June, samples were transported in backpacks from sampling locations to Isfjord radio for temporary storage at 4 °C. From Isfjord radio, the samples were transported un-refrigerated in aluminum boxes, by boat to UNIS. The air-temperature during sampling in June was < 8 °C, for the remaining sampling dates < 0 °C *(Table 2.2)*. Samples were stored at UNIS in cold room at 4 °C for up to 14 days until analysis, samples stored longer were kept in freezer room at -18 °C.

2.2 Reagents and standards

A complete list of qualities, producers and suppliers of reagents and solvents is supplied in *Table B.1* in appendix.

Conditioning/elution solution, referred to as *reagent A* below; 0.1 % ammonia in methanol, was prepared by diluting 225 µL of 25 % NH_4OH to 50 mL with methanol in a PP tube.

Methanol for conditioning and elution, referred to as *reagent B* below.

WAX-Water, referred to as *reagent C* below; 1 liter of MilliQ water was passed through a conditioned WAX cartridge without using vacuum and collected in a pre-cleaned HDPE/PP-bottle or a borosilicate glass-bottle burned at 450 °C. This water was used for all reagents and blanks.

Acetate buffer pH 4, 20 mM CH_3COOH/ 5 mM CH_3COONH_4, referred to as *reagent D*, used to condition/clean the SPE-cartridges: First a 0.025 mol L^{-1} Acetic acid solution was prepared by diluting 360 µL of 99.9 % acetic acid to 250 mL of WAX-water. Second, a 0.025 mol L^{-1} Ammonium acetate (NH_4OAc) solution was prepared by dissolving 0.0967 g NH_4OAc in 50 mL WAX-water. At last, 200 mL of the acetic acid solution was mixed with 50 mL of the NH_4OAc -solution.

Mobile phase A, 10 % methanol in aqueous 2 mM NH_4OAc. 0.157g of NH_4OAc was added to a 1000 mL volumetric flask along with 100 mL of methanol, some MilliQ water was added to completely dissolve the solution before the volume was adjusted to 1000 mL by MilliQ water.

Mobile phase B, 2 mM NH_4OAc in methanol. 0.157 of NH_4OAc was dissolved in 1000 mL of methanol.

All standards used where supplied by Wellington Laboratories (Guelph ON, Canada). Standards were diluted to their respective concentrations in methanol using variable automatic pipettes of different volumes.

As internal standards (ISTDs), ^{13}C-, ^{18}O- and ^{2}H-labeled homologues were used, for convenience these are referred with an M-prefix to the native homologue acronym in tables and figures, e. g. MPFBA for $^{13}C_4$-PFBA. Complete names for internal and native standards are provided in *Table B.4* in the appendix.

Concentrations of the diluted standard mixtures are supplied in the appendix; *Table B.5* for ISTD-mix A, *Table B.6* ISTD-mix B, *Table B.7* for the native spike-mix and *Table B.8* for the calibration standards.

2.3 Materials

Complete list of the equipment, materials and consumables including producer, supplier and part numbers, is supplied *Table B.2* and *Table B.3* in appendix.

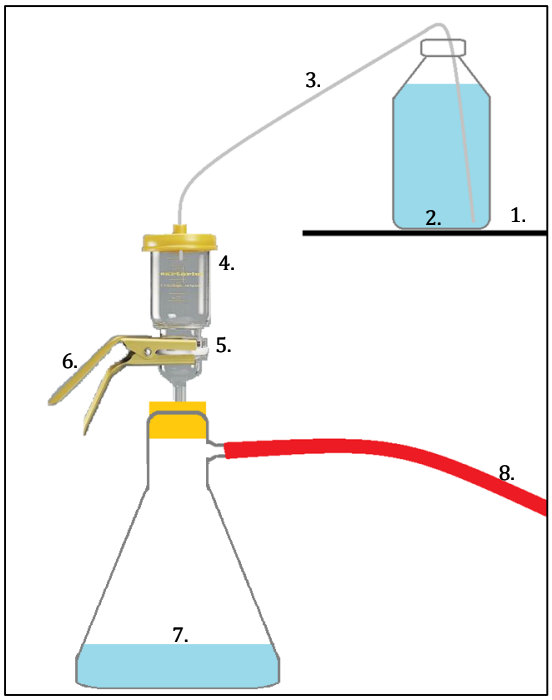
2.4 Sample extraction and clean up

Sample extraction and clean-up was done in the chemistry- and teaching laboratories at UNIS, (Longyearbyen, Svalbard). Sample extracts were then transported to Department of Food Safety and Infection Biology (MatInf) at the Norwegian University of Life Sciences (Oslo, Norway), where standards were prepared and some of the final treatment of the sample extracts was done.

Sample extraction was done by solid phase extraction (SPE), first described Moody and Field in 1999 for the extraction of PFHxA, PFHpA and PFOA in water (Moody & Field 1999), and later developed to include a range of short- and long-chain PFASs (Taniyasu et al. 2005; Yamashita et al. 2004). It was later adopted as an international standard for the determination of PFOS and PFOA, but with a rather high detection limits of 2 ng L^{-1} for PFOS and 10 ng L^{-1} for PFOA (ISO 2009). Ahrens et al. (2010) provided a guideline for PFAS analysis in different matrices (Ahrens et al. 2010). The method used in this study was based on the above mentioned, and mostly in compliance with the most recent method described by Ahrens et al.

2.4.1 Filtering of high-particulate samples

Samples containing high amounts of visible suspended particulates were filtered to avoid clogging of the SPE cartridges. The filtering assembly *(Figure 2.6)* consisted of a 47 mm fritted glass filter holder connected through a perforated silicone stopper to a 2 L suction flask, 250 mL filter funnel, clamp, silicone lid and vacuum tubing connected to a vacuum pump. The sample bottle was placed on an elevated lab jack, and sample was transferred by gravity, or by vacuum if needed, to the filter by a fitting length of polypropylene tubing (o.d. 1/8”).



1. Lab. Jack to elevate sample above filter
2. Sample reservoir
3. PP-tubing, o.d. = 1/8"
4. Filtration reservoir 250 mL
5. Glass filter holder with GF/C filter
6. Clamp
7. Suction flask for collection of filtrated sample.
8. Vacuum pump

Figure 2.6. Illustration of the filtration assembly.

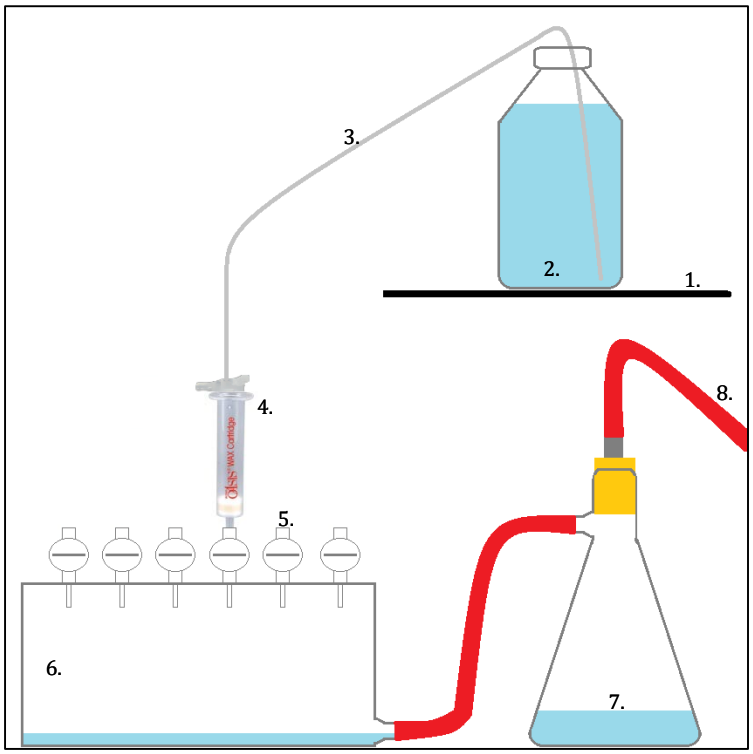
Before filtering, a clean GF/C glass fiber filter (burned at 400 °C for 6 hours in muffle furnace) was placed in the filter holder. If quantification of the suspended solids was of interest for further analysis, the sample bottle and filter was weighed in advance. The samples were homogenized by manual shaking. A fitting piece of aluminum foil was placed over the funnel opening and the sample bottle. The funnel opening was covered by the silicone lid. The sample was then connected to the filtering assembly with polypropylene tubing perforating the aluminum foil. The sample was loaded to the filter by starting the vacuum pump.

2.4.2 Pre-treatment

Frozen samples were thawed either over night at room-temperature or for a few days in a refrigerator at 4°C. The full sample bottles were weighed on a laboratory scale (5 - 6100 g, d =0. 1 g) and noted in the sample protocol. The samples were spiked with internal standards (*Table B.5* and *Table B.6* in the appendix), 50 µL of ISTD-mix A and 50 µL of ISTD-mix B. The samples were homogenized by manual shaking for approx. 10 seconds, and then sonicated for 15 minutes in an ultrasonic bath before extraction.

2.4.3 Sample extraction

Samples of water and melted snow were extracted by solid-phase extraction (SPE), using mixed mode reverse phase/weak anion exchange (WAX) resin. The SPE cartridges, Waters Oasis® WAX (500 mg, 6 cc, 60 µm), were placed on the vacuum manifold and conditioned with 4 mL *reagent A* followed by 4 mL of *reagent B* and *reagent C*. After conditioning, an additional 4 mL of *reagent C* was added and retained in the SPE-cartridge to prevent the cartridge from drying out during the first minutes of application of the sample. A reservoir adapter was placed on top of the cartridge and the cartridge was labeled with sample identity. As far as possible, sample triplicates and field blanks from each location were extracted at the same time. The sample bottle was placed on top of a lab jack elevated above the SPE-assembly, the bottle opening was covered by aluminum foil and the sample bottle was connected to the SPE cartridge through a fitting length of polypropylene tubing (o.d. 1/8”), see *Figure 2.7* for an illustration of the assembly. The loading of sample was started by vacuum pump, which was stopped after sample started to flow through the tubing. Loading speed was maximum 5 mL/min, or maximum 2 drops/second. Typical loading time for a 2 L sample was approx. 10 – 24 hours. The eluting water was thrown away.



1. Lab. Jack to elevate sample above SPE
2. Sample reservoir
3. PP-tubing, o.d. = 1/8"
4. SPE with reservoir adapter
5. SPE valves
6. Vacuum manifold
7. Suction flask for wastewater collection
8. Vacuum pump

Figure 2.7. Illustration of SPE assembly.

After samples were loaded, residual water was removed from the SPE cartridge by using vacuum for 30 seconds. The empty sample bottles were weighed with their original cap. Assuming the density was 1 g/mL for freshwater and 1.027 g/mL for saltwater, weight difference between full and empty bottles was used to calculate extracted volume. Weight and volume for each sample was noted in the sample protocol.

The SPE cartridges were cleaned/conditioned with 4 mL of *reagent D* in order to remove salts and other interferences and improve adsorption of target analytes to the sorbent (Taniyasu et al. 2005; Van Leeuwen et al. 2009), the eluate was thrown away. Afterwards, the cartridges were centrifuged at 1500*g* for 2 minutes to remove residual solution.

The cartridges were placed in two 15 mL polypropylene tubes per cartridge and eluted in two different fractions. Fraction 1, containing neutral PFASs, by using 4 mL of methanol *(reagent A)* and fraction 2, containing ionic PFASs, by 4 mL of 0.1% NH_3 in methanol *(reagent B)*. The polypropylene tubes were labeled with sample identity and fraction number, and stored in refrigerator at 4 °C before transportation and further treatment.

Figure 2.8. Sample extraction setup in the chemistry lab. at UNIS.

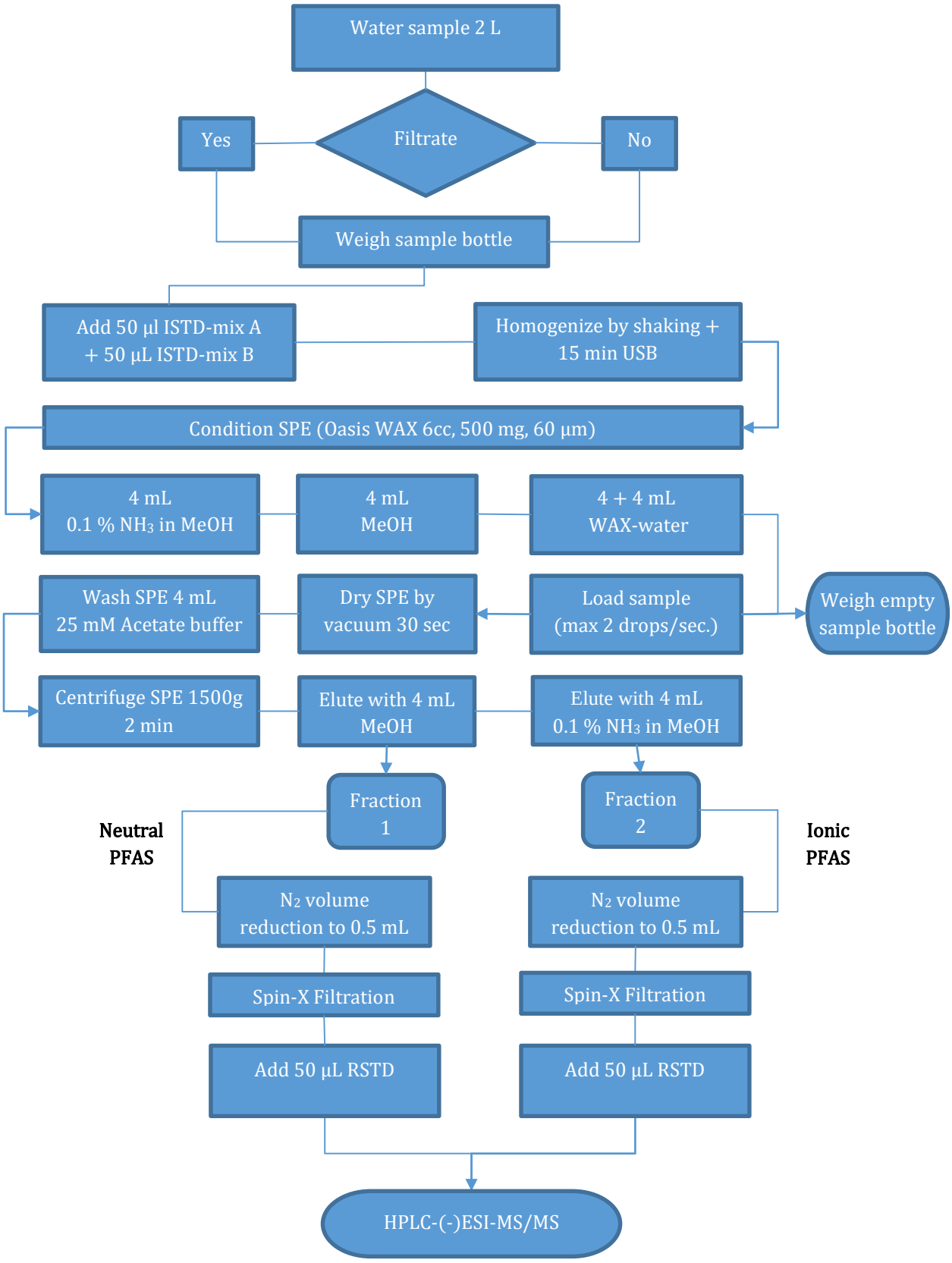


Figure 2.9. Flow chart of the extraction process.

2.4.4 Volume reduction

Because of limited time at UNIS for sample preparations, volume reduction of sample extracts was performed at different laboratories using slightly different techniques and equipment. The volume reductions were performed at UNIS, NMBU Campus Ås and NMBU Campus Adamstuen.

NMBU Campus Ås
Sample extracts were evaporated under nitrogen (5.0 quality) in a water bath at 35 °C using a TurboVap II (Biotage, Uppsala, Sweden) in 6 x 200 mL glass evaporation tubes with 0.5 mL endpoint sensor. The evaporation tubes were cleaned in dishwasher machine then cleaned using three portions of acetone and three portions of methanol.

TurboVap UNIS
In November 2014 some samples were evaporated under airflow from a motor driven fan in a water bath at 35 °C, using TurboVap 500 (Biotage, Uppsala, Sweden) in 2 x 500 mL glass evaporation tubes. The TurboVap system was cleaned by letting two tubes of acetone evaporate for 10 minutes. The evaporation tubes used for sample extracts were burned in a muffle furnace at 450 °C for 6 hours, and cleaned using three portions of acetone and three portions of methanol between each sample of similar expected PFAS concentration and matrix.

Before volume reduction of the sample extract, the tube containing the extract was vortexed and then transferred to the TurboVap tube. The sample tube was then rinsed with 1 mL of methanol, which also was transferred to the TurboVap tube

Nitrogen evaporator UNIS
In June 2015 some samples were evaporated under a stream of nitrogen in a water bath kept at 35±5 °C. The extracts were concentrated to <1 mL directly in the 15 mL PP-tube by a gentle stream of high purity nitrogen (5.0 quality). The sides of the PP-tube were rinsed by approx. ½ Pasteur pipette of methanol, the volume was again reduced to < 1 mL. This rinsing was repeated two times. The stainless steel needles were cleaned by 15 minutes of sonication in methanol and then rinsed by a Pasteur pipette of methanol.

NMBU Campus Adamstuen
Sample extracts were evaporated under a stream of nitrogen (5.0 quality) in a water bath kept at 35 °C using a TurboVap LV (Biotage, Uppsala, Sweden), directly in the 15 mL PP-tubes in up to 50 positions. A PP-tube with 500 µL of water was used as a reference to mark a 0.5 mL reference point on each tube. The extracts were then evaporated to approx. 0.4 mL.

At last, 50 µL of the RSTD-mix ($^{13}C_8$-PFOA, 196 pg μL^{-1}) was added, and the volume was adjusted to 0.5 mL by methanol. Before LC-MS/MS analysis, the sample extracts were filtered using Spin-X Nylon centrifuge filters, which were centrifuged at 5000 rpm/1.8*g* for 3 minutes.

2.5 Instrumental analysis

Instrumental analysis was done was done at the Department of Food Safety and Infection Biology (MatInf) at the Norwegian University of Life Sciences (Oslo, Norway).

Analyses were performed using an Agilent 1200 HPLC system coupled to an Agilent 6460 series triple quadrupole MS/MS system. Chromatographic separation were done on an Zorbax Eclipse Plus C-18 column (Agilent, 3. 5 µm 2. 1 x 150 mm) and a Supelguard Discovery C-18 guard column (Supelco , 2 cm x 2.1 mm, 5 µm). As mobile phase, 10 % methanol in water [A] and methanol [B] were used, both containing 2 mM

ammonium acetate as ionization aid (Ahrens 2009) . Two different instrument methods were used for PFCAs and for PFSAs, FASAs and FASEs, both with an acquisition time of 26 minutes.

10 µL of the sample extract was injected and the column oven was kept isotherm at 21 °C. Mobile-phase flow was constant at 0.2 mL min^{-1}.

For PFCAs, the gradient started with 85 % [B] held for 5 minutes, then increased linearly over 5 minutes to 99 % [B], this was held constant for 7 minutes then changed linearly over 1 minute to 1 % [B] until end of analysis at 26 minutes.

For PFSAs, FASAs and FASEs the gradient started with 85 % [B] held for 5 minutes, then increased linearly over 5 minutes to 99 % [B], this was held constant for 7 minutes then changed linearly over 1 minute to 10 % [B] and held for 7 minutes before increased linearly over 2 minutes to 85 % [B].

Detection was done by tandem mass spectrometry (MS/MS) in multiple reaction monitoring (MRM) mode. The triple quadrupole mass spectrometer was operated with the Agilent jet stream electrospray ionization (AJS-ESI) source. Ion source parameters, MS/MS parameters and MRM transitions are available in *Table C.1*, *Table C.2* and *Table C.3* in the appendix.

2.5.1 Data handling and integration

MRM chromatograms were processed by the Software "Agilent Mass Hunter Workstation: Quantitative Analysis" Version B.07.00, Build 7.0.457.0. The algorithm "Agilent 2" did peak-integration automatically; peak-integrations were inspected visually and adjusted by manual integration if necessary.

Signal to noise ratio (S/N) calculated by Mass Hunter according to the noise algorithm "ASTM" with a noise SD multiplier = 5.0.

2.5.2 Quantification

Quantification was done by ISTD method using ^{13}C, ^{2}H and ^{18}O labeled PFAS homologues. An ISTD-calibration curve of eight standards between 0.1 - 200 pg μL^{-1} were prepared for each target compound. For some compounds, the highest calibrations standard was excluded to obtain a better coefficient of regression (R^2) >0.99. Obvious outliers were excluded from the calibration curves. The origin treatment and weighing of the calibration curves where chosen to obtain the best achievable accuracy for the lower end calibration standards. The mid- and higher end calibration standards were not much affected by the choice of origin treatment and weighing of the curve. For quantification of PFUnDA and PFDoDA, the calibration curve of PFDA was used, and for Br-PFOS the calibration curve of PFOS was used. Results from these three compounds may be regarded as semi-quantitative. Calibration parameters can be found in *Table 2.4*, each single calibration curve is supplied in *Figure D.1* to *Figure D.16* in the appendix.

Equation 2.1. Internal standard calibration curves.

$$y = ax + b$$

Where:

$$y = \frac{A_i}{A_g} \qquad x = \frac{M_i}{M_g} \qquad b = constant$$

$A_{i/g}$ = Chromatographic peak area of native compound (*i*) or internal standard (*g*).

$M_{i/g}$ = Amount of native compound (*i*) or internal standard (*g*).

The criteria for identification was retention time within ±5 % of the calibration standards, and confirmation was done by ratio of qualifier/quantifier MRM-transition within ±20 % of the mean ratio observed in calibration standards. For some compounds, a second MRM-transition was not available as confirmation. Comparison of retention time of mass-labeled homologues was also used for confirmation.

Recovery of the ISTDs were calculated in every sample. A recovery of 40 – 120 % was regarded as acceptable, and between 20 – 40 % were regarded as semi-quantitative. Recoveries outside these ranges were regarded as questionable.

Results were calculated to nanograms analyte per liter sample for water samples, for snow samples per liters melted snow. Results were calculated with two significant digits.

Table 2.4. Calibration parameters.

Acronym	Linear Range	R^2	Origin treatment	Weight	y = ax + b	
	[pg/µL]				a	b
PFBA	1 - 100	0.9990	Include	1/x	0.0469	7.30E-02
PFPeA	0.1 - 25	0.9988	Include	1/x	0.0447	1.11E-02
PFHxA	0.1 - 100	0.9993	Include	1/x	0.0379	3.07E-03
PFHpA	0.1 - 100	0.9989	Include	1/x	0.0435	1.79E-03
PFOA	0.1 - 100	0.9991	Include	1/x	0.0556	5.83E-03
PFNA	0.1 - 100	0.9993	Include	1/x	0.0537	3.71E-03
PFDA	0.1 - 100	0.9995	Include	1/x	0.0510	1.29E-03
PFUnDA[a)]						
PFDoDA[a)]						
PFBS	0.088 - 88	0.9980	Include	1/x	0.0668	4.53E-02
PFHxS	0.094 - 94	0.9995	Include	1/x	0.0588	3.41E-03
Br-PFOS[b)]						
L-PFOS	0.096 - 168	0.9987	Force	1/x	0.0535	
6:2 FTSA	0.095 - 95	0.9985	Force	1/x	0.0130	
FOSA	0.1 - 100	0.9984	Force	none	0.0387	
MeFOSA	0.1 - 100	0.9969	Include	1/x	0.0053	3.20E-04
EtFOSA	0.1 - 100	0.9994	Include	1/x	0.0095	5.16E-04
MeFOSE	0.1 - 100	0.9951	Force	1/x	0.0090	
EtFOSE	0.1 - 100	0.9965	Force	1/x	0.0196	

a) Calibration curve from PFDA used.

b) Calibration curve from L-PFOS used.

2.6 Data-analysis and statistics

The Unscrambler® X version 10.3 (64 bit) was used for principal component analysis (PCA) to identify patterns and similarities in the composition profiles between samples and locations. For statistical analysis, all results above MDL were included. Results below MDL were set to half MDL (Johnson et al. 2015), except values very close to MDL, which were kept as their original value. To account for relativly large concentration differences, all result data was normalized by constant row-sum normalization to with a normalization variable = 1.0. Samples were automatically grouped by principal component 1 (PC-1) in the score plots (PC-1 vs. PC-2 and PC-2 vs. PC-3).

Excel 2013 with Analysis ToolPak was used for linear regression to determine the relationship between PFOA, PFNA and L-PFOS measured in this study and parallel samples at same time and location.

3 Quality assurance and Quality control

3.1 Contamination control

3.1.1 Sampling

Unused sample bottles were cleaned using three portions of 10 to 25 mL of methanol. Bottles previously used for similar samples were rinsed by three portions of approx. 25 mL of MilliQ-water before methanol rinsing.

Sample containers and equipment without fluoro-polymers were chosen. Contact between outdoor clothing containing fluoro-polymers and samples/sample-equipment were avoided. Nitrile gloves were used during all handling of the samples.

3.1.2 Sample preparations

All glassware was cleaned in dishwasher machine where the program included rinse with MilliQ water, then manually rinsed with acetone followed by methanol using Pasteur pipettes. The opening was covered with aluminum foil, before it was burned in a muffle furnace at 450 °C for 6 hours. Plastic tubes and other items that could not be burned, was cleaned thoroughly with methanol. Pre-cleaned equipment was packed in aluminum foil to avoid recontamination.

Fume hoods and other working surfaces were cleaned to remove visible dirt and dust, and then rinsed with methanol. Working surfaces were covered with aluminum foil, which was replaced regularly.

Contact between ambient air and liquid surfaces of samples, extracts and reagents was minimized as far as possible. Open waste containers were avoided in the same fume hood as sample extraction. All contact with fluoro-polymers, e.g. PTFE, was avoided.

Only MilliQ-water purified through Oasis WAX SPE-cartridges (WAX-water) was used for reagents and blanks.

3.1.3 Instrumental analysis

Previous studies have recommended replacing all fluorinated seals and tubings with non-fluorinated alternatives, and using a scavenger cartridge between pump and injector to remove contaminats from the degasser, connecting tubes and mobile phase (Ahrens 2011). However, no modifications were done to the instrument in this study.

For every tenth injection of sample or blank, and instrument blank consisting of pure methanol was injected.

3.2 Traceability

All samples were given unique identities, with consecutive numbers starting from “PFC-JSS-001”, and all information regarding each sample was noted in the sampling protocol (*Table E.1* in the appendix).

3.3 Blanks, detection- and quantification limits

Field blanks were prepared by filling 250 mL of WAX-water to pre-cleaned 1 L polyethylene- or 2 L polypropylene bottles. The cap of the field blanks were left open for the whole duration of sampling at each site (5 to 10 minutes). The field blanks were transported, stored, extracted and analysed as for regular samples.

Laboratory/method blank was prepared by adding 250 mL of WAX-water to three pre-cleaned 250 mL polyethylene bottles. They were further extracted and analysed as described for samples.

Filtration blank were prepared by filling 250 mL of WAX water into a 2 L polypropylene bottle, the blank was filtrated, extracted and analysed as described for samples.

Volume-reduction blank was prepared by adding 4 mL for methanol and 50 µL of each internal standard into a pre-cleaned 15 mL polypropylene tube. It was evaporated and further treated as described for sample extracts.

As instrumental blank, 10 µL of methanol was injected for every 10 samples or matrix blanks injected.

Instrument detection limit (IDL): determined by the amount that gave S/N = 3 in standard. Determined by the three lowest calibrations standards.

Method detection limit (MDL): determined by the amount in real samples that gives S/N = 3. Because of high blank contamination, MDL for PFBA was determined by mean amount in field blanks plus three times the standard deviation.

Limit of quantification (LOQ) was set to mean blank amount plus five times the standard deviation. For components not detected in field blanks, the amount giving S/N = 10 in real samples was used as LOQ.

Table 3.1. Detection and quantification limits.

Acronym	IDL [ng]	MDL [ng]	MDL 2L sample [ng/L]	LOQ [ng]	LOQ in 2L sample [ng/L]
PFBS	0.003	0.005	0.003	0.050[b]	0.025
PFHxS	0.003	0.011	0.0055	0.012	0.006
Br-PFOS	NA	0.023	0.012	0.038[c]	0.019
L-PFOS	0.003	0.029	0.015	0.040	0.020
6:2 FTSA	0.015	0.015	0.008	0.27	0.14
PFBA	0.084	1.00[a]	0.50	1.37	0.68
PFPeA	0.012	0.047	0.024	0.20	0.10
PFHxA	0.025	0.056	0.028	0.18	0.090
PFHpA	0.032	0.066	0.033	0.18	0.089
PFOA	0.059	0.061	0.031	0.28	0.14
PFNA	0.026	0.042	0.021	0.17	0.085
PFDA	0.017	0.016	0.008	0.071	0.036
PFUnDA	NA	0.018	0.009	0.025	0.12
PFDoDA	NA	0.009	0.005	0.032[d]	0.016

a. Determined by average fieldblank + 3SD
b. Set to same the lowest calibration level.
c. In order to get LOQ>MDL, LOQ was determined by average field blank + 10 SD.
d. No blank contamination, LOQ set to S/N = 10 in real sample.
NA = no standards were available for the calculation.

All blank values are supplied in *Table E.11* to *Table E.15* in the appendix, and selected chromatograms are available in *Figure G.1* to *Figure G.18* in the appendix. PFBA was the major contaminant observed in the field blanks- and laboratory blank, with mean amount detected at respectively 436±186 and 624±46 pg. Average amount in field blank for other PFCAs were ranging from 23 to 64 pg, for PFSAs 4 to 10 pg and 27 pg for 6:2 FTSA. Similar amounts were found in laboratory blanks. All samples were initially analysed with an instrument where PFBA had been used as an ion-pairing reagent. This instrument was most likely the source of PFBA contamination, and possibly other PFCAs. This brings some concerns towards over-estimations of PFBA in samples caused by added contamination. However, compared with results from

Rakovic et al. in *section 3.6*, PFBA was slightly under-estimated. This comparison indicated that an appropriate MDL and LOQ was chosen in order to account for contamination issues. Rakovic et al. used the same facilities and equipment for extraction of water samples at UNIS, and observed significantly lower contamination of PFBA, lower contamination of PFHxA, PFHpA, PFOA, PFBS and PFOS, and no contamination of other PFCAs and PFSAs (Rakovic et al. in prep.). These results indicate that contamination from the first instrument used for analysis was the major source of contamination, and not the sampling and extraction procedures.

3.4 Recovery

Recoveries of the internal standards (ISTDs) added before extraction relative to the recovery standard (RSTD) added before instrumental analysis were calculated for all samples and matrix blanks in this study. ISTD recoveries between 40 and 120 % were considered acceptable. Recoveries between 20 – 40 % were regarded as questionable, and results from these should be regarded as semi-quantitative.

Absolute recoveries of native analytes were examined in samples from one sample location at Lake Linnévatnet in June 2015 and in blank samples. The native-spiked sample matrix was prepared by dividing each of two 2L samples from the same site into two sub-samples of approx. 1L each in PP-bottles, in total four sub-samples. These four sub-samples were then spiked with 50 µL of the native spike-mix (*Table B.7* in the appendix), and mixed manually by shaking. The preparation of the native-spiked blanks sample is described under *section 3.5*. Native-spiked samples were extracted as described for samples. Absolute recoveries were calculated relative to the recovery standard (RSTD); spiked samples were corrected for background levels *(Equation 3.1A)*.

Equation 3.1. Calculation of the recovery of (A) native and (B) ISTD compounds and their RFFs (C and D).

A)
$$\eta_i\ (\%) = \left(\left(\frac{M_{RSTD} \cdot A_i \cdot RFF_i}{A_{RSTD}}\right) - (C_{sample} \cdot V_{sample})\right) \cdot \frac{1}{M_{i(spiked)}} \cdot 100\%$$

B)
$$\eta_g\ (\%) = \frac{M_{RSTD} \cdot A_g \cdot RFF_g}{M_{g(spiked)} \cdot A_{RSTD}} \cdot 100\%$$

C)
$$RFF_i = \frac{M_i \cdot A_{RSTD}}{M_{RSTD} \cdot A_i}$$

D)
$$RFF_g = \frac{M_g \cdot A_{RSTD}}{M_{RSTD} \cdot A_g}$$

$\eta_{i/g}$ (%) = Absolute recovery in percent of added native compound (*i*) or internal standard (*g*) added to sample.

$RFF_{i/g}$ = Relative response factor for native compound (*i*) or internal standard (*g*) relative to the recovery standard (RSTD) (These response factors were not used for quantification in samples).

$M_{i/g/RSTD}$ = amount added in nanograms of individual native compound (*i*), internal standard (*g*) or recovery standard (RSTD).

$A_{i/g/RSTD}$ = Chromatographic peak area of individual native compound (*i*), internal standard (*g*) or recovery standard (RSTD).

C_{sample} = concentration (ng L^{-1}) of native compound (*i*) in sample calculated by same RFF_i as for the recovery.

V_{sample} = volume of spiked sample in liters.

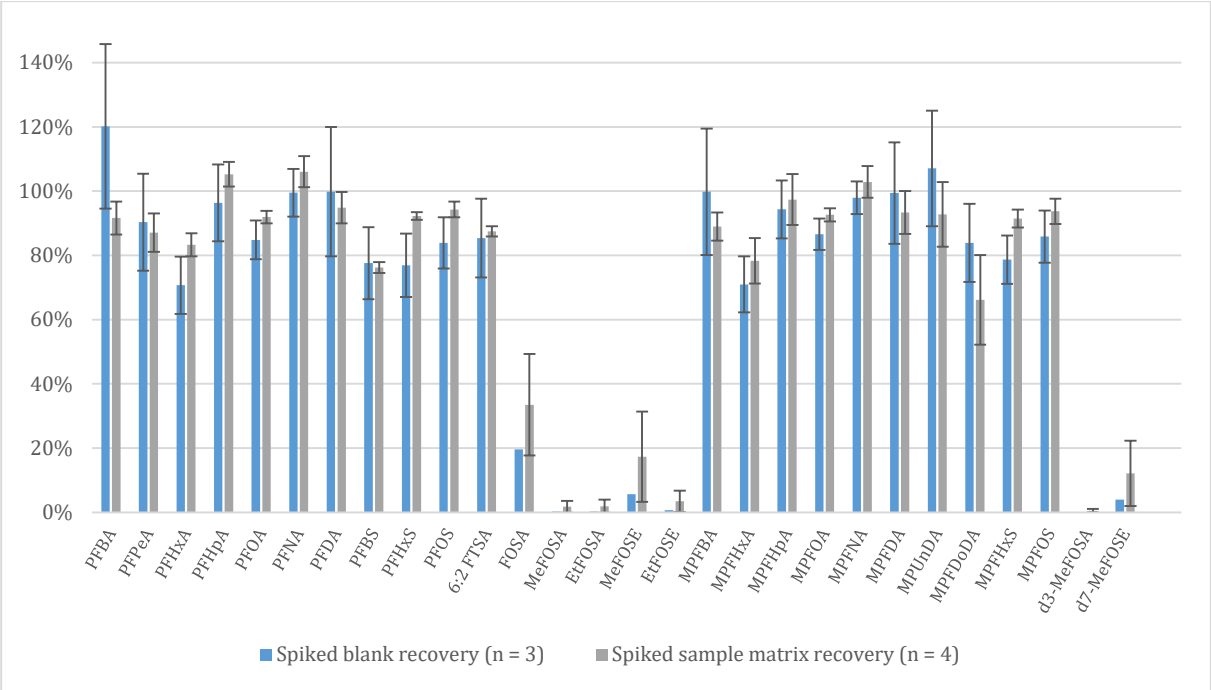


Figure 3.1. Absolute recovery of native and mass-labeled standards spiked in sample matrix and blanks.

Table 3.2. Mean native- and ISTD recoveries in samples and blanks.

Acronym	Spiked blank (n = 3)		Spiked sample matrix (n = 4)		Samples (n =30 / 61[a])		Field blanks (n = 4 / 12[a])		Lab. Blanks (n = 4 / 6[a])	
	Mean (%)	SD (%)	Mean (%)	SD (%)	Mean (%)	SD (%)	Mean (%)	SD (%)	Mean (%)	SD (%)
PFBA	120	26	92	5.1						
PFPeA	90	15	87	6.0						
PFHxA	71	8.9	83	3.6						
PFHpA	96	12	105	3.9						
PFOA	85	6.0	92	1.9						
PFNA	99	7.4	106	4.9						
PFDA	100	20	95	4.9						
PFBS	78	11	76	1.7						
PFHxS	77	9.9	92	1.2						
PFOS	84	8.0	94	2.4						
6:2 FTSA	85	12	87	1.6						
FOSA	20		34	16						
MeFOSA	0.3		1.8	1.8						
EtFOSA	0.3		1.9	2.0						
MeFOSE	5.7		17	14						
EtFOSE	0.7		3.4	3.3						
MPFBA	100	20	89	4.4	81	19	90	6.3	87	6
MPFHxA	71	8.7	78	7.1	66[a]	21	57[a]	16	63[a]	17
MPFHpA	94	9.0	97	7.9	84[a]	24	78[a]	20	82[a]	24
MPFOA	87	4.9	93	2.0	88	13	86	5.3	87	5.4
MPFNA	98	5.1	103	4.9	94	15	85	7.3	99	5.5
MPFDA	99	16	93	6.6	88	16	83	4.2	88	5.9
MPUnDA	107	18	93	10	84	20	79	1.4	87	7.8
MPFDoDA	84	12	66	14	62	18	54	11	67	13
MPFHxS	79	7.5	91	2.8	78	13	80	4.3	86	4.3
MPFOS	86	8.1	94	3.9	82	14	72	5.6	82	3.8
d3-MeFOSA	0.1		0.5	0.6						
d7-MeFOSE	3.9		12	10						

a. For the first samples extracted (sample ID from PFC-JSS-001 to 042) only ISTD-mix A was added before extraction, ISTD-mix B was added after extraction and used for quantification.

ISTD-mixture B was not acquired until June 2015, therefor samples extracted before this were added ISTD-mix B prior to instrumental analysis and used for the quantification of corresponding compounds. For these samples, MPFHxA and MPFHpA were used to assess extraction efficiency.

Mean recoveries for native PFCAs, PFSAs and 6:2 FTSA in sample matrix was in the range of 76 to 106 %, and for native FOSAs and FOSEs 1.8 to 34 %. Mean recoveries of internal standards for PFCAs and PFSAs in samples were in the range of 66 to 94 %, and recoveries for $^{2}H_{7}$-MeFOSE and $^{2}H_{3}$-MeFOSA in spiked sample matrix were 12 and 0.5 % respectively. Recoveries in field- and laboratory blanks were in a similar range. Recoveries of each ISTD in individual samples are provided in *Table E.2* in the appendix.

Higher and less variable recoveries for PFCAs ($6 \leq C \leq 9$) and PFSAs were observed in spiked samples compared to spiked blanks. This observation might be attributed to higher solubility of PFASs in de-ionized water, at thus higher break-through.

Most of the observed low recoveries, could be explained by discrepancies reported in the analytical protocol (*Table E.1* in the appendix). Some examples will be mentioned; two samples were by accident eluted with 1.44 mL instead of 4 mL, and obtained recoveries between 38.2 and 53.0 % for MPFHxA and MPFHpA. One extract was accidentally spilled in the fume hood during volume reduction, and attempted recovered in the vial, obtained recoveries between 14.6 and 24.1 % for PFCAs and PFSAs. Accidental evaporation to dryness did however not seem to adversely affect the recoveries of PFCA and PFSA ISTDs. Recoveries in five samples, of which extracts were accidentally evaporated to dryness, obtained recoveries in the range of 62.8 to 106.1 % for MPFHxA and MPFHpA.

In samples from downstream the FFTS at the airport, recoveries of both below 20 % and above 120 % were observed in the same samples. This was consistent throughout three sample replicas. These observations might be caused by matrix-effects yielding ion-suppression or ion-enrichment in the MS. The affected ISTDs (and their recoveries) were MPFBA (15.0 – 16.4 %), MPFHxA (43.2 – 47.1 %), PFDA (111 – 134 %), PFUnDA (143 – 155 %) and PFDoDA (154 – 174 %). Since both MPFBA and MPFHxA were affected, it is likely also for PFPeA, of which no mass-labeled ISTD was available for this study. Results for analytes using these ISTDs were included in the study because of their significant contributions to the total PFAS content, despite unacceptable recoveries. They should however be regarded as semi-quantitative.

Matrix effects are compound dependent, and is caused by the competition between matrix substances and the analytes to access the droplet surface for transfer to the gas phase in the electrospray (Taylor 2005). Various matrix properties can affect ionization, such as surface tension (Apffel et al. 1995), and humic and fulvic acids, which elute early when using a high aqueous mobile-phase (Cullum et al. 2004). In a 2007 inter-laboratory comparison study by Van Leeuwen et al., some participating laboratories observed ion-suppression for PFBA to PFHpA (highest for PFBA). This was explained by possible co-elution of early eluting organic acids and complexes (e. g. humic acids) from the sample matrix (Van Leeuwen et al. 2009). Extracts of the above-mentioned FFTS-samples were yellow in color, possibly indicating presence of humuc/fulvic acids, which might explain ion-suppression for short-chain PFCAs eluting early. High concentrations of detected PFASs, and possibly unknown PFASs from AFFF-emissions, might have reduced the surface tension, thus caused ion-suppression/enrichment. Possible preventative measures would have been to reduce sample volume to minimize amount of co-extracted matrix, dilution of the sample extracts, a more thorough clean-up step for the SPE or further clean-up of the sample extracts.

Previous studies, of which the extraction procedure in this study was based on, have been using 150 mg of WAX sorbent in SPE cartridges (Ahrens et al. 2010). In this study, 500 mg sorbent was used without modifying the elution volumes and no experiments were done to validate appropriate elution volumes. However, acceptable recoveries of the internal standards for the ionic PFASs indicate that the elution volumes were suitable for these compounds.

Very low and highly variable recoveries were obtained for the neutral PFASs. In fraction two, containing the ionic PFASs, peaks of internal standards from fraction one, $^{2}H_{7}$-MeFOSE and $^{2}H_{3}$-MeFOSA, were observed. These low recoveries and observation of FOSA and FOSE ISTDs in fraction two, could indicate insufficient elution volume for the neutral PFASs, however other analytical challenges such as volatilization during volume-reductions of extracts seems to be of more importance to the low recoveries of these compounds. Because of these low and fluctuating recoveries observed, mass-labeled internal standard for each single compound should have been chosen in order to identify compound-specific losses during sample extraction and analysis. In a 2007 inter-laboratory comparison study by Van Leeuwen et al., they concluded that $^{2}H_{3}$-MeFOSA was unsuitable as an internal standard for FOSA after several different laboratories reported significant losses. They hypothesized that losses were caused by degradation of MeFOSA when in contact with water or losses due to low solubility. Experiments showed that sorption to the LC-vial caused significant decrease in concentration (Van Leeuwen et al. 2009). In this study, a recovery of 34±16 % was found for native FOSA spiked in sample matrix (n=4), indicating that FOSA could have been quantified using an appropriate internal standard, e.g. $^{13}C_{8}$FOSA from Wellington Laboratories (Guelph, Ontario, Canada).

Because of low recoveries, the neutral PFASs will not be further discussed in this study.

3.5 Break-through

Three polypropylene bottles, each containing 2 L of WAX-water as a blank, was spiked with 5 or 50 ng of each native compounds, depending on the concentration in the native spike mix (*Table B.7* in the appendix, 50 µL of the spike mix). The bottles were weighed, added ISTDs and extracted as for samples subsequently on two Oasis WAX 6cc 500 mg cartridges placed on top of each other connected by a reservoir adapter. Break-through was determined by calculating the percentage of the chromatographic peak area of each compound in the lower cartridge compared to the top cartridge. The top cartridge was also used to determine recovery of native and mass-labeled compounds in a blank sample.

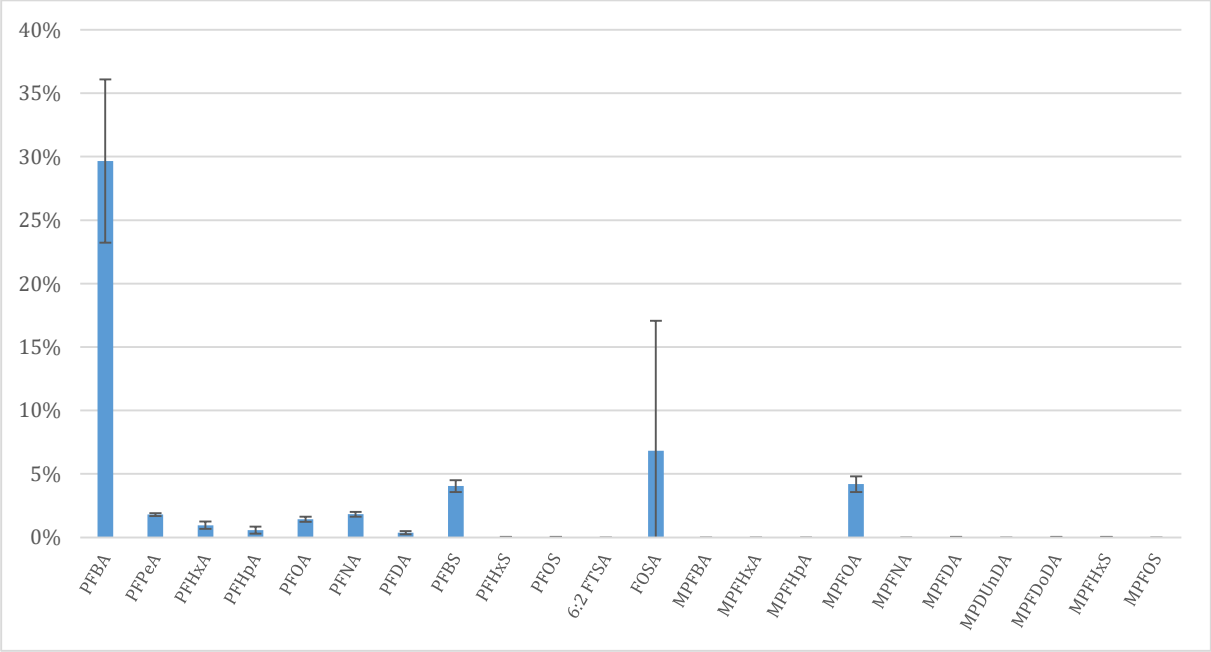


Figure 3.2. Breakthrough results.
Breakthrough from first to second SPE of native and mass-labeled PFASs spiked into 2 L of WAX water.

Breakthrough was not calculated for Me/Et-FOSA/FOSE compounds because of low recoveries.

The high amount of observed breakthrough for PFBA was most likely a blank issue and not breakthrough, because no breakthrough of the ^{13}C-labeled PFBA was observed. This blank issue was most likely also the case for the observed signal of the native PFCAs. PFPeA, PFBS and FOSA did not have ^{13}C-labeled homologues, thus it was difficult to conclude if the observed signal was a blank signal or breakthrough. For MPFOA ($^{13}C_4$ PFOA), parts of the observed breakthrough was likely originating from the $^{13}C_8$PFOA used as RSTD, which in the analytical certificate had reported a 2.1 % impurity of $^{13}C_4$ PFOA.

Based on this breakthrough experiment, the capacity of the SPE-sorbent was sufficient for sample volumes selected for extraction in this study.

3.6 Repeatability and reproducibility

Repeatability was determined by the mean RSDs of sample replicas from the same site. Reproducibility was determined by the mean percent difference between parallel samples taken at same time and location by Rakovic et al. , analysed separately in a different laboratories(Rakovic et al. in prep.). Only results above LOQ were included for comparison.

Mean RSDs were all below 30 %. The mean between-laboratory difference was below 30 % for most compounds, except PFBA, PFHxA and PFUnDA. For PFNA, which had one of the highest detection frequencies in both studies, the mean inter-laboratory difference was 3.0 % and the mean RSD was 12 %.

In an inter-laboratory comparison in 2009 with 20 different laboratories from 9 different countries participating, they found repeatability (within laboratory precision) in the range of 3 – 11 % and reproducibility (inter-laboratory precision) in the range of 7 – 31 % for various PFASs in surface water (Taniyasu et al. 2013a). For PFOS (6.63 ng L^{-1}) and PFOA (5.08 ng L^{-1}) in river water, repeatability was 6 % for both, and reproducibility was 27 and 29 % respectively.

It was challenging to achieve good repeatability and reproducibility in this study, because many of the results were close and even below the detection limits. However, the mean between-laboratory difference in this study was in the same range as reproducibility at much higher concentrations in the inter-laboratory comparison by Taniyasu et al. Based on this, the precision of the method used in this study can be considered acceptable.

Figure 3.3 show correlation plots for PFOA, PFNA, PFOS with results from this study compared to Rakovic et al. , these particular compounds where selected for their high detection frequencies in samples from both studies. The results show a significant linear relationship ($p < 0.05$) with R^2 values between 0.75 and 0.93. For PFNA it seems to be a stronger linear relationship at lower concentrations, as differences increase with higher concentrations.

Table 3.3. Repeatability and reproducibility results.
Repeatability determined as mean RSD for sample replicas and reproducibility as mean percent between-laboratory difference (Rakovic et al. in prep.).

	Repeatability						Reproducibility					
Acronym	n	Mean RSD (%)	Median RSD (%)	SD (%)	Min (%)	Max (%)	n	Mean difference. (%)	Median difference (%)	SD (%)	Min (%)	Max (%)
PFBA	6	11	7.4	10	1.8	30	5	-31	-37	19	-44	1.9
PFPeA	3	20	22	5.9	13	24	2	-9.6	-9.6	6.6	-14	-5.0
PFHxA	6	14	13	8.5	5.8	30	5	40	3.0	97	-31	209
PFHpA	9	17	14	13	4.3	37	5	-19	-28	34	-51	37
PFOA	11	14	12	8.9	2.6	28	9	-27	-25	15	-57	-1.0
PFNA	9	12	12	7.4	1.6	22	10	3.0	-6.4	27	-37	50
PFDA	8	13	12	9.6	3.1	28	5	16	6.4	48	-34	95
PFUnDA	0	NA	NA	NA	NA	NA	2	74	74	117	-9.2	157
PFDoDA	6	19	21	8.8	3.3	28	0	NA	NA	NA	NA	NA
PFBS	2	27	27	36	1.8	53	0	NA	NA	NA	NA	NA
PFHxS	10	26	24	26	0.1	94	0	NA	NA	NA	NA	NA
Br-PFOS	10	14	7.9	12	4.5	40	0	NA	NA	NA	NA	NA
L-PFOS	11	15	13	13	3.9	40	10	9.5	-15	49	-32	103
6:2 FTSA	1	2.0	2.0	NA	2.0	2.0	0	NA	NA	NA	NA	NA
ΣPFCA	11	19	7.3	23	1.6	73	10	-30	-39	41	-67	73
ΣPFSA	11	20	11	27	0.9	98	10	-9.9	-23	53	-92	103
ΣPFAS	11	13	6.8	17	0.1	57	10	-24	-39	45	-59	92

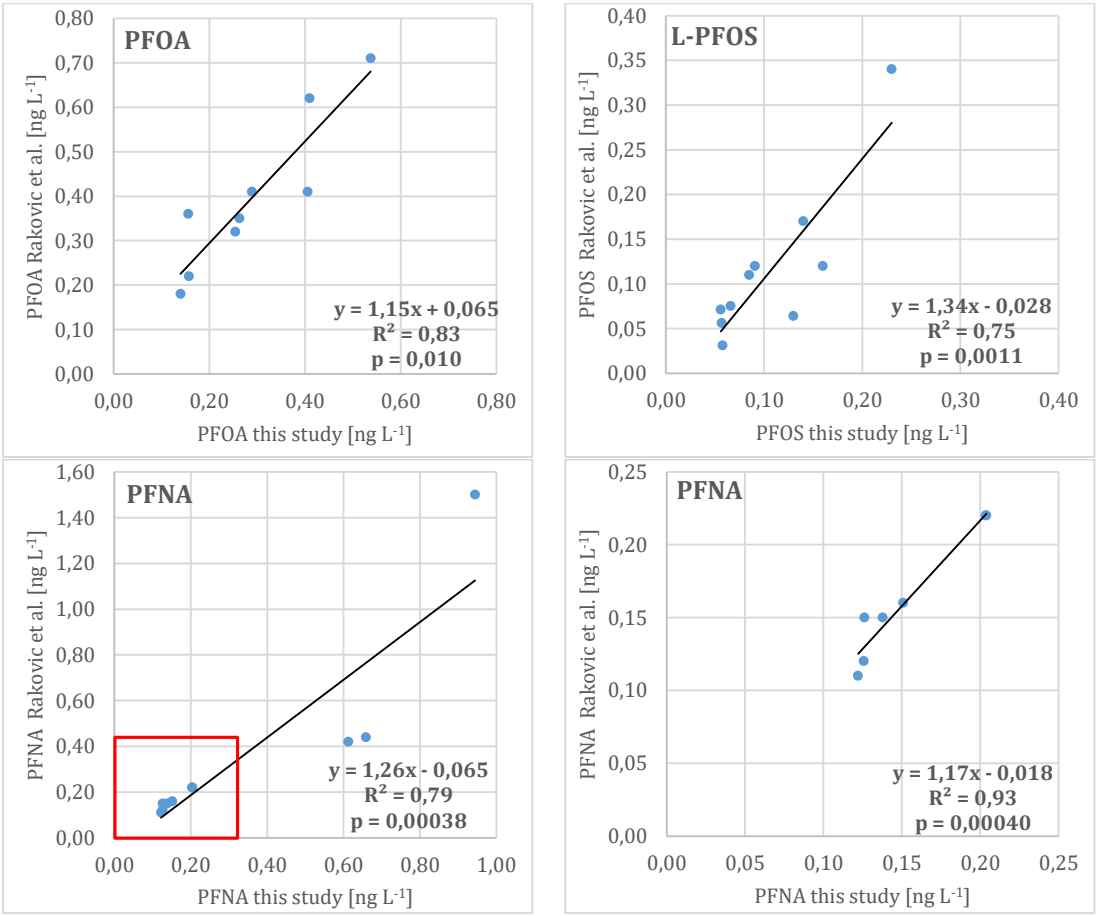


Figure 3.3. Correlation plots between selected compounds from this study and Rakovic et al.

4 Results

4.1 Water characteristics

The analytical method used, and detailed results for water characteristics can be found in the appendix. Calcium, magnesium, sulfate and bicarbonate are the dominating ions in the water. The overall ion content was 40 % higher in April 2015 compared to levels determined in August 1968. However, the ion composition profile is similar. This observed difference was probably caused by the lack of meltwater inflow to dilute the surface water of the lake in April, thus making the surface water more saline. The bedrock in the catchment area mainly consists of Carboniferous-Permian limestones/gypsum and sandstones (Svendsen et al. 1989). Sulfate is accounting for approx. 60 % of the anions, meaning the lake can be classified as a typical sulfate lake according to Bøyum & Kjensmo. High levels of calcium, magnesium and sulfate is probably originating from gypsum in the bedrock (Bøyum & Kjensmo 1978).

Table 4.1. Depth in meters, conductivity in µS cm^{-1} and ion concentrations in meq L^{-1}.

Date	Depth	pH	Cond	Ca	Mg	Na	K	HCO_3	SO_4	Cl
Apr 18, 2015[a]	0.2	7.97	305,7	2.04	0.81	0.1923	0,0086	1.003	2.04	0.1633
Aug 20, 1968[b]	1	7.4	158	1.449	0.663	0.154	0.007	0.726	1.313	0.147

a. this study, sample site L4
b. (Bøyum & Kjensmo 1978)

Table 4.2. Relative ion-composition in Lake Linnévatnet.

Date	Ca	Mg	Na	K	HCO_3	SO_4	Cl
Apr 18, 2015[a]	33 %	13 %	3.1 %	0.14 %	16 %	33 %	2.6 %
Aug 20, 1968[b]	32 %	15 %	3.5 %	0.16 %	16 %	29 %	3.3 %

4.2 Sample results

Results from the FASAs, and FASEs, were rejected due to of their low recoveries, results for the remaining 14 analytes were reported. Results are presented as the median, minimum and maximum concentrations (ng L^{-1}) for sample site were replicate samples were collected, or as single results if not.

Results for Lake Linnévatnet are presented in *Table 4.3* and *Figure 4.1*, and remaining samples in *Table 4.4* and *Figure 4.1*. Figures illustrating the spatial distribution in Lake Linnévatnet in April 2015 and June 2015 are provided in *Figure 4.2* and *Figure 4.3*, and a figure illustrating the temporal variation between March 2014, April 2015 and June 2015 is provided in *Figure 5.1*. Individual sample results are available in *Table E.9* in the appendix. Example chromatograms are presented in *Figure G.1* to *Figure G.18* in the appendix. Reported values for sum PFAS include all 14 PFASs analysed with values above the quantification limit, sum PFCA include nine PFCAs ranging from C_4 through C_{12}, Sum PFSA include PFBS, PFHxS, PFOS (branched and linear) and 6:2 FTSA. 6:2 FTSA was included in the sum PFSA because it was the only FTSA analyzed, however levels were below the quantification limit in most samples.

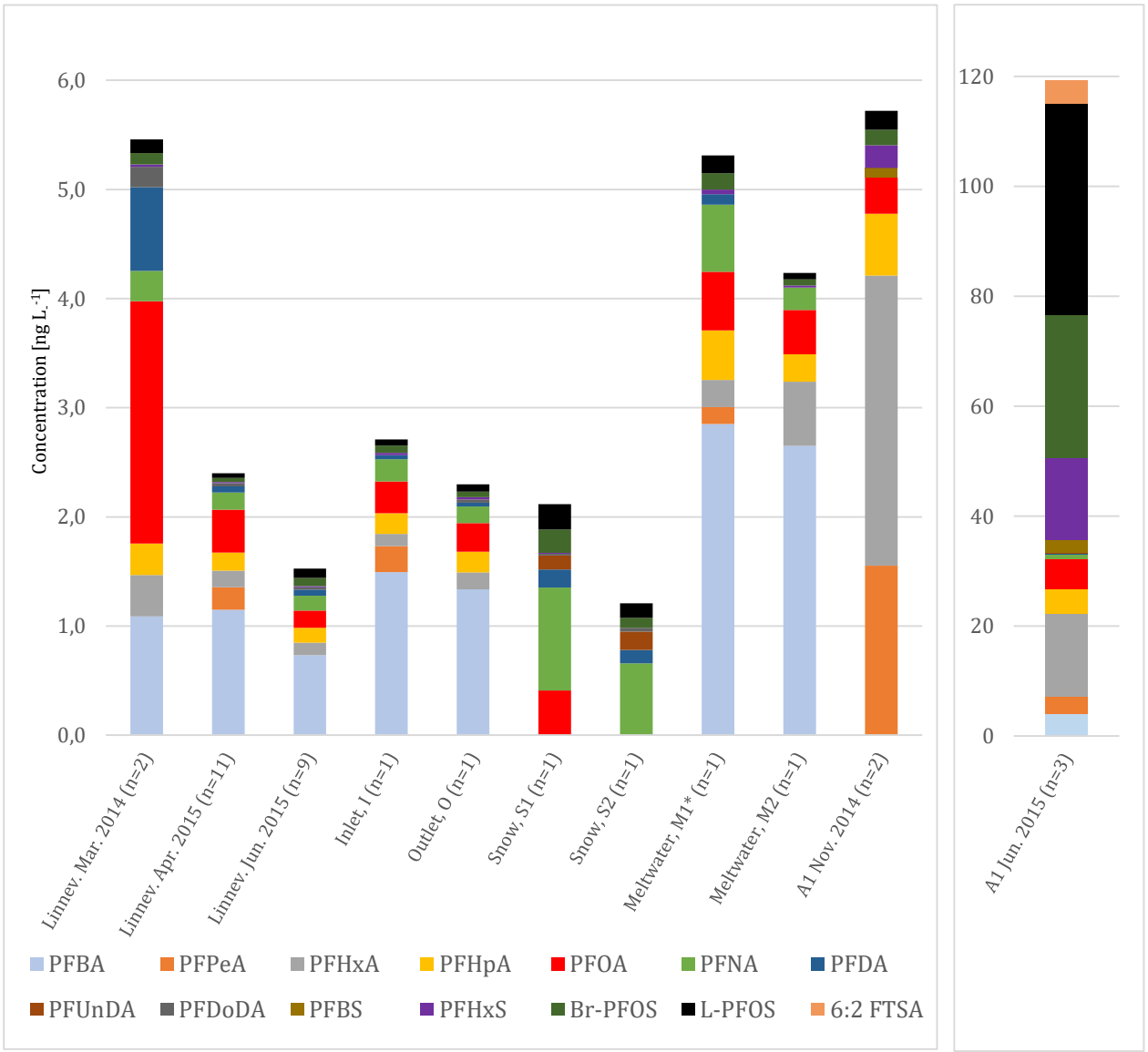


Figure 4.1. Graphical result overview of median concentrations at each site.

Table 4.3. Sample results from Lake Linnévatnet from March 2014, April 2015 and June 2015. Concentrations in ng L^{-1}.

Analyte	L5 March 2014 (n = 2)			Linnévatnet April 2015 (n = 12)			Linnévatnet June 2015 (n = 11)		
	Median	*Min.*	*Max.*	Median	*Min.*	*Max.*	Median	Min.	Max.
PFBA	1.1	*<0.69*	*1.09*	1.1	*0.86*	*5.2*	ND	*ND*	*0.89*
PFPeA	<0.10	*<0.10*	*<0.10*	<0.099	*ND*	*0.21*	ND	*ND*	*<0.090*
PFHxA	0.38	*0.34*	*0.41*	0.14	*<0.080*	*0.38*	<0.081	*ND*	*0.13*
PFHpA	0.29	*0.26*	*0.32*	0.17	*0.13*	*0.53*	<0.080	*<0.078*	*0.15*
PFOA	2.2	*1.78*	*2.66*	0.39	*0.18*	*1.36*	0.16	*0.13*	*0.30*
PFNA	0.28	*0.24*	*0.32*	0.16	*0.10*	*0.32*	0.14	*0.11*	*0.16*
PFDA	0.77	*0.61*	*0.92*	0.056	*<0.034*	*0.12*	0.057	*0.048*	*0.086*
PFUnDA	<0.13	*<0.13*	*<0.13*	<0.12	*<0.11*	*<0.25*	<0.11	*<0.11*	*<0.11*
PFDoDA	0.19	*0.16*	*0.22*	0.016	*ND*	*0.047*	0.021	*<0.014*	*0.026*
PFBS	<0.025	*<0.025*	*<0.026*	<0.024	*ND*	*<0.050*	<0.022	*ND*	*<0.023*
PFHxS	0.023	*0.022*	*0.023*	0.013	*<0.006*	*0.17*	0.011	*ND*	*0.016*
Br-PFOS	0.10	*0.083*	*0.12*	0.037	*0.028*	*0.11*	0.073	*0.035*	*0.095*
L-PFOS	0.12	*0.11*	*0.14*	0.041	*0.024*	*0.069*	0.085	*0.054*	*0.15*
Σ-PFOS	0.23	*0.19*	*0.27*	0.068	*0.044*	*0.18*	0.16	*0.11*	*0.23*
6:2 FTSA	<0.14	*<0.14*	*<0.14*	<0.12	*ND*	*<0.14*	<0.12	*<0.12*	*<0.12*
Σ_9-PFCA	4.7	*4.5*	*4.8*	1.9	*1.6*	*8.0*	0.60	*0.36*	*1.5*
Σ_5-PFSA	0.25	*0.21*	*0.29*	0.070	*0.051*	*0.35*	0.18	*0.12*	*0.24*
Σ_{14}-PFAS	4.9	*4.7*	*5.1*	2.0	*1.6*	*8.3*	0.77	*0.49*	*1.7*

Table 4.4. Sample results for sites A1, I, O, M1-2 and S1-2, concentrations in ng L^{-1}.

Analyte	A1 Nov. 2014 (n = 3)			A1 Jun. (n = 3)			I (n = 1)	O (n = 1)	M1 (n = 1)	M2 (n = 1)	S1 (n = 1)	S2 (n = 1)
	Median	*Min.*	*Max.*	Median	*Min.*	*Max.*						
PFBA	ND			4.0	*3.9*	*4.1*	1.5	1.3	2.9	2.7	ND	ND
PFPeA	1.6	*1.3*	*2.2*	3.2	*3.1*	*3.9*	0.24	<0.080	0.2	<0.086	ND	ND
PFHxA	2.7	*2.6*	*3.0*	15.2	*14.8*	*16.5*	0.11	0.15	0.25	0.59	<0.088	ND
PFHpA	0.57	*0.40*	*0.81*	4.3	*4.07*	*4.48*	0.19	0.19	0.46	0.25	ND	ND
PFOA	0.31	*ND*	*0.36*	5.5	*5.35*	*5.62*	0.29	0.26	0.54	0.41	0.41	<0.12
PFNA	<0.085	*ND*	*<0.092*	0.86	*0.85*	*0.87*	0.20	0.15	0.61	0.20	0.94	0.66
PFDA	ND	*ND*	*ND*	0.17	*0.15*	*0.19*	0.036	0.035	0.10	<0.031	0.17	0.12
PFUnDA	<0.13	*<0.12*	*<0.14*	<0.13	*<0.12*	*0.13*	<0.11	<0.10	<0.11	<0.11	0.13	0.17
PFDoDA	ND			<0.015	*<0.015*	*<0.016*	<0.014	0.030	ND	ND	0.017	0.035
PFBS	0.035	*<0.025*	*0.14*	2.40	*2.33*	*2.41*	<0.022	<0.020	ND	<0.022	<0.024	<0.022
PFHxS	0.21	*0.014*	*0.43*	15	*15*	*15*	0.022	0.021	0.041	0.020	0.007	ND
Br-PFOS	0.088	*ND*	*0.20*	26	*25*	*27*	0.066	0.051	0.15	0.057	0.21	0.092
L-PFOS	0.10	*ND*	*0.24*	39	*37*	*41*	0.057	0.066	0.16	0.058	0.23	0.13
Σ-PFOS	0.19	*ND*	*0.44*	65	*62*	*68*	0.12	0.12	0.31	0.12	0.45	0.22
6:2 FTSA	ND			4.3	*4.2*	*4.3*	<0.12	ND	ND	ND	<0.13	<0.12
Σ_9-PFCA	5.3	*4.8*	*5.6*	33	*33*	*35*	2.6	2.2	5.0	4.1	1.7	0.98
Σ_5-PFSA	0.43	*0.014*	*1.0*	86	*83*	*90*	0.15	0.14	0.35	0.14	0.45	0.22
Σ_{14}-PFAS	5.6	*5.3*	*6.3*	121	*117*	*122*	2.7	2.3	5.3	4.2	2.1	1.2

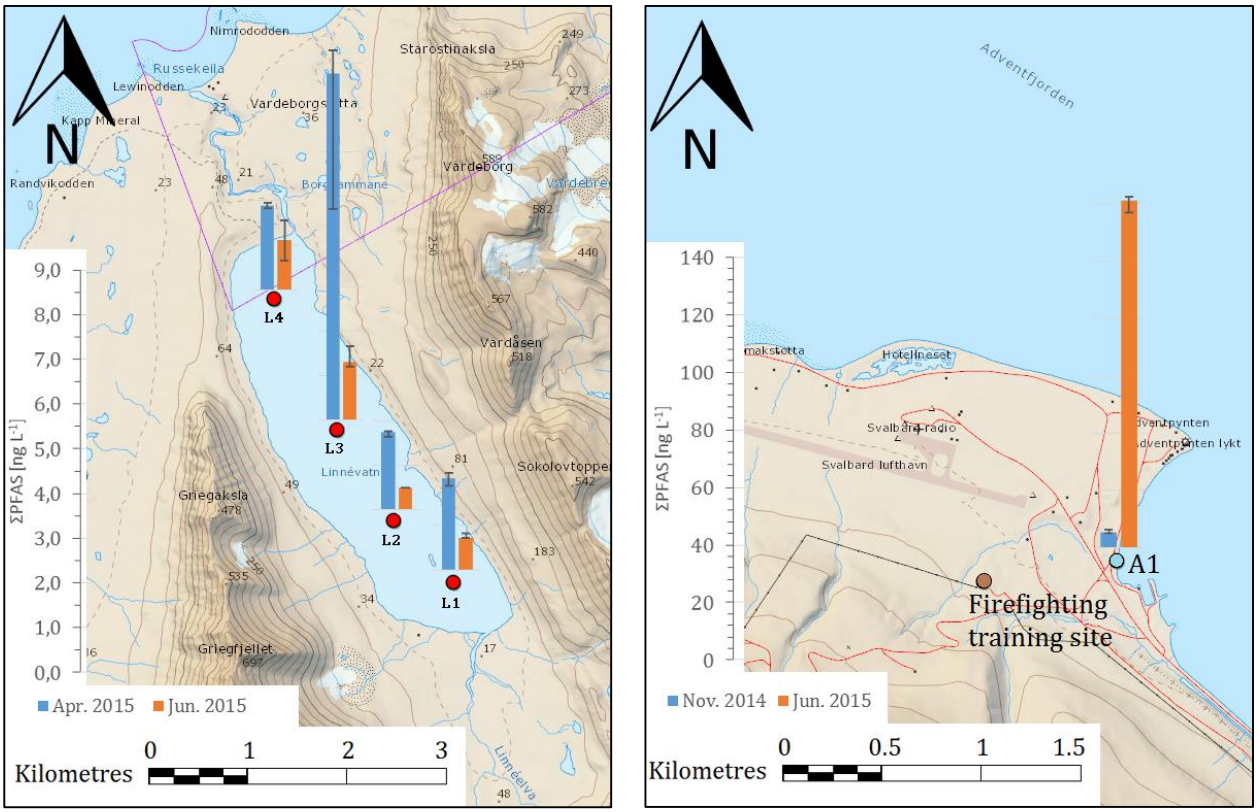


Figure 4.2. Spatial distribution of ΣPFAS in Linnévatnet and Svalbard Airport. Median ΣPFAS, whiskers represent max. and min. values. Left: results from lake Linnévatnet in April (L1: n=3, L2: n=3, L3: n=3, L4: n=2) and June 2015 (L1: n=3, L2: n=2, L3: n=3, L4: n=2). Right: Svalbard Airport (A1) in November 2014 (n = 3) and June 2015 (n = 3). Map adapted from Topo Svalbard (NPI 2015).

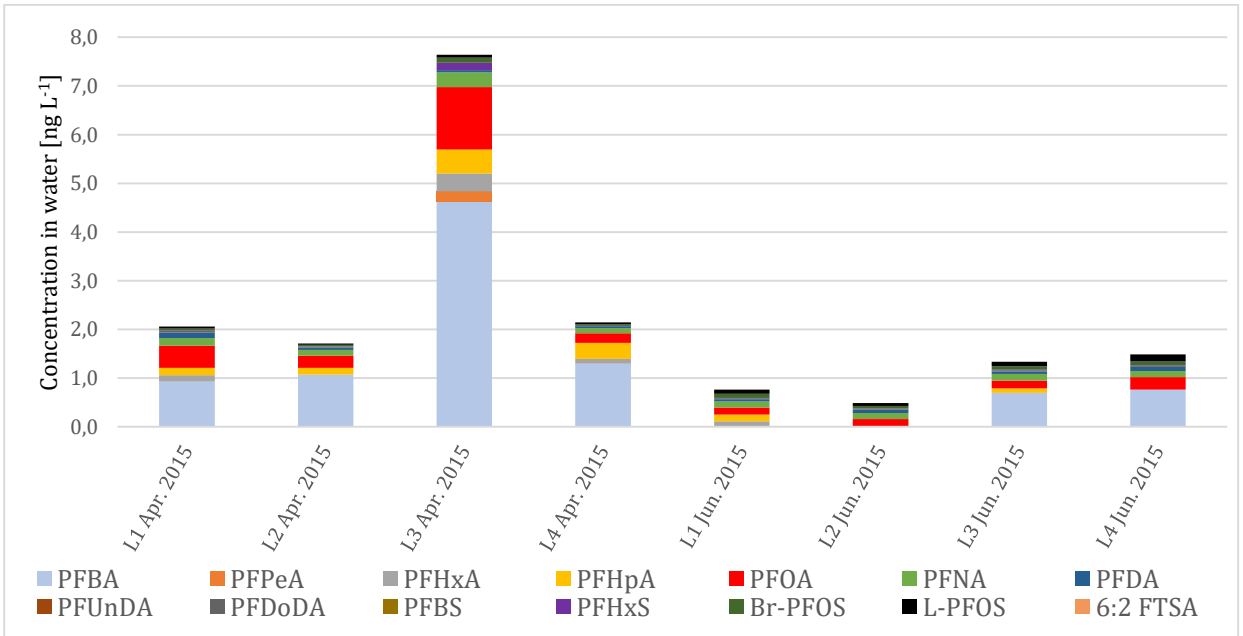


Figure 4.3. Spatial distribution of individual [PFAS] in Lake Linnévatnet from April and June 2015. Median values used.

4.3 Statistics

Principal component analysis (PCA) is a multivariate statistical method widely used in almost all scientific disciplines, including environmental chemistry. The objective of PCA is du reduce number of dimensions in a data set with a large number of inter-correlated variables. The data is transformed into a new set of orthogonal variables called principle components (PC), where the first PC explains the largest amount of variance and following PCs progressively accounts for a smaller variance in the data set (Johnson et al. 2015). Scores are new values for the observations, geometrically interpreted as projections of observations onto the principal components (Abdi & Williams 2010). Loadings are defined as the correlation between an initial variable and a principal component, and can be used to visualize which variable account for observed differences between scores(Abdi & Williams 2010).

Score plots and their corresponding loading plots of the results from this study, is presented in *Figure 4.4* and *Figure 4.5* for principal component one and two (PC-1 and PC-2) and *Figure 4.6* and *Figure 4.7* for principal component two and three (PC-2 and PC-3). Four principal components explain together 97.5 % of the variance, PC-1 (58.8 %), PC-2 (19.0 %), PC-3 (12.3) and PC-4 (7.4 %), meaning PC-1 explain the largest amount of variation in the dataset.

Scores represent individual samples from the different sample locations. Different colors represent automatic grouping by separation along PC-1. The closer a variable is to center of the loading plot, the less important it is for the first two components. Variables opposite to each other through the origin are inversely correlated.

First component indicate PFBA is inversely correlated with PFBS and PFHxS, second component seems to represent the proportion of long-chain PFCAs *(Figure 4.5)*. The samples from downstream the FFTS near the airport (A1, November 2014 and June 2015) are both grouped in clusters in the left side of the PC-1 vs. PC-2 plot *(Figure 4.4)*, clearly separated from the other sample sites. The samples from November clustered in the upper left quadrant, influenced by short-chain PFCAs PFHxA and PFPeA. The June samples clustered in the lower left quadrant, influenced by Br-/L-PFOS, PFBS, PFHxS and 6:2 FTSA.

A bit further right in the lower left quadrant, two clusters containing samples S1, and S2 and L5-1 and L5-2 together with all replicas of L1 from June, both clusters influenced by PFOS (linear and branched).

One replica of L2 and two replicas of L4 from June are clustered close to the origin in the lower right quadrant, slightly influenced by PFOA.

Remaining samples from Linnévatnet from April and June, meltwater samples, inlet and outlet are grouped in two different clusters along PC-1 axis influenced by PFBA.

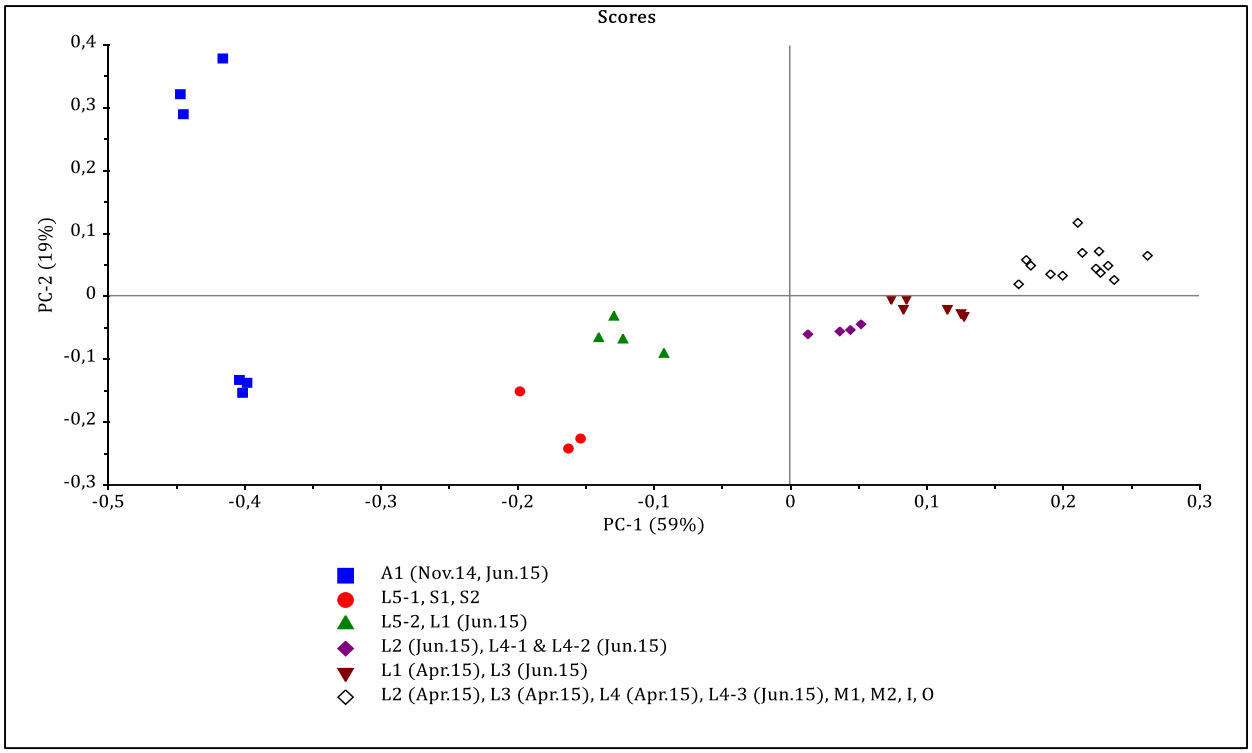


Figure 4.4. Score plot PC-1 and PC-2.
Different colors represent groping of individual samples by PC-1 (explained in legend).

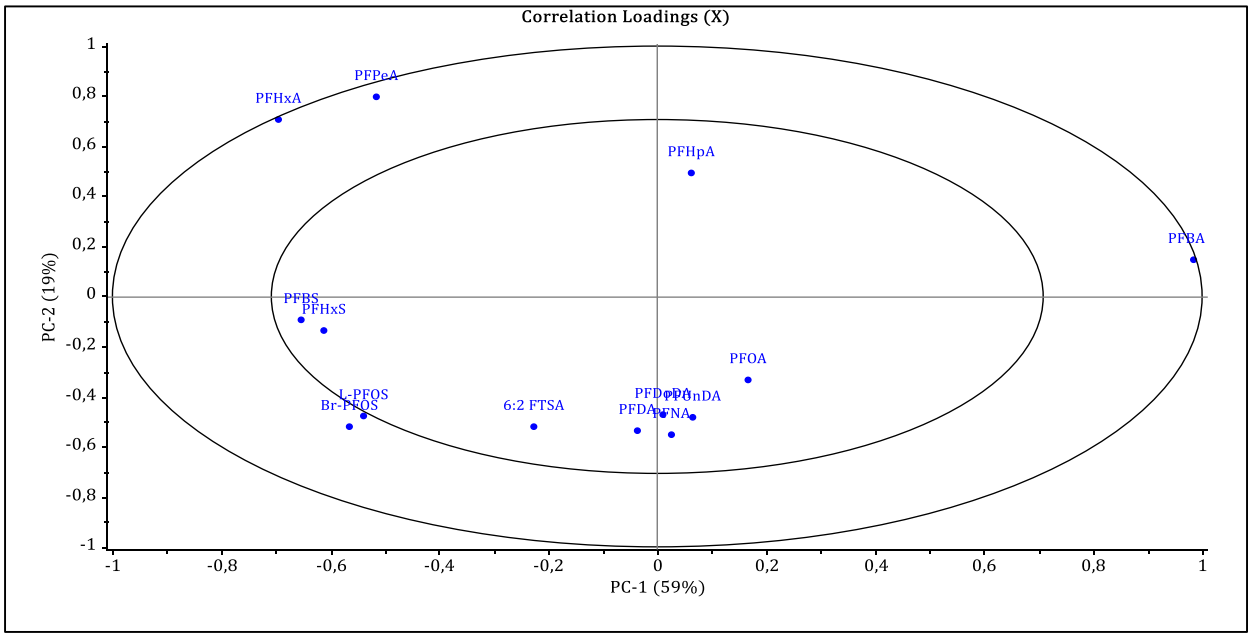


Figure 4.5. Loading plot PC-1 and PC-2.

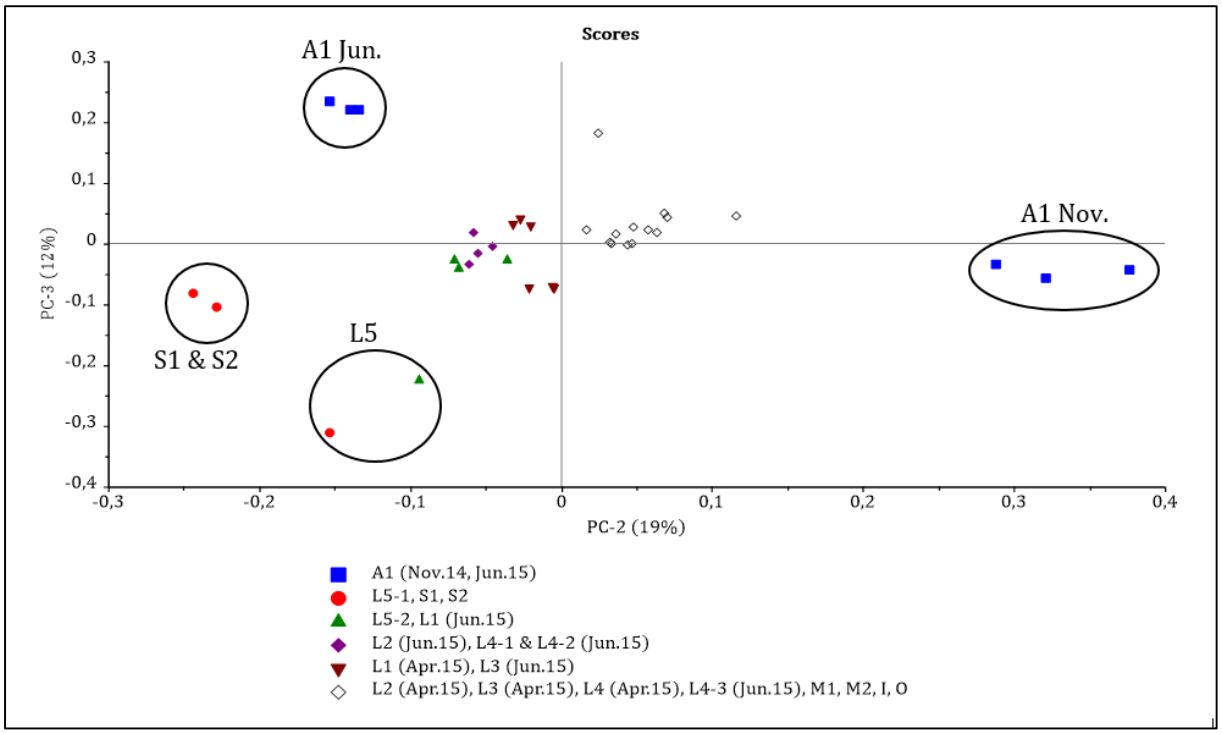


Figure 4.6. Score plot PC-2 and PC-3.
Different colors represent groping of individual samples by PC-1 (explained in legend).

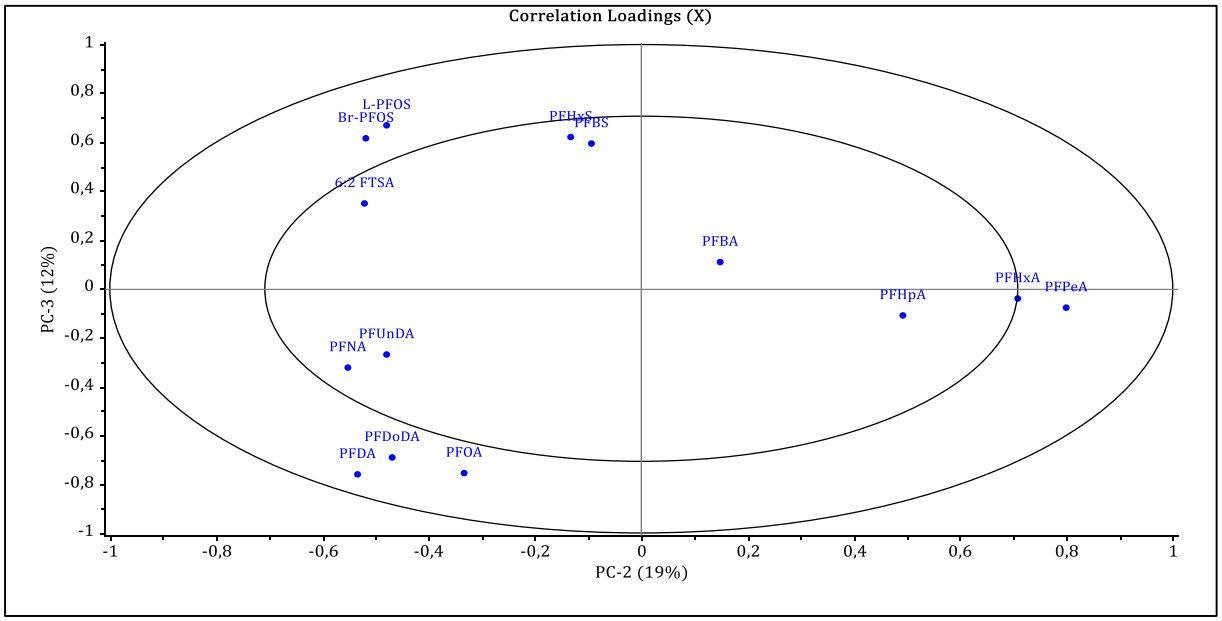


Figure 4.7. Loading plot PC-2 and PC-3.

Four distinct clusters appear in the PC-2 vs. PC-3 plot *(Figure 4.6)*. Both replicas of L5 cluster together in the lower left quadrant influenced by even numbered long-chain PFCAs (PFOA, PFDA and PFDoDA).

Both snow samples cluster together in lower left quadrant, influenced by odd numbered long-chain PFCAs; PFNA and PFUnDA.

All replicas of A1 from November were grouped high in the lower right quadrant close to the PC-2 axis, influenced by short-chain PFASs (PFPeA, PFHxA and PFHpA).

All replicas of A1 from June grouped together in the upper left quadrant, influenced by a high proportion of PFOS (both branched and linear), 6:2 FTSA, PFBS and PFHxS. Illustrating a distinct difference in patterns compared to the November 2014 samples from the same locations.

The rest of the samples, including all samples from Lake Linnévatnet in April and June 2015, inlet and outlet of lake Linnévatnet and meltwater samples, are grouped together in the same clusters as for the PC-1 vs. PC-2 plot close to the origin, indicating that no district single variable are explaining their position in the plot.

Based on the principal component analysis, the samples can be categorized in five major groups;

1) those mainly influence by PFBA
2) those mainly influences by PFOS (linear and branched)
3) those mainly influenced by short-chain PFCAs (PFPeA, PFHxA, PFHpA)
4) those mainly influenced by even numbered long-chain PFCAs (PFOA, PFDA and PFDoDA)
5) those mainly influenced by odd-numbered long-chain PFCAs (PFNA and PFUnDA)

5 Discussion

5.1 Levels in the studied sample sites

For the lake samples PFBA was in general the dominating compound in lake Linnévatnet, except in March 2015 where PFOA dominated. PFBA was also dominating river and meltwater samples, with sligtly higher concentrations than in the lake. PFBA was not detected in snow samples, where PFNA dominated. In samples from downstream the firefigting training site at the airpiort, a distict difference with PFPeA and PFHxA dominating in November 2014 and much higher concentrations with PFOS dominating in June 2015.

Similar concentrations were found between sample replica and locations in Lake Linnévatnet within each sampling campaign. In April 2015, the observed ΣPFAS was approx. 4 times higher at site L3 compared to the other sites, and levels of all quantified PFASs, except PFDA, were higher than the other sites sampled in the same campaign. This could be caused by contamination during sampling, extraction or analysis. However, almost identical composition profile as other samples from the same sampling campaign suggests a similar source as other samples from the lake. Also, repeatable results between replicas and no additional contamination in field blank weigh against this. One possibility could be contamination by nearby snow falling into the water of the drill hole. Meltwater from snow in June was found to have the same composition profile as the lake samples, but higher concentrations.

Concentrations of PFBA were in general lower in June compared to April, with concentrations ranging from 0.86 – 5.2 ng L^{-1} in April and <MDL – 0.89 ng L^{-1} in June. Most of the observed difference in ΣPFAS between sample sites in June could be explained by PFBA being below the method detection limit at two sites. Detected PFBA in June was very close to the detection and quantification limits (0.50 and 0.68 ng L^{-1}). The observed difference in ΣPFAS would possibly have been significantly smaller, if the above-mentioned contamination by PFBA giving higher detection limits had been avoided.

PFOA concentrations were more variable in April compared to June, with concentrations ranging from 0.18 – 1.4 ng L^{-1} in April and 0.13 – 0.30 ng L^{-1} in June.

Samples from Lake Linnévatnet in March 2014 showed a distict difference in both concentration-levels and composition patterns compared to samples collected later. It was dominated mainly by even numbered long-chain PFCA, PFOA being the main contributor and not PFBA and short-chain PFCAs as observed in samples from Lake Linnevatnet in April and June 2015. However, PFBA was in the same concentration range in March 2015 as for later samples, even if the relative contirbution was lower. The high contribution of even numbered long-chain PFCAs could possibly be an indication of recent atmospheric deposition of telomer-based precursors from a high- contamination source area.

Lower total PFAS concentrations was observed in June, especially at sites L1 and L2 closer to the inflow where PFBA was not detected. It was difficult to explain this by dilution from inflowing meltwater, because concentrations in the inflowing river was higher than in the lake, with a PFBA concentration of 1.5 ng L^{-1}. One explanation might be turbulent flows causing an increased vertical mixing with water of lower PFBA concentrations from deeper layers of the lake (Veillette et al. 2012).

Similar concentrations and composition pattern were observed for inlet and outlet, both slightly higher concentrations than observed in the lake samples. ΣPFAS was 2.7 ng L^{-1} for inflow and 2.3 ng L^{-1} for outflow, the lake samples ranged between 0.49 and 1.7 ng L^{-1}.

In a 2012 study by Veillette et al., they observed a layer of lower salinity and temperature in the upper 2 m beneath the ice-cover of the lake during spring melt. They suggested that the less saline meltwater would flow relatively uninterrupted underneath the ice from the inflow to the outflow. They refer to this as a short-circuit conduit, which would transport feed contaminants relatively unchanged through the lake without significant mixing with underlying water layers. In contrast, when the lake is ice-free, wind-induced

mixing will result in mixing with deeper layers of the lake, this giving a different composition in outflow compared to inflow (Veillette et al. 2012). The results from this study showed very similar compositions in inflow and outflow of Lake Linnévatnet, indicating a similar short-circuit conduit was taking place during sampling in June 2015. Conductivity measurements could have been a helpful tool to assess the influence of low-saline meltwater versus more saline lake water at each site samples, which might explain some of the observed similarities between inflow and outflow, and the difference to the lake samples in June 2015. Conductivity along with pH and major ion composition was however measured at only one sample site in April 2015 *(Table 4.1).*

The PFAS composition in the ice cover itself might have influenced lake samples, since samples were not collected not deep enough to get below the ice cover. Possible enrichment of PFASs could occur on or near ice-surfaces and water surfaces. In a 2008 study by Ju et al., they found PFOS being enriched by a factor of 24-109 in the surface microlayer (50 µm thickness) compared to the corresponding sub-surface water layer (>30 cm depth) (Ju et al. 2008). Even if such extreme differences were not observed, some ice-water interactions might have affected PFAS composition and concentration in the drill-holes sampled. Ice-thickness in June was approx. 1 meter, sampling depth was approx. 5 to 20 cm below the surface. For future sampling, tools to collect samples deep enough to reach approx. 0.5 – 1 meter below the ice would be helpful to identify a such ice-water interaction, e. g. by using a Niskin sampler.

In snow, PFNA, PFDA, PFUnDA and PFOS were the dominating compounds. PFOA was above the LOQ in one of the two snow samples, no shorter-chain PFCAs were detected (except PFHxA <LOQ in S1). Snow act as a temporary storage resevoir for contaminants scavanged from the atmosphere during the winter, these are released in fractions during melt according to their water solubility and sorption to snow (Daly & Wania 2004). The stages of metamorphosis and melting affect the PFAS composition profiles in the snow and eluting meltwater, where short-chain PFAAs elute early during melting leaving long-chain PFASs in an aged snowpack (Codling et al. 2014; Plassmann et al. 2011). PFCAs show the same elution patterns as PFSAs with one perfluorocarbon less, indicating the sulfonate moiety increase sorption to snow, which also have been observed for sediments (Higgins & Luthy 2006; Plassmann et al. 2011). Sorptive capacity of snow decrease during melt as specific surface area (SSA) decrease and pH increases (Plassmann et al. 2011). The high observed concentrations long-chain compared to short-chain PFAAs in the snow samples agrees well with compositions in an aged snowpack in a late stage of melting, and also agrees with visual observations of wet and coarse-grained snow during sampling.

Meltwater was dominated by PFBA and short-chain PFASs with a similar composition pattern as for lake samples, but higher concentrations. ΣPFAS was ranging from 4.2 to 5.3 ng L^{-1}, PFBA was ranging from 2.7 to 2.9 ng L^{-1}. The composition pattern was not reflecting the predominantly long-chain PFASs found in the corresponding snow-pack. However, some of the meltwater could have originated from snow at an earlier stage of melt higher in the mountainslope. It must be noted that the sample extract of M1 was spilled, and attempted recovered. Recoveries were below 20 %, but results were kept because they were at comparable concentrations.

Distinct differences were observed between November 2014 and June 2015 in samples from the contaminated reference site downstream the FFTS at the airport (A1). In November 2014, PFPeA and PFHxA were dominating with median values of 1.6 and 2.7 ng L^{-1}, and ΣPFAS was between 5.3 and 6.3 ng L^{-1}. PFOS (linear and branched) was the dominating compound in June 2015, at concentrations in the range of 62 – 68 ng L^{-1} for total PFOS, and ΣPFAS was between 117 and 122 ng L^{-1}. However, even if they were sampled only a few meters apart they are probably not directly comparable. The November samples were sampled in saltwater, and is likely to be affected by a strong dilution effect and possibly other local PFAS sources.

The observed concentrations in November were higher, and composition patterns were different compared to results from Adventfjorden by Rakovic et al., which indicate influence by local contamination also in November. However, the composition profile were very different from June, indicating different sources.

High concentrations of PFPeA were consistent with observations by Kwok et al. in 2006, which was assumed to originate from a local source (Kwok et al. 2013). The elevated concentrations observed in June were probably caused by AFFF-contaminated runoff from the FFTS located up-stream.

5.1.1 Seasonal variability within Linnévatnet

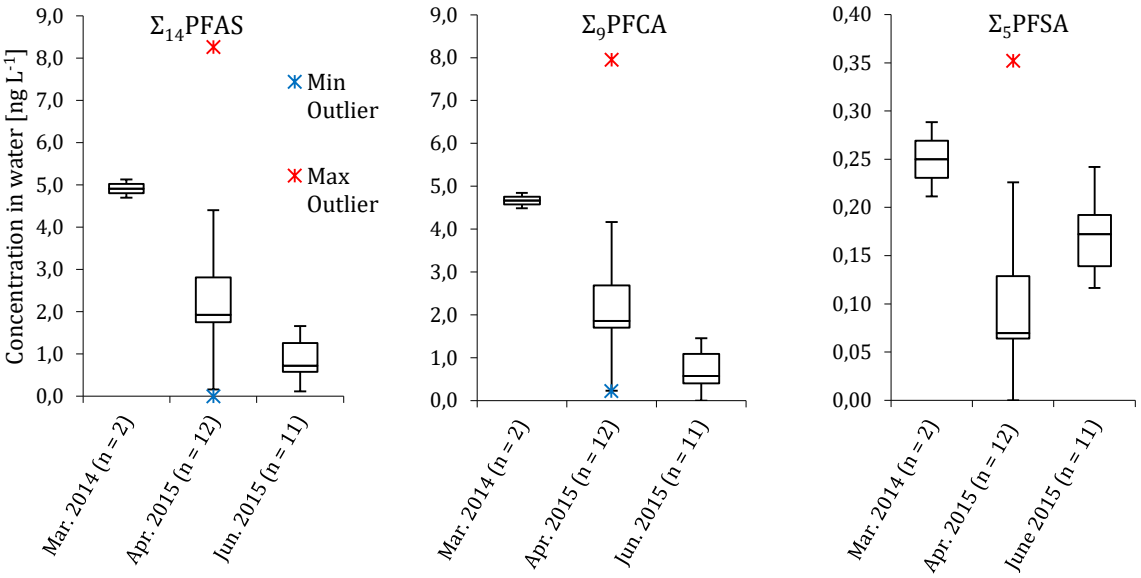


Figure 5.1. Temporal trends for total PFAS, PFCAs and PFSAs at Lake Linnévatnet.

Higher ΣPFAS concentrations were observed in March 2014 compared to April and June 2015, the lowest concentrations were observed in June (Figure 5.1). Most of these observed differences can be explained by variable ΣPFCA. Observed ΣPFSA were in a more similar range between the three sampling times, with lowest concentrations observed in April 2015. Results from April had a much higher variability for both ΣPFCA and ΣPFSA compared to June. March 2014 had only two sample results, thus it is difficult to say anything about the variability.

The higher PFCA levels in winter in general could be an indication of PFASs recently deposited in snow and surface of lake or PFASs concentrating close to ice-surface because of little or no mixing in the water body underneath the ice-cover. These elevated surface concentrations could later be diluted and more evenly mixed in the waterbody as meltwater runoff starts in spring/summer and by wind-induced mixing as ice-cover disappears. Another possibility could be contamination originating from the sampling method. For instance, sample bottles were not rinsed with sample before being filled in November 2014 and April 2015. In these sample bottles, residual methanol in rinsed bottles could act as a trap for neutral PFAS precursors from the air, which degrades to PFCAs. It is not known how sample bottles were pre-cleaned for samples in March 2014. Contamination by storage is another possibility. Field blanks from April were kept in the same freezer as the samples until extraction in June. Field blanks indicate slightly higher blank contamination for PFOA in April compared to June, other components seem to be in the same range. Field blanks were not included for March 2014 samples, thus it is difficult to conclude if samples were contaminated.

PFAS concentrations in the surface water might have an annual cycle depending on the mixing of fresh depositions in the water body based on the above-mentioned assumption of higher concentrations under the ice surface in winter when no mixing occurs. Hence, my hypothesis would be that PFAS concentrations in the surface water would be lowest and most homogenous in autumn after periods of ice-free lake surface

and wind-induced mixing. The observed results somehow contradicts a study from Arctic snow which predicts a maximum concentration in spring-summer (Young et al. 2007).

5.2 Levels and patterns in the Arctic and Antarctic environment.

A comparison levels from five different studies from the Arctic and Antarctic, including this study, is provided in *Table 5.1* for lake water, melt water, river water, snow, surface water and seawater. The comparison of results from different studies should be done with caution, because of different sampling methods, extraction methods and methods for instrumental analysis (Ahrens et al. 2009a). In addition, physical and chemical characteristics of the sample are of importance, e.g. pH, contents of organic carbon and particulate matter (Ahrens et al. 2009a). For snow and corresponding meltwater samples, the stages of metamorphosis and melting affect the composition profiles (Codling et al. 2014; Plassmann et al. 2011).

Concentrations found in studies compared below *(Table 5.1)*, ranged from tens of pg to low ng per liters for individual compounds. PFBA was the dominating compound in lake water, river water and snow, in concentrations ranging from hundreds of pg to low ng per liter. PFPeA was in general around or below 0.1 ng L^{-1}, higher concentrations found around Longyearbyen, Svalbard, was explained by likely local contamination (Kwok et al. 2013). PFHxA, PFHpA, PFOA and PFNA were in general found at concentrations of tens to low-hundreds pg per liter.

Lower median concentrations of PFHxA were found in Linnévatnet compared to other locations, however the range was similar. PFHpA concentrations seems to be slightly higher in Svalbard compared to other locations (Kwok et al. 2013; Rakovic et al. in prep.). PFOA was higher in lake samples from the Canadian Arctic than those in Svalbard, lower concentrations were observed in King Georg's Island. Levels of PFNA were higher in Svalbard compared to King George Island and Northern Sweden. PFDA concentrations were in a similar range throughout the Arctic and Antarctic, but higher in snow in this study. This however, is probably reflecting the age of the snow-pack more than geographical differences. PFUnDA was below detection/quantification limits in most studies, however similar results were observed between snow samples from Svalbard and the Antarctic (Cai et al. 2012b; Rakovic et al. in prep.). PFBS showed similar results throughout different studies and matrices, most results <0.035 ng L^{-1}. The same was the case for PFHxS, where most concentrations were in the range of <0.030 ng L^{-1}. Except river water from Longyearbyen, were PFHxA concentration was 0.16 ng L^{-1}, indicating a possible local source (Kwok et al. 2013). PFOS concentration observed in studies throughout the Arctic and Antarctic was in general in the order of tens of pg per liter. PFOS-levels reported in freshwater from Svalbard was in the range of low-hundreds pg per liter, approx. one order of magnitude higher than reported concentrations in the Canadian high Arctic, northern Sweden and Antarctica, indicating elevated PFOS concentrations in Svalbard. Linear PFOS was used for the comparison from this study and from Rakovic et al.; however other studies did not report weather they included branched isomers in total PFOS or exclusively reported linear PFOS.

In their 2015 study, Lescord et al. examined a lake, Meretta, strongly influenced by local contamination from an airport (Lescord et al. 2015). They found PFOS concentrations of 41 ± 9.3 ng L^{-1}, similar results were found in this study of FFTF runoff water with L-PFOS concentrations between 37 and 41 ng L^{-1}. Concentrations of PFHxS, PFBS, PFHxA and PFDA were also in a similar range, and the ratio of PFHxS/PFHxA was equal to one in both studies. These similarities indicate a similar source of contamination, probably caused by AFFF usage at the airport.

Apart from the differences discussed, PFAS concentrations seems to be in a similar range throughout the Arctic and Antarctic sites studied. Concentrations in seawater were in general lower for each compound compared to the different freshwater matrices, probably caused by dilution. These spatial similarities emphasizes the ubiquitous distribution of PFASs in the aquatic environment, and is an indicator for long-range transport as the source.

Table 5.1. A comparison of selected PFAS concentrations (ng L^{-1}) at different locations in the Arctic and Antarctic. References and explanation of the table symbols can be found on the next page.

Location	Year	Matrix	PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnDA	PFDoDA	PFBS	PFHxS	PFOS
Linnévatnet, Svalbard. (n = 23) [a]	2015	LW	0.86 (ND - 5.2)	<0.089 (ND - 0.21)	<0.089 (ND - 0.38)	0.14 (ND - 0.53)	0.22 (0.13 - 1.4)	0.14 (0.10 - 0.32)	0.052 (ND - 0.12)	<0.11	0.016 (ND - 0.047)	<0.023	0.010 (ND 0.17)	0.057 (ND - 0.15)
Linnévatnet, Svalbard (n=4) [b]	2015	LW	0.89 (0.51 - 2.4)	0.12 (0.061 - 0.18)	0.13 (0.12 - 0.17)	0.16 (0.094 - 0.30)	0.34 (0.22 - 0.36)	0.14 (0.11 - 0.16)	0.062 (0.054 - 0.073)	ND	ND	0.025 (0.019 - 0.032)	ND	0.10 (0.071 - 0.17)
Longyearbyen, Svalbard. (n = 1) [c]	2006	LW	0.43	1.4	0.073	0.061	0.17	0.13	0.018	0.012	0.006		0.063	0.14
Lake Char, Canadian high Arctic. mean ± SD. (n = 5) [d]	2010 - 2011	LW			0.43 ± 0.15		0.62 ± 0.27		0.040 ± 0.040				0.12 ± 0.010	0.050 ± 0.010
Lake 9 mile, Canadian high Arctic. mean ± SD. (n = 5) [d]	2010 - 2011	LW			0.43 ± 0.090		0.69 ± 0.31		0.080 ± 0.030			0.070 ± 0.010	ND	0.020 ± 0.010
Lake Meretta (local pollution), Canadian high Arctic. mean ± SD. (n = 5) [d]	2010-2011	LW			30 ± 4.7		17 ± 1.2		0.13 ± 0.050			4.9 ± 1.00	30 ± 3.5	41 ± 9.3
King George Island, Antarctica (n = 4) [g]	2011	LW	2.26 (1.71 - 2.67)	0.053 (0.019 - 0.089)	0.12 (0.81 - 0.20)	0.068 (0.052 - 0.083)	0.076 (0.046 - 0.097)	0.023 (0.020 - 0.028)	<0.018	0.012 (<0.011 - 0.012)	<0.0043	0.038 (<0.0083 - 0.050)		0.017 (0.012 - 0.022)
Kapp Linnè, Svalbard (n = 2) [a]	2015	MW	2.7 - 2.9	<0.086 - 0.15	0.25 - 0.59	0.25 - 0.46	0.41 - 0.54	0.20 - 0.61	<0.031 - 0.036	<0.11	ND	ND - <0.022	0.020 - 0.041	0.058 - 0.16
Kapp Linnè, Svalbard (n=3) [b]	2015	MW	3.6 (2.8 - 4.6)	0.12 (0.11 - 0.18)	0.22 (0.19 - 0.24)	0.55 (0.35 - 0.57)	0.71 (0.41 - 0.82)	0.42 (0.22 - 0.49)	ND	ND	ND	0.027 (0.014 - 0.031)	ND	0.15 (0.12 - 0.90)
Linnévatnet (inflow and outflow), Svalbard. (n=2) [b]	2015	RV	0.79 - 2.3	ND - 0.25	0.092 - 0.16	0.10 - 0.30	0.18 - 0.41	0.15 - 0.22	ND	ND	ND	0.019 - 0.034	ND	0.056 - 0.11
Linnévatnet (inflow and outflow), Svalbard (n=2) [a]	2015	RV	1.34 - 1.50	<0.080 - 0.24	0.11 - 0.15	0.19 - 0.19	0.26 - 0.29	0.15 - 0.20	0.035 - 0.036	<0.11	<0.014 -0.030	<0.022	0.021 - 0.022	0.057 - 0.066
Longyearbyen, Svalbard. Mean ± SD. (n = 6) [c]	2006	RV	1.20 ± 1.30	1.00 ± 1.30	0.26 ± 0.082	0.15 ± 0.073	0.31 ± 0.19	0.10 ± 0.049	0.019 ± 0.009	0.011 ± 0.011	0.008 ± 0.0048		0.16 ± 0.20	0.29 ± 0.37
Kapp Linnè, Svalbard. (n=2) [a]	2015	SN	ND	ND	ND - <0.066	ND	<0.12 - 0.41	0.66 - 0.94	0.12 - 0.17	0.13 - 0.17	0.017 - 0.035	<0.024	ND - 0.007	0.13 - 0.23
Kapp Linnè, Svalbard. (n=3) [b]	2015	SN	ND (ND - 0.14)	ND	ND (ND - 0.10)	0.052 (ND - 0.11)	0.61 (ND - 0.62)	0.48 (0.44 - 1.5)	0.25 (0.063 - 0.69)	0.14 (0.065 - 0.15)	ND (ND - 0.091)	ND (ND - 0.010)	ND	0.17 (0.064 - 0.34)
Longyearbyen (downstream glacier), Svalbard. mean ± SD. (n = 5) [c]	2006	SN	0.25 ± 0.11	0.080 ± 0.017	0.090 ± 0.031	0.12 ± 0.051	0.40 ± 0.16	0.25 ± 0.11	0.090 ± 0.041	0.035 ± 0.013	0.016 ± 0.0063		0.018 ± 0.0075	0.12 ± 0.051
Northern Sweden. (n = 24) [f]	2009	SN	0.34 (ND - 0.82)	0.17 (ND - 0.59)	0.47 (0.18 - 0.15)	0.0021 (ND - 0.042)	0.067 (ND - 0.12)	0.027 (0.0054 - 0.25)	0.017 (0.0037 - 0.15)			0.099 (ND- 2.16)	0.025 (ND- 0.65)	0.021 (0.0026 - 0.25)
King George Island, Antarctica (n = 4) [g]	2011	SN	0.52 (0.077 - 1.11)	0.099 (<0.010 - 0.20)	0.31 (0.14 - 0.68)	<0.0056	0.20 (0.11 - 0.38)	0.048 (0.018 - 0.11)	0.067 (<0.018 - 0.11)	0.16 (<0.011 - 0.26)	0.19 (<0.0043 - 0.19)	0.017 (<0.0083 - 0.017)		0.018 (0.017 - 0.020)
Surface water, Canadian high Arctic. (n = 11) [e]	2007 - 2008	SFW				0.059 - 0.19	0.085 - 0.25	0.057 - 0.19	0.003 - 0.027			0.011 - 0.024	0.003 - 0.024	0.013 - 0.071
Grønfjorden, Svalbard (n=5) [b]	2015	SW	0.63 (0.47 - 1.4)	0.057 (ND - 0.33)	0.064 (ND - 0.091)	0.10 (0.068 - 0.16)	0.24 (0.21 - 0.30)	ND (ND - 0.061)	ND	ND	ND	0.032 (0.030 - 0.042)	ND	0.041 (0.017 - 0.094)
Longyearbyen, Svalbard. mean ± SD. (n=3) [c]	2006	SW	0.057 ±0.0 48	0.35 ± 0.034	0.056 ± 0.007	0.015 ± 0.025	0.070 ± 0.020	0.039 ± 0.0021	<LOQ	<LOQ	<LOQ		0.030 ± 0.032	0.11 ± 0.069

Remarks to Table 5.1. Concentrations presented as median and range (min. - max), or mean ± standard deviation if stated.
LW = lake water, MW = meltwater stream, RV = River, SN = Snow, SFW = Surface water, SW = seawater.
a) This study, b) (Rakovic et al. in prep.), c) (Kwok et al. 2013), d) (Lescord et al. 2015), e) (Veillette et al. 2012), f) (Codling et al. 2014), g) (Cai et al. 2012b).

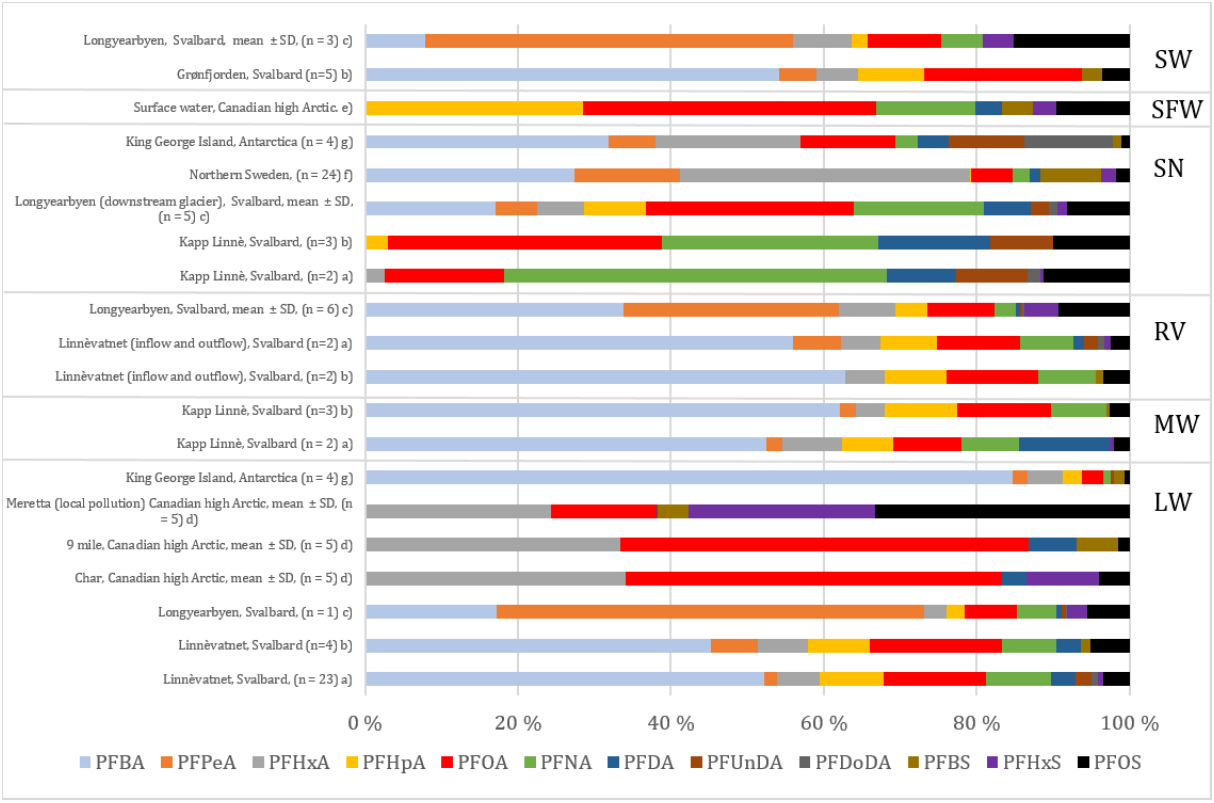


Figure 5.2. PFAS composition profile in various aqueous matrices at Arctic and Antarctic locations.
LW = lake water, MW = meltwater stream, RV = River, SN = Snow, SFW = Surface water, SW = seawater.
a) This study, b) (Rakovic et al. in prep.), c) (Kwok et al. 2013), d) (Lescord et al. 2015), e) (Veillette et al. 2012), f) (Codling et al. 2014), g) (Cai et al. 2012b).

A comparison between PFAS composition profiles from selected Arctic and Antarctic studies is provided in *Figure 5.2*. It is difficult to compare composition profiles between studies where different methods were used with different target analytes included and different LODs/LOQs. Lescord et al. and Veillette et al. did, not report PFBA concentrations (Lescord et al. 2015; Veillette et al. 2012). Since PFBA was the main contributor in many studies, these composition profiles will not be discussed in detail.

In general, PFBA is the dominating compound in lake, meltwater, river, surface water and seawater. PFPeA is contributing largely in all aquatic matrices near Longyearbyen, indicating a local source (Kwok et al. 2013). The contribution of PFPeA, PFHxA, PFHpA, PFOA and PFNA show a similar pattern that can be recognized in most studies from Svalbard. A similar pattern for these four compounds also appear in results from lake water in King George Island, Antarctica, however PFBA is much more dominating by more than 80 % contribution (Cai et al. 2012b). The composition pattern from Grønfjorden (Rakovic et al. in prep.), a fjord approx. 10 km east of lake Linnévatnet showed a very similar composition pattern as lake water, river water and meltwater from this study, but contained no long-chain PFCA where C ≥9.

Svalbard snow samples showed a large contribution of long-chain PFCAs (C_8 to C_{12}) and higher contribution of PFOS than in Northern Sweden and Antarctica. However, these differences might reflect the age and stage of melt of the snow pack, rather than geographic differences.

5.3 Composition profiles and congener patterns in the studied sample sites.

The same five distinct groups as observed in the principal component analysis also appear in Figure 5.3:

1) Samples dominated by PFBA
2) Samples dominated by even numbered long-chain PFCA
3) Samples dominated by odd-numbered long-chain
4) Samples dominated by short-chain PFPeA and PFHxA
5) Samples dominated by PFOS

Samples from Linnévatnet in April and June 2015, lake inlet and outlet and meltwater samples can be placed in the first category. They were dominated by 65 – 80 % short-chain PFCAs, where PFBA contribution was approx. 50 % of ΣPFAS. Long-chain PFASs contributed approx. 10 – 25 % and PFSAs 5 – 10 %, where PFOS was the main contributor. The PFOS contribution was higher in June samples compared to April, and PFOA was slightly higher in April compared to June.

Samples from Linnévatnet in March 2014 (L5) can be placed in the second category. They were dominated by the long-chain PFCAs at approx. 65 %, where PFOA was the major contributor at approx. 40 %. PFCAs with an even number of carbons were found in higher concentrations than their odd-numbered homologues with one more carbon in the chain, e.g. PFOA>PFNA and PFDA>PFUnDA. The contribution of PFSAs was similar to the first category at approx. 5 %, where PFOS was the main contributor.

The third category included the snow samples. They contained no short-chain, and were dominated by approx. 80 % long-chain PFCAs, where PFNA (45 – 55 %)> PFOA>PFUnDA>PFDA>PFDoDA. PFOA was only quantified in S1 contributing 20%. PFCAs with an odd number of carbons were found in higher concentrations than their even-numbered homologues with one more carbon in the chain, e.g. PFNA>PFDA and PFUnDA>PFDoDA. PFOS contribution was approx. 20 %. The results from snow samples containing mostly long-chain PFCAs were consistent with old, metamorphosed snow late in the melting stage (Codling et al. 2014; Plassmann et al. 2011).

The fourth category included samples from A1 in November 2014. These were seawater, because of no run-off during the winter. This site was dominated by approx. 80 % short-chain PFCAs, PFHxA>PFPeA>PFHpA. PFHxA was the main contributor at approx. 45 %, and PFPeA approx. 25 %. Relatively high proportions of PFPeA and PFHxA were also found in seawater close to Longyearbyen in 2006, indicating a local source for these short-chain PFCAs separate from the FFTS run-off (Kwok et al. 2013).

The fifth category included samples from a small stream downstream the FFTS at the airport (A1) in June 2015. These samples were dominated by PFSAs at approx. 70 % of ΣPFAS. PFOS was dominating at more than 50 %, followed by PFHxS>6:2 FTS>PFBS. PFHxA was the dominating carboxylate with a similar contribution as for PFHxS.

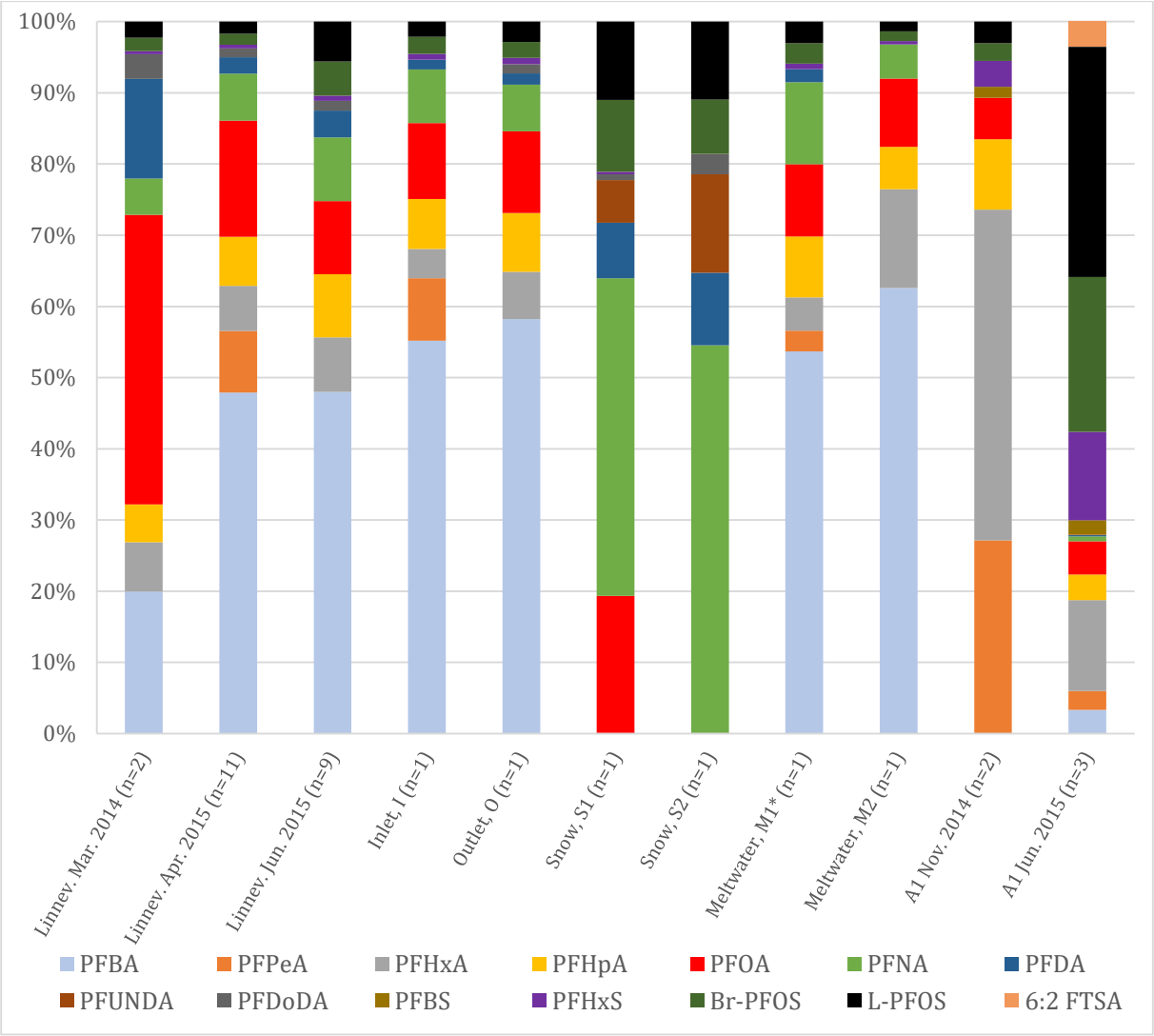


Figure 5.3. Composition profiles based on median concentrations at each sample location.

Ratios of ΣPFCA/ΣPFSA observed *(Figure 5.4)* in Linnévatnet was 19±3.1 in March 2014 (n=2), 25±4.2 in April 2015 (n=11) and 4.4±1.9 in June 2015 (n=10). A1 was 0.31±0.024 in June 2015 (n=3). Higher ratios were in general observed in samples with higher ΣPFAS, except in A1 where PFSAs was the main contributor to the ΣPFAS.

The percentage of branched PFOS relative to total PFOS is provided in *Figure 5.4*. The percentage of branched PFOS (all sample sites except A1) was 49±7.6 %, and for A1 in June 2015, when influence of local contamination was highest, 39.9±0.31 %. For Linnévatnet, the proportions of branched PFOS were 45±1.5 % in March 2014 (n=2), 55±5.3 % in April 2015 (n=10) and 44±7.6 % in June 2015 (n=11). Technical mixtures produced by the ECF-process contained approx. 70 % of the linear isomer (Arsenault et al. 2008). The quantification of branched PFOS was probably more uncertain than for the linear isomer, as no calibration standard was available in this study for the branched isomers. Ionization yield could possibly be higher for Br-PFOS, giving a higher response. In water samples from Lake Ontario in 2002, Houde et al. found an enrichment of branched isomers compared to lake biota and their PFOS-standard (Houde et al. 2008). They found 43 – 56 % of L-PFOS in water, which is comparable to observations in this study. The branched isomers could be selectively enriched in surface water, giving these elevated ratio (Ahrens 2011). McMurdo suggested an isomeric separation of PFOA by partitioning between aerosol and gas phase based on different Henry's Law constant and pK_a of the isomers (McMurdo et al. 2008). They assumed branched

isomers of PFOA would tend to partition less to the gas phase, thus branched isomers would be observed at lower concentrations at remote locations far from a source. Similar isomeric separation might influence PFOS. However, if the assumption by McMurdo et al. is correct, the high percentage of branched PFOS could be an indication of influence by a local pollution source.

PFOA/L-PFOS ratios showed both seasonal and spatial variations *(Figure 5.4).* In Linnévatnet ratios of 18±1.2 were observed in March 2014 (n=2), 13±4.7 in April 2015 (n=10) and 2.0±0.52 in June 2015 (n=10). For A1 in June PFOA/L-PFOS ratio was 0.14±0.0089, which probably indicate influence by local contamination. In comparison, PFOA/L-PFOS ratios calculated by data obtained from Rakovic et al. where 7±4.5 for Grønfjorden (close to Barentsburg) (n=5) and 11±6. 2 for Adventfjorden (close to Longyearbyen)(n=3). From other studies, a ratio of 2.65 was observed from a waste water treatment plant effluent and a ratio of 3.10 for open-ocean seawater (Ahrens 2011). In the Canadian Artic, ratios of 3.4 were observed in Lake Amituk and 5.9 observed in Lake A (Veillette et al. 2012). In a study at King Georges Island, Antarctica by Cai. et al., they found PFOA/PFOS ratios in lake samples between 3.1 to 7.7. They concluded this mainly reflected atmospheric deposition of PFOS and local input of PFOA (Cai et al. 2012b). Results from Linnévatnet in June from this study is consistent the above mentioned ratios observed elsewhere, but ratios observed in March 2014 and April 2015 were much higher.

Mean PFOA/PFNA ratios *(Figure 5.4)* observed in Linnévatnet was 7.9±0.49 in March 2014 (n=2), 2.8±0.98 in April 2015 (n=10) and 1.3±0.41 in June 2015 (n=10). A1 June was 6.4±0.15 (n=3). Similar ratios as observed in June have been observed in recent studies. Kwok et al. observed average ratios of 1.9±0.7 and 1.3±0.4 in two ice-cores from a glacier in Svalbard (Kwok et al. 2013), and Young et al. observed a ratio of 1.5±0.8 in samples of an ice-cap in the Canadian Arctic (Young et al. 2007). Armitage et al. modelled PFOA/PFNA ratios in oceans based on direct aquatic emissions and oceanic transport, assuming $pK_a = 0$ and no emissions to air, modelled ratios for oceans near Svalbard was in the range of 3 to 6 (Armitage et al. 2009). Differences from these modelled ratios might indicate atmospheric origin as opposed to oceanic. However, observed ratios were in the same range, especially in March 2014 and April 2015.

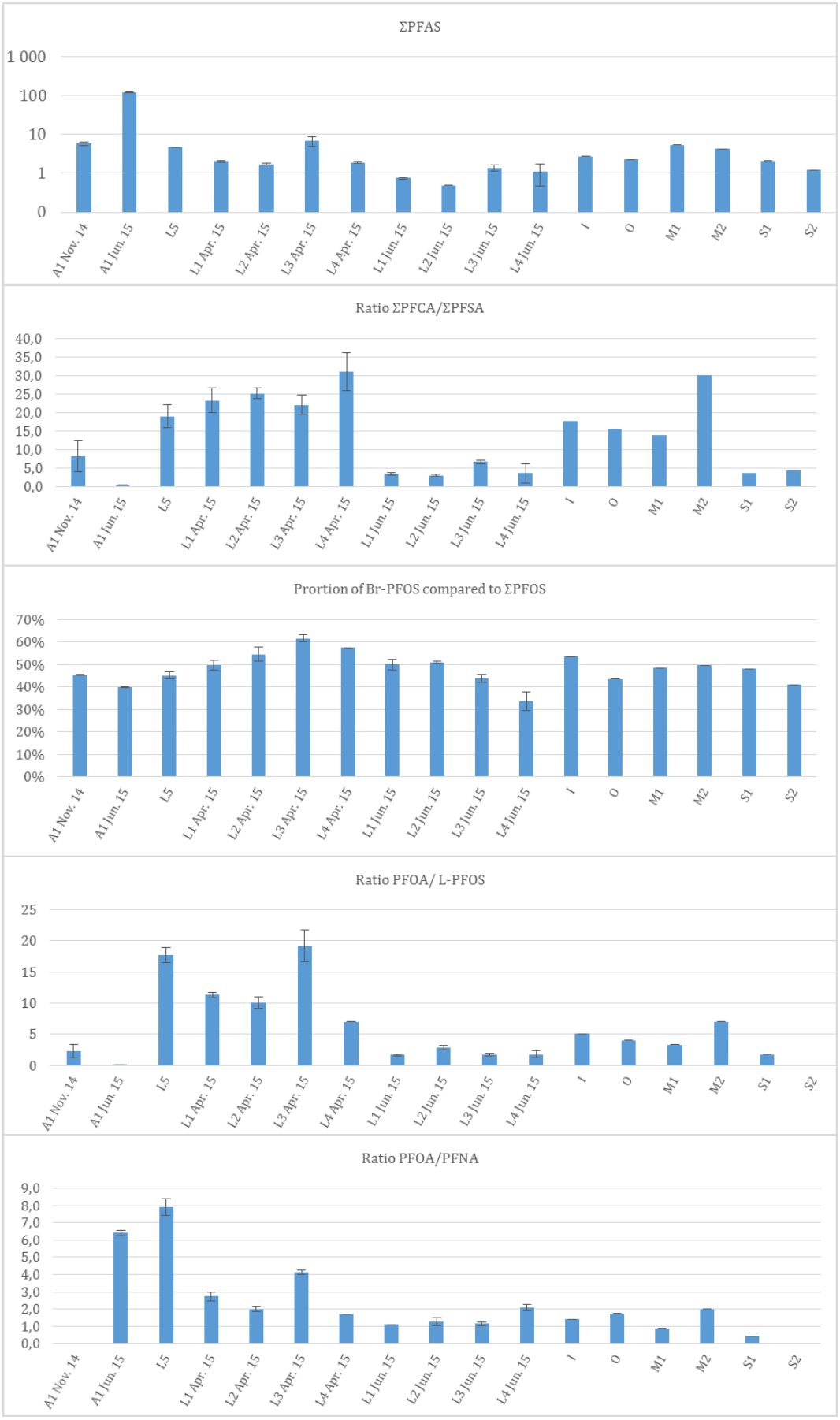


Figure 5.4. Various congener ratios for the individual sample sites.

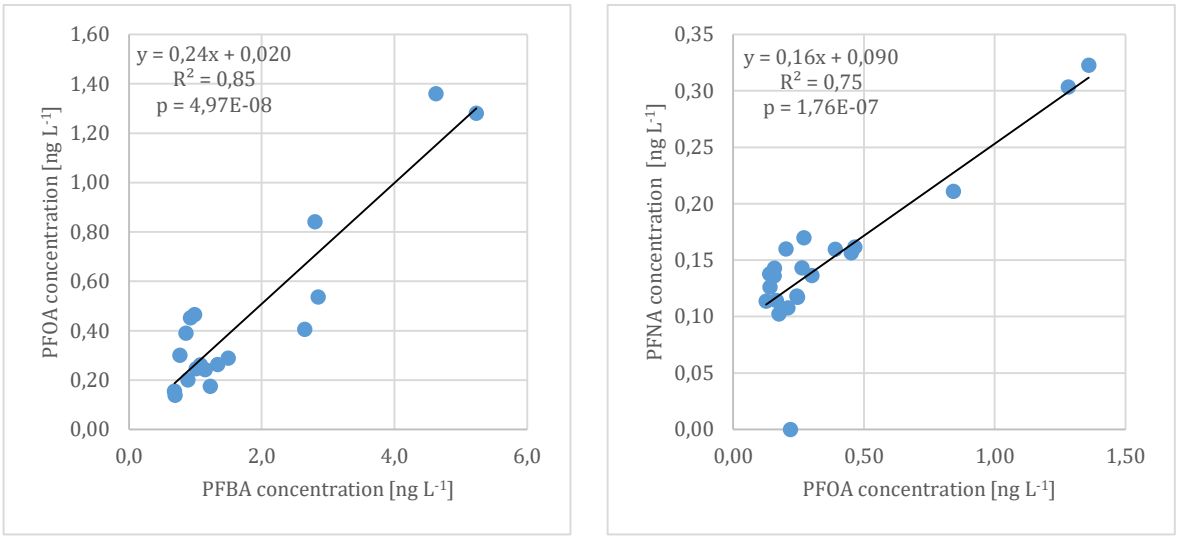


Figure 5.5. Correlation-plot for PFBA and PFOA (left) and for PFOA and PFNA (right). PFBA values >LOQ from Linnévatnet, meltwater and river samples in April and June 2015 were used for PFBA/PFOA-plot (n=18). Results >LOQ from all sample sites at Lake Linnévatnet in 2015 were used for PFOA/PFNA plot (n=22).

A significant linear relationship was observed between PFBA and PFOA (R^2=0.85, p<0.01), and for PFOA and PFNA (R^2=0.75, p<0.01, *Figure 5.5*). This indicate a common source of the PFBA and PFOA, and for PFOA and PFNA (Kwok et al. 2013). Similar relationship between PFOA and PFNA have been observed in surface snow by Kwok et al. (R^2=0.61, p<0.01) and in ice-cores from an Arctic ice-cap by Young et al. (R^2 =0.40) (Kwok et al. 2013; Young et al. 2007).

Observation of similar ratios of PFOA/PFNA as previously found and the significant linear correlation between the two, indicate that long-range atmospheric transport and oxidation of 8:2 FTOH could be a possible source of the observed levels of PFOA and PFNA (Ellis et al. 2004; Young et al. 2007). Recent studies have shown 8:2 FTOH to be the most abundant precursor PFAS found in Arctic atmosphere (Cai et al. 2012a; Del Vento et al. 2012; Shoeib et al. 2006; Xie et al. 2015). In open ocean waters, reported concentrations of PFOA are approx. one order of magnitude higher than of PFNA, suggesting marine aerosols is not the main source (Young 2007). Correlation between sodium content in samples and individual PFASs could have been used as an indication of marine origin (Kwok et al. 2013; Young et al. 2007), but ion composition was only measured for one sample site in April 2015.

N-methyl perfluorobutane sulfonamidoethanol (MeFBSE) and N-methyl perfluorobutane sulfonamide (MeFBSA) have been the most abundant C_4-based precursor reported Arctic and Antarctic atmosphere (Cai et al. 2012a; Del Vento et al. 2012; Xie et al. 2015). MeFBSE have been shown to degrade by oxidation through MeFBSA to PFBA (D'Eon et al. 2006). Thus, long-range atmospheric transport and oxidation of MeFBSE might be a possible source of PFBA to the catchment of Lake Linnévatnet. Higher concentrations of PFBA than PFOA and PFNA were generally found in samples, but MeFBSE and MeFBSA precursor are generally found in lower concentrations in the atmosphere than 8:2 FTOH. It is possible 4:2 FTOH could be the main precursor for PFBA by a similar mechanism as described above, but it have not been widely reported from Arctic atmospheric samples. A common telomer-based source could also explain the linear relationship between PFBA and PFOA. Another possibly relevant atmospheric pathway could be FTOs which by ozonolysis produces odd-numbered PFCAs (Prevedouros et al. 2006).

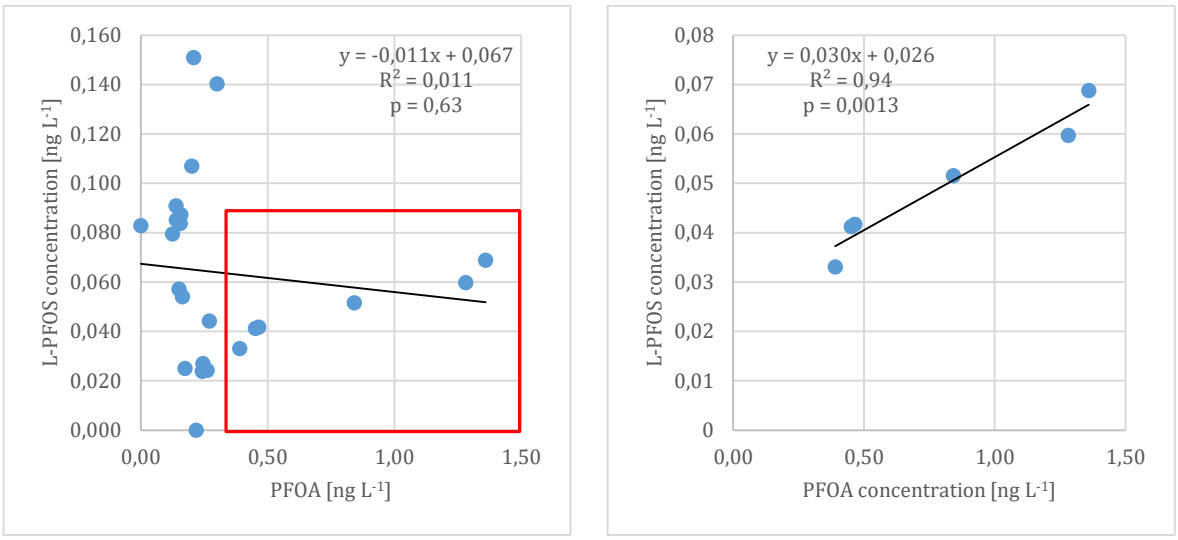


Figure 5.6. Correlation-plots for PFOA and L-PFOS.
All sample sites at Lake Linnévatnet in 2015 (left, n=23), and sites where PFOA >0.39 ng L^{-1} (right, n=6).

No significant linear relationship between PFOA and L-PFOS was observed when all sites were combined *(Figure 5.6).* However, for samples where PFOA concentration > 0.39 ng L^{-1}, a sigificant linear relationship was observed. These levels were observed in samples from all relicas of sites L1 and L3 in April 2015, and also for L5 which is not included in the regression analysis above. This observed difference with increasing concentration could be an indication of different origin of sources, different mixing at sampling sites or a common source of contamination during sampling og sample analysis. The observed increase in correlation with elevated concentrations of PFOA could indicate recent deposition from a common pathway, were no significant mixing with sourrounding waters yet have occoured. In comparison, Kwok et al. reported a significant linear relationship between PFOA and PFOS (R^2=0.63, p<0.01), but did not observe the lack of linear correlation at lower concentrations (Kwok et al. 2013).

Because of the predominant winds from NE and frequent wind from east, local settlements Barentsburg and Longyearbyen might be possible local sources of PFAS. Possible local sources can be domestic wastewater, paints on buildings and vehicles containing perfluoro-surfactants and use of AFFF for firefighting and training at airports (Cai et al. 2012b; DeRosa 2012). Fires have been reported in in Barentsburg coal mine in 1997 and 2008, and a long-term fire in an open coal storage pile 2006. It is not known if AFFF was used to extinguish these fires. If it was, PFASs from the AFFF could possibly be sorbed to aerosols and transported the 10 km from Barentsburg to the Lake Linnévatnet catchment by the easterly winds. A similar composition profile between Linnévatnet and Grønfjorden, which was different from Adventfjorden, could be an indication of the settlement Barentsburg being a local source.

6 Conclusions

The increasing number of studies documenting the presence of PFASs in remote Arctic lakes emphasize the ubiquitous distribution in the aquatic environment.

Total PFAS concentration in Lake Linnévatnet was 4.7 – 5.1 ng L^{-1} in March 2014, 1.6 – 8.3 ng L^{-1} in April 2015 and 0.49 – 1.7 ng L^{-1} in June 2015. The major components found in Linnévatnet in April and June was PFBA, PFHxA, PFHpA, PFOA and PFNA, together contributing approx. 90 % of the total PFAS concentration. Different composition profiles reviled five distinct groups of samples. Samples from Linnévatnet in April and June, meltwater and river water which were dominated by PFBA. Samples of Linnévatnet from March 2014 were dominated by even numbered long-chain PFCA. Snow samples were dominated by odd-numbered long-chain PFCAs. Samples influenced by local pollution and no meltwater dominated by short-chain PFPeA and PFHxA and surface water influenced by local pollution was dominated by PFOS.

Results indicate a seasonal variation with the highest concentrations in winter, mostly explained by variable PFCA concentrations.

Similar concentrations, composition profiles and PFOA/PFNA ratios in Linnévatnet as other remote areas indicate long-range atmospheric transport as the source. A significant linear relationship between PFBA/PFOA and PFOA/PFNA suggests a similar source. Input from local sources in nearby settlements Barentsburg and Longyearbyen should not be ruled out.

Validation of the analytical method used was found it suitable for ionic PFASs, though some potential for future improvement was identified. A contamination issue was identified which gave high detection and quantification limits for PFBA. This increased the variability in total PFAS concentrations in June, when PFBA concentrations measured was close to the detection limit. No significant breakthrough indicate the amount of WAX sorbent in the SPE cartridges was suitable for the extracted sample volumes. Procedural recoveries were good for the ionic PFASs, with mean absolute recoveries in the range of 76 to 106 % for native PFCAs, PFSAs and 6:2 FTSA in sample matrix, and 66 to 94 % for their internal standards. Low recoveries obtained for the neutral PFASs excluded them for further analysis. The repeatability was acceptable, with mean RSDs between sample replicas $\leq$27 %. Mean between-laboratory difference of parallel samples collected in June 2015 used to assess reproducibility showed a difference below 30 % for most compounds, except PFBA, PFHxA and PFUnDA. Reproducibility was comparable to results reported in a recent inter-laboratory comparison.

7 Future perspectives

Minor method improvements should be implemented in order to deal with above-mentioned issues in this study. Contamination sources from sampling, sample extraction and instrumental analysis should be identified before the handling of unknown samples. To increase recoveries of the FASEs and FASAs, elution volumes and volume reduction should be validated to find optimal volumes and procedure. In order to save time on the instrument, the two fractions eluted from the SPE can be combined since calibration curves obtained for FASA and FASE standards were good using the selected instrument method and mobile phases. Individual mass-labeled internal standard should be chosen for each single FASA and FASE compound because of the highly variable recoveries observed between the native compounds.

For sampling on ice, water should be collected underneath the ice surface, e.g. using a Niskin sampler to access the desired depth. For best representation of lake concentrations, sampling on an ice-free lake in the

autumn when mixing is at its highest should be considered. Analysis of conductivity and major ions should be done for each sample site. Conductivity in order to assess the influence of low-saline meltwater versus more saline lake water. Correlation between of individual PFASs and marine sodium would indicate transport by ocean currents and marine aerosols.

Continued monitoring of environmental matrices should be done to strengthen our knowledge of PFASs in the Arctic. Future studies of Lake Linnévatnet should aim to identify whether local sources, long-range atmospheric or oceanic transport is the main source. Local sources can be identified by sampling air, water and soil in nearby settlements Longyearbyen and Barentsburg. A reference site at the east coast of Spitsbergen, which is probably less affected by local contamination because of the predominate wind directions, should be included for air, water, precipitation and snow. The use of passive air and water samplers could be an alternative for more time and cost efficient sampling. The use of SIP-disk passive air samplers have been developed for both neutral and ionic PFASs in air (Genualdi et al. 2010). The use of POCIS with WAX sorbent as passive sampler in water have been shown effective for a range of short and long-chain PFASs (Kaserzon et al. 2012).

Non-target methods can be used to identify new unknown PFASs of possible concern. In a 2007 study by Miyake et al, they analyzed total fluorine, extractable organic fluorine and inorganic fluorine in sea water by combustion ion chromatography and known PFASs by LC-MS/MS. They found that 60 to 90 % of the organic fluorine still remain unknown (Miyake et al. 2007).

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Appendix

Contents

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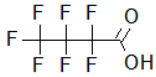
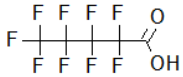
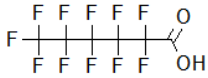
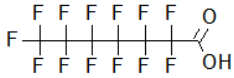
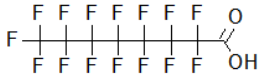
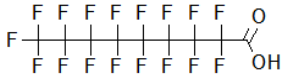
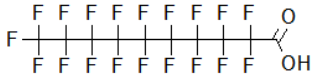
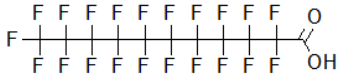
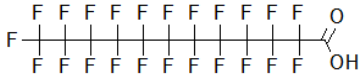
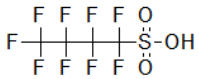
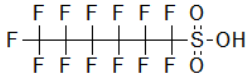
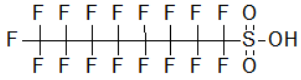
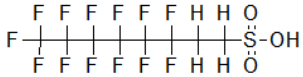
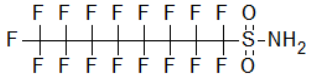
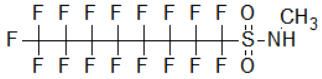
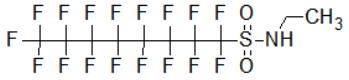
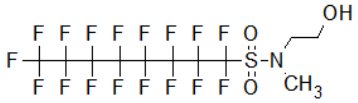
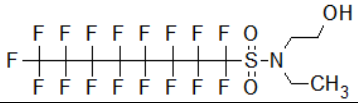
A Chemical structures

Table A.1. Structures drawn using ACD/ChemSketch (Freeware) 2015 (ACD/Labs 2015)

Analyte	Acronym	Structure
PFCAs		
Perfluorobutanoic acid	PFBA	
Perfluoropentanoic acid	PFPeA	
Perfluorohexanoic acid	PFHxA	
Perfluoroheptanoic acid	PFHpA	
Perfluorooctanoic acid	PFOA	
Perfluorononanoic acid	PFNA	
Perfluorodecanoic acid	PFDA	
Perfluoroundecanoic acid	PFUnDA	
Perfluorododecanoic acid	PFDoDA	
PFSAs		
Perfluorobutanoic sulfonate	PFBS	
Perfluorohexanoic sulfonate	PFHxS	
Perfluorooctanoic sulfonate	PFOS	
FTSAs		
6:2 Fluorotelomer sulfonate	6:2 FTSA	
FASAs		
Perfluorooctane sulfonamide	FOSA	
N-methyl-perfluorooctane sulfonamide	MeFOSA	
N-ethyl-perfluorooctane sulfonamide	EtFOSA	
FASEs		
N-methyl perfluorooctane sulfonamidoethanol	MeFOSE	
N-ethyl perfluorooctane sulfonamidoethanol	EtFOSE	

B Materials, chemicals and standards

Table B.1. List of chemicals used in this study.

Name	Quality	Purity ≥ %	CAS#	Producer	Supplier	LOT#	Size	Used for
Acetic aceid (glacial)	EMPARTA ACS (for analysis)	99.7	64-19-7	Merck KGaA, Darmstadt, Germany	VWR International AS, Oslo, Norway	K42116130 112	2.5 L	Acetate buffer
Acetone	SupraSolv	99.8	67-64-1	Merck KGaA, Darmstadt, Germany	VWR International AS, Oslo, Norway	I553112 033	2.5 L	Rinsing of equipment.
Ammonium acetate	trace metals basis	99.99	631-61-8	Sigma-Aldrich, Milwaukee, Wisconsin, USA	Sigma-Aldrich, Oslo, Norway	MKBP5146V	50 g	Acetate buffer
Ammonium acetate	pro analysi, p.a.	98,0	631-61-8	Merck KGaA, Darmstadt, Germany		A334416	1 kg	Acetate buffer (from chemical storage at NMBU, Ås, only used in November 2014).
Ammonium hydroxide solution, Fluka	Puriss. p.a. plus	25	1336-21-6	Sigma-Aldrich, Seelze, Germany	Sigma-Aldrich, Oslo, Norway	SZBA282P	1 L	Eluting- and conditioning solutions (from chemical storage at NMBU, Ås, only used in November 2014).
Ammonium hydroxide solution, Fluka	Puriss. p.a. plus	25	1336-21-6	Sigma-Aldrich, Seelze, Germany	Sigma-Aldrich, Oslo, Norway	SZBF075PV	1 L	Eluting- and conditioning solutions
Methanol	SupraSolv (for gas chromatography)	99.8	67-56-1	Merck KGaA, Darmstadt, Germany	VWR International AS, Oslo, Norway	I621411 202	2.5 L	Extraction, rinsing of equipment.
Methanol	LiChrosolv (gradient grade for liquid chromatography)	99.9	67-56-1	Merck KGaA, Darmstadt, Germany	VWR International AS, Oslo, Norway	I743607 427	2.5 L	Extraction, rinsing of equipment.
Methanol	HiPerSolv Chromanorm for HPLC	99.9	67-56-1	VWR Prolabo	VWR International AS, Oslo, Norway	L1434902	2.5 L	Std. dilution, rinse of consumables, instrument blank, lab. blank Adamstuen, adjusting volumes in extracts.
Methanol	LiChrosolv (gradient grade for liquid chromatography)	99.9	67-56-1	Merck KGaA, Darmstadt, Germany	VWR International AS, Oslo, Norway	l626707208	2.5 L	Rinsing of sample bottles.
Nitrogen 5.0	5.0	99.999	7727-37-9	AGA, Oslo, Norway				

Table B.2. List of materials and instruments.

Name/description	Producer	Supplier	Cat#	LOT#
Finnpipette Focus Adjustable Volume Pipettors 30-300 µL	Thermo Scientific, Waltham, MA, USA		4600240	
Agilent 1200 Series UPLC system	Agilent Technologies, Santa Clara, CA, USA	Matriks AS, Oslo, Norway		
6400 Series Triple Quadrupole LC/MS	Agilent Technologies, Santa Clara, CA, USA	Matriks AS, Oslo, Norway	G6460A	
Agilent 1200 Series High Performance Autosampler	Agilent Technologies, Santa Clara, CA, USA	Matriks AS, Oslo, Norway	G1367C	
Agilent 1200 Series Binary Pump	Agilent Technologies, Santa Clara, CA, USA	Matriks AS, Oslo, Norway	G1312B	
Agilent 1200 Series Thermostatted Column Compartment	Agilent Technologies, Santa Clara, CA, USA	Matriks AS, Oslo, Norway	G1316B	
MassHunter Workstation Software: Quantitative analysis for QQQ version B.07.00 / Build 7.0.457.0	Agilent Technologies, Santa Clara, CA, USA	Matriks AS, Oslo, Norway		
MassHunter Workstation Software: Qualitative analysis for QQQ version B.06.00 / Build 6.0.633.10	Agilent Technologies, Santa Clara, CA, USA	Matriks AS, Oslo, Norway		
Motorized ice drill, Stihl BT121 1.3 kW engine	Andreas Stihl AG & C, Waiblingen, Germany			
Stuart Reciprocating shaker, SSL2	Bibby Scientific Ltd., Staffordshire, UK			
Proline 10 - 100 µL	Biohit, Helsinki, Finland			4063354
Proline 100 - 1000 µL	Biohit, Helsinki, Finland			12539649
Proline 20 - 200 µL	Biohit, Helsinki, Finland			6132923
Proline 5 - 50 µL	Biohit, Helsinki, Finland			13516958
200 mL tubes, 0.5 mL Endpoint	Biotage, Uppsala, Sweden			
200 mL tubes, 1 mL Endpoint	Caliper LifeSciences, Hopkinton, MA, USA			
TurboVap 500 Concentration Workstation	Caliper LifeSciences, Hopkinton, MA, USA			
Research® plus 0.5-5 mL	Eppendorf, Hamburg, Germany	Eppendorf Norge AS, Oslo, Norway		
Research® plus 100-1,000 µL	Eppendorf, Hamburg, Germany	Eppendorf Norge AS, Oslo, Norway	3120000062	
Universal 16 R Sentrifuge	Hettich, Beverly, MA, USA	Nerliens Meszansky AS, Oslo, Norway		
Laboratory Dish washer machine	Ken Hygiene Systmes, Broby, Denmark		211LAB	47914 05
Vacuum pump	KNF Neuberger, Freiburg Germany		N840FT.18	
Glass filter holder assembly with funnel, fritted base, stopper, clamp, 47 mm	Merck Millipore, Billerica, Massachusetts, USA	Merck Life Science AS, Oslo, Norway	XX1004700	
Glass filter holder assembly with funnel, fritted base, stopper, clamp, 47 mm	Merck Millipore, Billerica, Massachusetts, USA	Merck Life Science AS, Oslo, Norway	XX1004700	
Millipak Express 20 (0.22 µm filter)	Merck Millipore, Billerica, Massachusetts, USA	Merck Life Science AS, Oslo, Norway	MPGP02001	
Q-guard 1 (MilliQ water purification)	Merck Millipore, Billerica, Massachusetts, USA	Merck Life Science AS, Oslo, Norway	QGARD00R1	
MagIC Net 3.1	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway		

Conductivity detector (Intelligent high-performance conductivity detector), Digital signal processing, range 0-15000 µS/cm	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway	2.850.9010	
853 «MCS» – CO2 Suppressor	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway	2.853.0010	
Metrohm 788 IC Filtration Sample Processor	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway		
Metrohm 940 Professional IC Vario	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway		
Analytical scale XP204 (max. 220 g, d = 0.1 mg)	Mettler Toledo, Greifensee, Switzerland			
Laboratory Scale PL6001-S (5 - 6100 g, d =0.1 g), e=1 g)	Mettler Toledo, Greifensee, Switzerland			
Muffle Furnace 30 - 3000°C, Controller B170	Nabertherm GmbH, Lilienthal, Germany			
N-EVAP 111 OA Heat Analytical Nitrogen Evaporator	Organomation Assoc. Inc., Berlin, MA, USA		5085	
Stainless steel needles 19 gauge, 4" long, blunt end.	Organomation Assoc. Inc., Berlin, MA, USA		NA0603	
Vacuum manifold, 12 position	Phenomenex, Torrance, California, USA			
Mora ice Arctic Power Drill, 150 mm	Rapala VMC Corporation, Vääksy, Finland		en-2-3939	
Mora ice Arctic Power Drill, 200 mm	Rapala VMC Corporation, Vääksy, Finland		en-2-3959	
Power Drill Extender, 500 mm	Rapala VMC Corporation, Vääksy, Finland		en-2-3197	
Laboratory jack, Swiss Boy 253 - 629 mm height (alt. 120 - 500 mm)	Rudolf Grauer AG, Degersheim, Switzerland	Sigma-Aldrich, Oslo, Norway	245-1170	
Stopper for 2 l suction flask 16672	Sartorius AG, Göttingen, Germany		17174	
Suction flask, 2 l, glass	Sartorius AG, Göttingen, Germany		16672	
Proline 100 - 1000 µL	Sartorius AG, Göttingen, Germany			14577995
Voilé Telepro T6 Avalanche Shovel	Voilé Manufacturing, Salt Lake City, UT, USA		402-EX	
Ultrasonic Cleaner USC600T	VWR International, Leuven, Belgium		142-6007	
VWR mixer mini vortex 230V EU	VWR International, Radnor, PA, USA	VWR International AS, Oslo, Norway	12620-848	
VWR 1207 digital microcentrifuge with 12 (12 x 1.5/2.0 ml) place rotor, EU plug	VWR International, Radnor, PA, USA	VWR International AS, Oslo, Norway	521-2830	
Aluminum boxes, various sizes	Zarges, Weilheim in Oberbayern, Deutschland			

Table B.3. List of consumables.

Name/description	Producer	Supplier	Cat#	LOT#
PELTOR™ Optime™ III Ear Muffs	3M Company, Maplewood, Minnesota, USA	3M Personlig verneutstyr,Skjetten, Norway	H540A	
Agilent ZORBAX Eclipse Plus C18 (USP L1) 3.5 µm 2.1 x 150 mm	Agilent Technologies, Santa Clara, CA, USA	Matriks AS, Oslo, Norway	959763-902	
Polypropylene 80D tubing, 1/8" OD, AP9003000714, 100 FT	Ark-Plas Products, Inc., Flippin, AR, USA	Cole Parmer Norge, Bergen, Norway	95875/01 (EW-95875-01)	
2L Reagent bottle, reusable plastic, non-sterile polypropylene, PP	Corning Inc., Corning, NY, USA	Sigma-Aldrich, Oslo, Norway	1500P-2L	21412001
Costar 8169 Spin-X Centrifuge Tube Filter, 0.22 µm Nylon, 2 mL tube, non-sterile polypropylene. 100/pack, 200/case	Corning Inc., Corning, NY, USA	VWR International AS, Oslo, Norway	525-3415	30814000
epT.I.P.S.® Standard, Eppendorf Quality™, 0.1 – 5 mL L, 120 mm, violet, 500 tips (5 bags x 100 tips)	Eppendorf, Hamburg, Germany	Eppendorf Norge AS, Oslo, Norway	30000978	
Metrosep A SUPP 4/5 Guard/4.0	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway	6.1006.500	
Metrosep A Supp 4 - 250/4.0	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway	6.1006.430	
Precolumn Metrosep C 4 Guard	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway	6.1050.500	
Cation column Metrosep C 4 – 150	Metrohm AG, Herisau, Switzerland	Metrohm Nordic AS, Høvik, Norway	6.1050.420	
Supelguard Discovery 18,2 cm x 2,1 mm, 5 µm	Supelco Bellefonte, PA, USA		505188	5829
Bottle wide neck + cap, round, LDPE, 1000 mL	VWR International, Radnor, PA, USA	VWR International AS, Oslo, Norway	215-5634	
Nitrile gloves	VWR International, Radnor, PA, USA	VWR International AS, Oslo, Norway	112-2373	
VWR HIGH PERFORMANCE 15 ml, CONICAL BOTTOM CENTRIFUGE TUBES, Polypropylene, 25 tubes per rack, 2 racks/pack, 10 packs/case	VWR International, Radnor, PA, USA	VWR International AS, Oslo, Norway	525-0401	
Srew cap 9mm rubber, red/orange/TEF	VWR International, Radnor, PA, USA	VWR International AS, Oslo, Norway	548-0032	123006
Vials 1,5 mL PP, screw cap	VWR International, Radnor, PA, USA	VWR International AS, Oslo, Norway		
Oasis WAX 6cc 500 mg	Waters, Milford, MA, USA	Waters Norge, Oslo, Norway	186004647	002535054A, 002334148A, 002334080A
SEP-PAK Reservoir adaptor	Waters, Milford, MA, USA	Waters Norge, Oslo, Norway	WAT054260	
VALVE(STOPCOCK)W/NEEDLE TIP	Waters, Milford, MA, USA	Waters Norge, Oslo, Norway	WAT200685	
2-stroke gasoline				
Polypropylene vials, screw cap, 1.5 mL		Holger Hartmann, Oslo, Norway	LPP-11 19 1205	30156

B.1 Standards

All analytical standards were produced by Wellington Laboratories (Guelph ON, Canada) and supplied by Greyhound Chromatography and Allied Chemicals (Merseyside, England). Dilutions were prepared with various volume pipettes (*Table*) in methanol (*Table*).

Table B.4. Standards used for quantification and identification.

Acronym	Compound	Concentration [µg/mL]	Uncertainty (U_c, k = 2) [µg/mL]	Chemical purity (%)	LOT #
PFBA	Perfluoro-n-butanoic acid	5.0	0.25	>98	PFACMXA0514
PFPeA	Perfluoro-n-pentanoic acid	5.0	0.25	>98	PFACMXA0514
PFHxA	Perfluoro-n-hexanoic acid	5.0	0.25	>98	PFACMXA0514
PFHpA	Perfluoro-n-heptanoic acid	5.0	0.25	>98	PFACMXA0514
PFOA	Perfluoro-n-octanoic acid	5.0	0.25	>98	PFACMXA0514
PFNA	Perfluorono-n-nonanoic acid	5.0	0.25	>98	PFACMXA0514
PFDA	Perfluoro-n-decanoic acid	5.0	0.25	>98	PFACMXA0514
L-PFBS	Potassium perfluoro-1-butanesulfonate	5.0 (4.4 as the anion)	0.25 (0.22)	>98	PFACMXA0514
L-PFHxS	Sodium perfluoro-1-hexanesulfonate	5.0 (4.7 as the anion)	0.25 (0.24)	>98	PFACMXA0514
L-PFOS	Sodium perfluoro-1-octanesulfonate	5.0 (4.8 as the anion)	0.25 (0.24)	>98	PFACMXA0514
6:2 FTSA	Sodium 1H, 1H, 2H, 2H-perfluorooctanoic sulfonate	50 (47.4 as the anion)	2.5 (2.4)	>98	62FTSA1014
FOSA	Perfluoro-1-octanesulfonamide	50	2.5	>98	FOSA1113l
MeFOSA	N-methylperfluoro-1-octanesulfonamide	50	2.5	>98	NMeFOSA0114M
EtFOSA	N-ethyl-perfluoro-1-octanesulfonamide	50	2.5	>98	NEtFOSA0714M
MeFOSE	2-(N-methylperfluoro-1-octanesulfonamido)-ethanol	50	2.5	>98	NMeFOSE0314M
EtFOSE	2-(N-ethyl perfluoro-1-octanesulfonamido)-ethanol	50	2.5	>98	NEtFOSE0114M
4:2 FTOH	2-perfluorobutyl ethanol	50	2.5	>98	FBET0807
6:2 FTOH	2-perfluorohexyl ethanol	50	2.5	>98	FHET0313
8:2 FTOH	2-perfluorooctyl ethanol	50	2.5	>98	
[$^{13}C_4$]-PFBA	Perfluoro-n-[1,2,3,4-$^{13}C_4$]butanoic acid	2.0	0.10	>98	MPFACMXA0214
[$^{13}C_5$]-PFHxA	Perfluoro-n-[1,2,3,4,6-$^{13}C_5$]hexanoic acid	50	2.5	>98	M5PFHxA0810
[$^{13}C_2$]-PFHxA	Perfluoro-n-[1,2-$^{13}C_2$]hexanoic acid	2.0	0.10	>98	MPFACMXA0214
[$^{13}C_4$]-PFHpA	Perfluoro-n-[1,2,3,4-$^{13}C_4$]heptanoic acid	50	2.5	>98	M4PFHpA1213
[$^{13}C_4$]-PFOA	Perfluoro-n-[1,2,3,4-$^{13}C_4$]octanoic acid	2.0	0.10	>98	MPFACMXA0214
[$^{13}C_8$]-PFOA	Perfluoro-n-[1,2,3,4,5,6,7,8-$^{13}C_8$]octanoic acid	49	2.45	97.9	M8PFOA0514
[$^{13}C_5$]-PFNA	Perfluoro-n-[1,2,3,4,5-$^{13}C_5$]nonanoic acid	2.0	0.10	>98	MPFACMXA0214
[$^{13}C_2$]-PFDA	Perfluoro-n-[1,2-$^{13}C_2$]decanoic acid	2.0	0.10	>98	MPFACMXA0214
[$^{13}C_2$]-PFUnDA	Perfluoro-n-[1,2-$^{13}C_2$]undecanoic acid	2.0	0.10	>98	MPFACMXA0214
[$^{13}C_2$]-PFDoDA	Perfluoro-n-[1,2-$^{13}C_2$]dodecanoic acid	2.0	0.10	>98	MPFACMXA0214
[$^{18}O_2$]-PFHxS	Sodium perfluoro-1-hexane[$^{18}O_2$]sulfonate	2.0 (1.89 as the anion)	0.10 (0.095)	>98	MPFACMXA0214
[$^{13}C_4$]-PFOS	Sodium perfluoro-1-[1,2,3,4-$^{13}C_4$]octanesulfonate	2.0 (1.91 as the anion)	0.10 (0.096)	>98	MPFACMXA0214
d_3-MeFOSA	N-methyl-d3-perfluoro-1-ocanesulfonamide	50	2.5	>98	dNMeFOSA0114M
d_7-MeFOSE	2-(N-methyl-d3-perfluoro-1-octanesulfonamido)ethan-d4-ol	50	2.5	>98	d7NMeFOSE1213M
$^{13}C_2$, d2-6:2 FTOH	2-Perfluorohexyl-[1,1-$^2H_2$]-[1,2-$^{13}C_2$]-ethanol	50	2.5	>98	MFHET0513

Table B.5. Internal standard mixture B (ISTD-mix A).

Abbreviation	Primary concentration [µg/mL]	U_{rel} (k=2) (%)	U_{abs} (k=2) [µg/mL]	Diluted concentration [ng/mL]	U_{rel} (k=2) (%)	U_{abs} (k=2) [ng/mL]
[$^{13}C_5$]-PFHxA	50	5.0	2.5	200	7.6	15
[$^{13}C_4$]-PFHpA	50	5.0	2.5	200	7.6	15
[$^{2}H_2$],[$^{13}C_2$]-6:2 FTOH	50	5.0	2.5	2000	5.1	102
[$^{2}H_3$]-MeFOSA	50	5.0	2.5	2000	5.1	102
[$^{2}H_7$]-MeFOSE	50	5.0	2.5	2000	5.1	102

Table B.6. Internal standard mixture B (ISTD-mix B).

Abbreviation	Primary concentration [ng/mL]	U_{rel} (k=2) (%)	U_{abs} (k=2) [ng/mL]	Diluted concentration [ng/mL]	U_{rel} (k=2) (%)	U_{abs} (k=2) [ng/mL]
[$^{13}C_4$]-PFBA	2000	5.0	100	200	12	24
[$^{13}C_2$]-PFHxA	2000	5.0	100	200	12	24
[$^{13}C_4$]-PFOA	2000	5.0	100	200	12	24
[$^{13}C_5$]-PFNA	2000	5.0	100	200	12	24
[$^{13}C_2$]-PFDA	2000	5.0	100	200	12	24
[$^{13}C_2$]-PFUnDA	2000	5.0	100	200	12	24
[$^{13}C_2$]-PFDoDA	2000	5.0	100	200	12	24
[$^{18}O_2$]-PFHxS	1890	5.0	94,5	189	12	23
[$^{13}C_4$]-PFOS	1910	5.0	95,5	191	12	23

Table B.7. Native spike-mix.

	Added volume std. [µL]	Cons. Std [ng/mL]	Conc. diluted [ng/mL]	Akk. vol [µL]
PFAC-MXA:	30			30
PFBA	-	5000	100	-
PFPeA	-	5000	100	-
PFHxA	-	5000	100	-
PFHpA	-	5000	100	-
PFOA	-	5000	100	-
PFNA	-	5000	100	-
PFDA	-	5000	100	-
L-PFBS	-	4400	88	-
L-PFHxS	-	4700	94	-
L-PFOS	-	4800	96	-
FOSA	30	50000	1000	60
N-EtFOSA	30	50000	1000	90
N-MeFOSA	30	50000	1000	120
N-MeFOSE	30	50000	1000	150
N-EtFOSE	30	50000	1000	180
6:2 FTSA	30	47400	948	210
Metanol	1290			1500

Table B.8. Calibration standards (from Excel sheet analytter.xlsx)

Acronym	Level 1 [pg/µL]	Level 2 [pg/µL]	Level 3 [pg/µL]	Level 4 [pg/µL]	Level 5 [pg/µL]	Level 6 [pg/µL]	Level 7 [pg/µL]	Level 8 [pg/µL]
Native standards								
PFBA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
PFPeA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
PFHxA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
PFHpA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
PFOA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
PFNA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
PFDA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
L-PFBS	0,088	0,44	0,88	8,80	17,6	44,0	88,0	154
L-PFHxS	0,094	0,47	0,94	9,40	18,8	47,0	94,0	165
L-PFOS	0,096	0,48	0,96	9,60	19,2	48,0	96,0	168
6:2 FTSA	0,095	0,47	0,95	9,48	19,0	47,4	94,8	166
FOSA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
MeFOSA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
EtFOSA	0,10	0,50	1,00	10,0	20,0	50,0	100	175
MeFOSE	0,10	0,50	1,00	10,0	20,0	50,0	100	175
EtFOSE	0,10	0,50	1,00	10,0	20,0	50,0	100	175
4:2 FTOH	0,10	0,50	1,00	10,0	20,0	50,0	100	175
6:2 FTOH	0,10	0,50	1,00	10,0	20,0	50,0	100	175
8:2 FTOH	0,10	0,50	1,00	10,0	20,0	50,0	100	175
Recovery standard								
[$^{13}C_8$]-PFOA	19,6	19,6	19,6	19,6	19,6	19,6	19,6	17,2
Internal standards								
[$^{13}C_4$]-PFBA	20,0	20,0	20,0	20,0	20,0	20,0	20,0	17,5
[$^{13}C_5$]-PFHxA	20,0	20,0	20,0	20,0	20,0	20,0	20,0	17,5
[$^{13}C_4$]-PFHpA	20,0	20,0	20,0	20,0	20,0	20,0	20,0	17,5
[$^{13}C_4$]-PFOA	20,0	20,0	20,0	20,0	20,0	20,0	20,0	17,5
[$^{13}C_5$]-PFNA	20,0	20,0	20,0	20,0	20,0	20,0	20,0	17,5
[$^{13}C_2$]-PFDA	20,0	20,0	20,0	20,0	20,0	20,0	20,0	17,5
[$^{13}C_2$]-PFUnDA	20,0	20,0	20,0	20,0	20,0	20,0	20,0	17,5
[$^{13}C_2$]-PFDoDA	20,0	20,0	20,0	20,0	20,0	20,0	20,0	17,5
[$^{18}O_2$]-PFHxS	18,9	18,9	18,9	18,9	18,9	18,9	18,9	16,5
[$^{13}C_4$]-PFOS	19,1	19,1	19,1	19,1	19,1	19,1	19,1	16,7
d3-N-MeFOSA	200	200	200	200	200	200	200	175
d7-N-MeFOSE	200	200	200	200	200	200	200	175
$^{13}C_2$, d2-6:2 FTOH	200	200	200	200	200	200	200	175

C Instrumental parameters

Table C.1. Retention times, MRM transitions and MS/MS parameters.

Acronym	ISTD used	Retention time [min]	Precursor ion (m/z)	Product ion 1 (Quantifier) (m/z)	Product ion 2 (Qualifier) (m/z)	Qualifier relative abundance (%)	CE (V)	Fragmentor (V)
PFBA	$[^{13}C_4]$-PFBA	9.23	213	169			1	61
PFPeA	$[^{13}C_5]$-PFHxA	9.91	263	219			1	61
PFHxA	$[^{13}C_5]$-PFHxA	10.42	313	269	119	4.6	0 (12)	66
PFHpA	$[^{13}C_4]$-PFHpA	10.90	363	319	169	13.2	0 (8)	71
PFOA	$[^{13}C_4]$-PFOA	11.39	413	369	169	30.1	0 (12)	76
PFNA	$[^{13}C_5]$-PFNA	11.94	463	419	219	9.9	4 (8)	86
PFDA	$[^{13}C_2]$-PFDA	12.48	513	469	219	12.9	4 (12)	86
PFUnDA	$[^{13}C_2]$-PFUnDA	13.03	563	519			4	86
PFDoDA	$[^{13}C_2]$-PFDoDA	13.50	613	569			4	96
PFBS	$[^{18}O_2]$-PFHxS	8.63	299	99	80	39.9	25 (33)	121
PFHxS	$[^{18}O_2]$-PFHxS	9.73	399	99	80	52.1	45	151
Br-PFOS	$[^{13}C_4]$-PFOS	10.69	499	99	80	16.7	61	166
L-PFOS	$[^{13}C_4]$-PFOS	10.83	499	99	80	46.2	61	166
6:2 FTSA	$[^{18}O_2]$-PFHxS	10.35	427	407	81	14.3	15	145
FOSA	$[^{2}H_3]$-MeFOSA	13.15	498	78			33	141
MeFOSA	$[^{2}H_3]$-MeFOSA	14.94	512	169			25	126
EtFOSA	$[^{2}H_3]$-MeFOSA	15.58	526	169			25	121
MeFOSE	$[^{2}H_7]$-MeFOSE	14.95	616	59			9	96
EtFOSE	$[^{2}H_7]$-MeFOSE	15.55	630	59			9	81
Recovery standard								
$[^{13}C_8]$-PFOA		11.39[a] / 10.33[b]	421	376			0	76
Internal standards								
$[^{13}C_4]$-PFBA		9.23	217	172			1	61
$[^{13}C_5]$-PFHxA		10.42	318	273			0	66
$[^{13}C_4]$-PFHpA		10.90	367	322			0	66
$[^{13}C_4]$-PFOA		11.39	417	372			0	76
$[^{13}C_5]$-PFNA		11.94	468	423			4	76
$[^{13}C_2]$-PFDA		12.48	515	470			4	86
$[^{13}C_2]$-PFUnDA		13.03	565	520			4	96
$[^{13}C_2]$-PFDoDA		13.50	615	570			4	96
$[^{18}O_2]$-PFHxS		9.73	403	84			49	146
$[^{13}C_4]$-PFOS		10.83	503	80			61	180
$[^{2}H_3]$-MeFOSA		14.92	515	169			25	136
$[^{2}H_7]$-MeFOSE		14.88	623	59			9	96

a. PFCA instrument method.
b. PFSA/FASA/FASE instrument method.
Fragmentor voltages in parenthesis represent qualifier transition, if different from quantifier.

Table C.2. Ion source parameters PFCAs.

Gas Flow [L/min]	5
Gas temp [°C]	300
Nebulizer [psi]	25
Sheath Gas Flow [mL/min]	8
Sheath Gas Heater [°C]	400
Capillary [V]	+5000 / -2500
Charging [V]	+2000 / -500

Table C.3. Ion source parameters PFSAs, FASAs and FASEs.

Gas Flow [L/min]	9
Gas temp [°C]	350
Nebulizer [psi]	30
Sheath Gas Flow [mL/min]	8
Sheath Gas Heater [°C]	400
Capillary [V]	+5000 / -4000
Charging [V]	+2000 / 0

D Calibration curves.

All calibration curves were obtained from Agilent Mass Hunter QQQ Quantitative analysis. Black dots represent relative response of the calibration points that have been used, green quadrates represent ISTD response and white circles represent rejected calibration points.

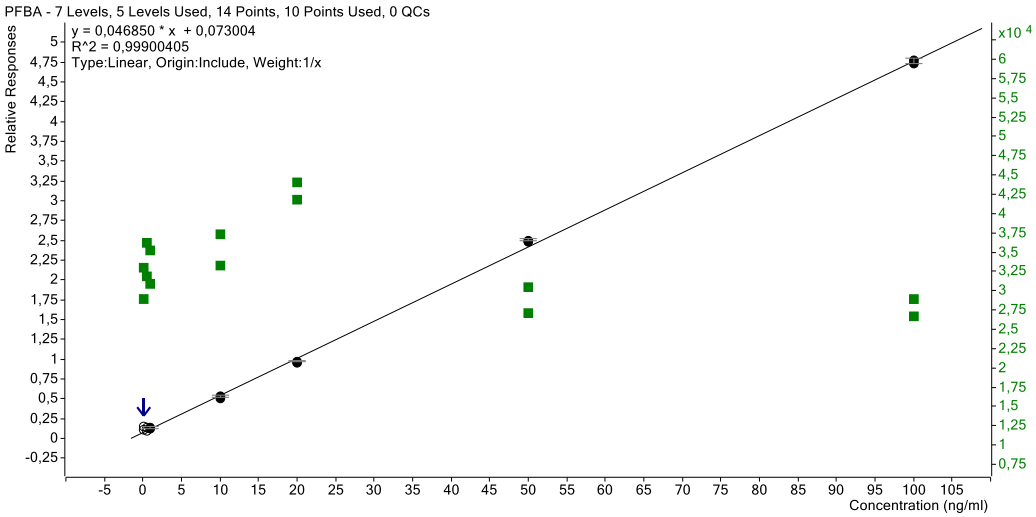


Figure D.1. Calibration curve for PFBA.

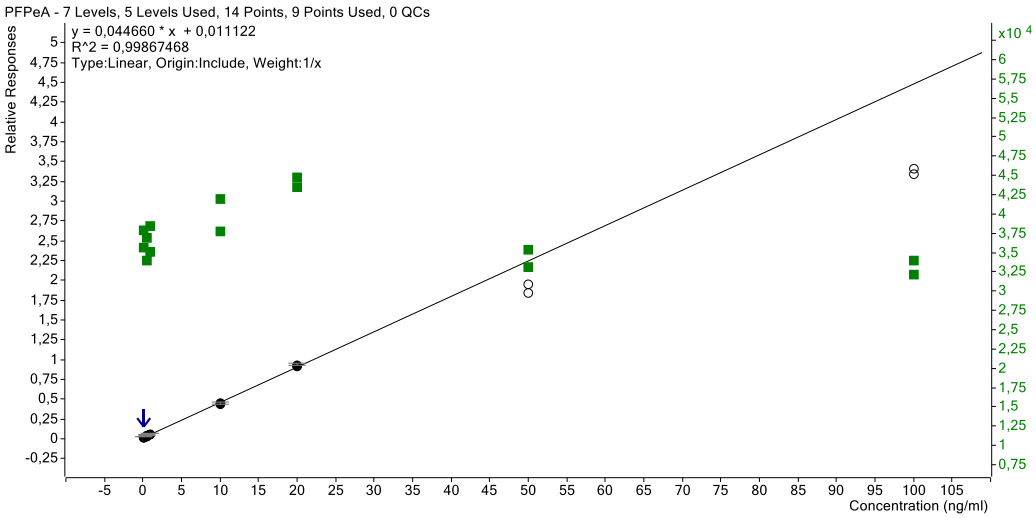


Figure D.2. Calibration curve for PFPeA.

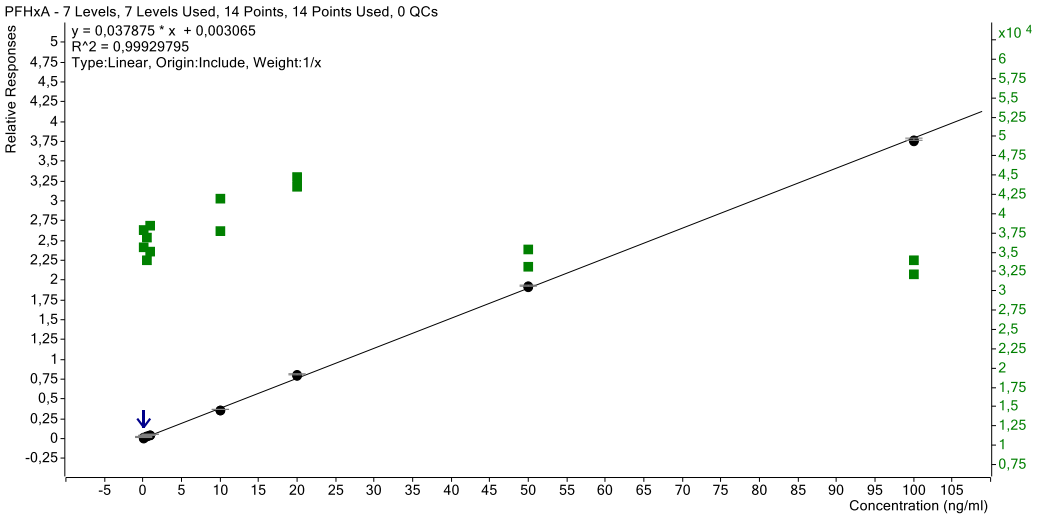


Figure D.3. Calibration curve for PFHxA.

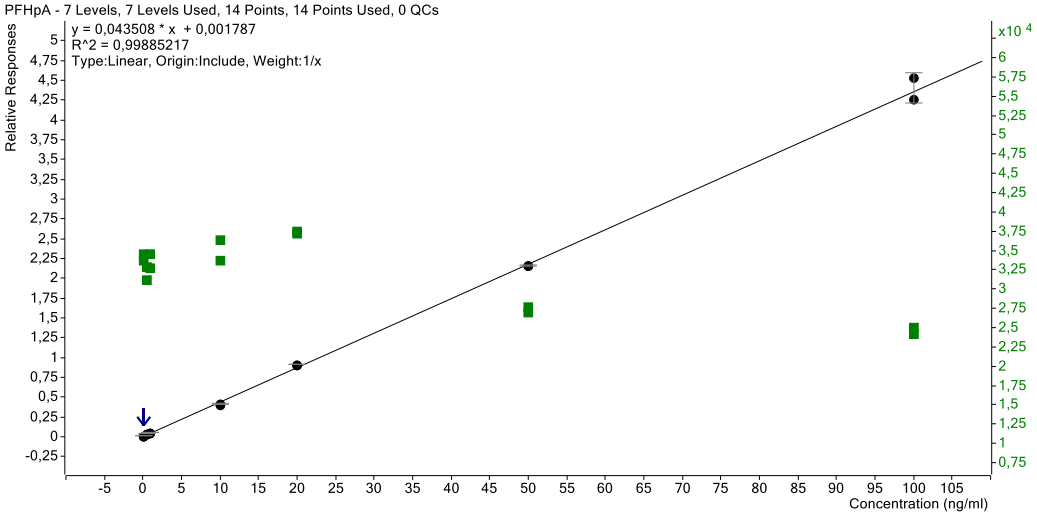


Figure D.4. Calibration curve for PFHpA.

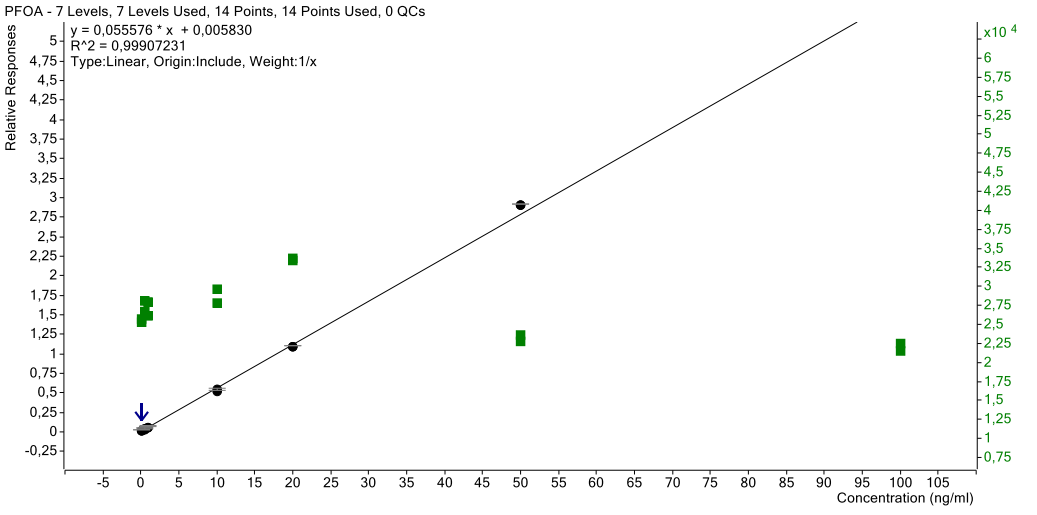


Figure D.5. Calibration curve for PFOA.

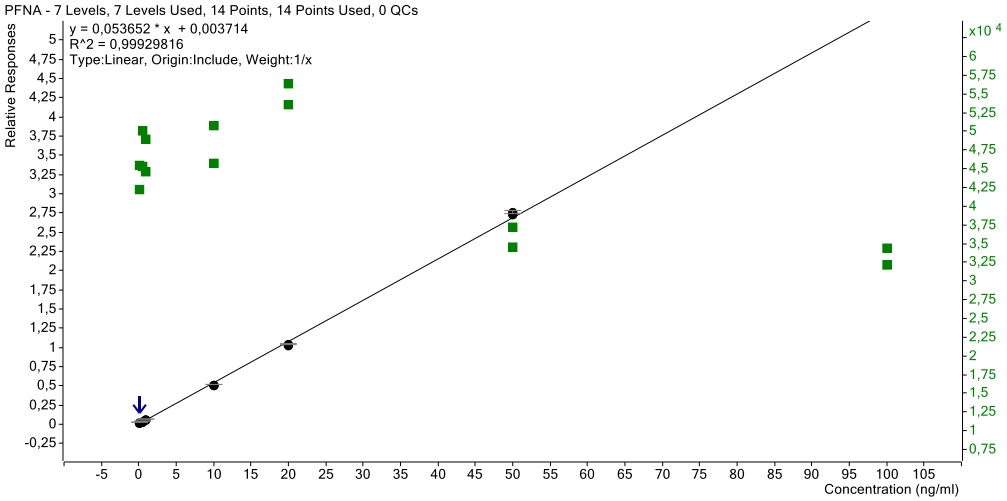


Figure D.6. Calibration curve for PFNA.

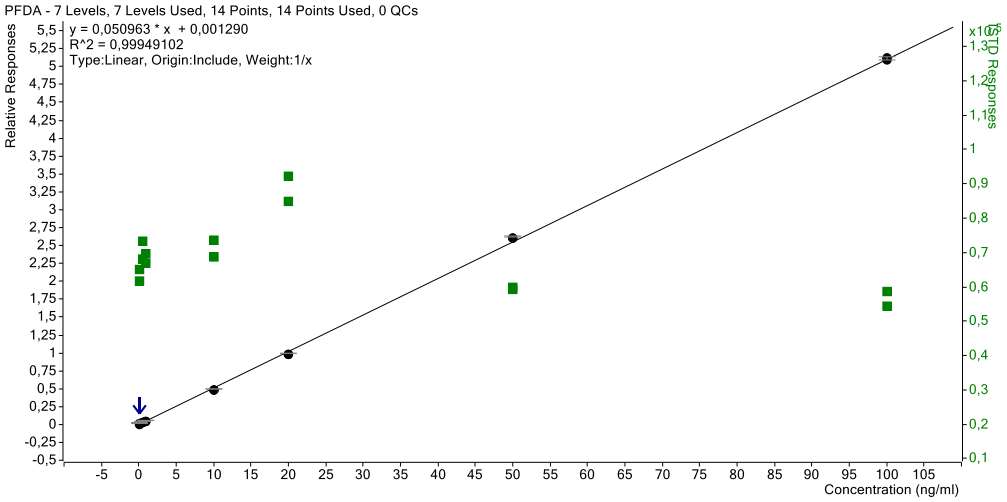


Figure D.7. Calibration curve for PFDA.

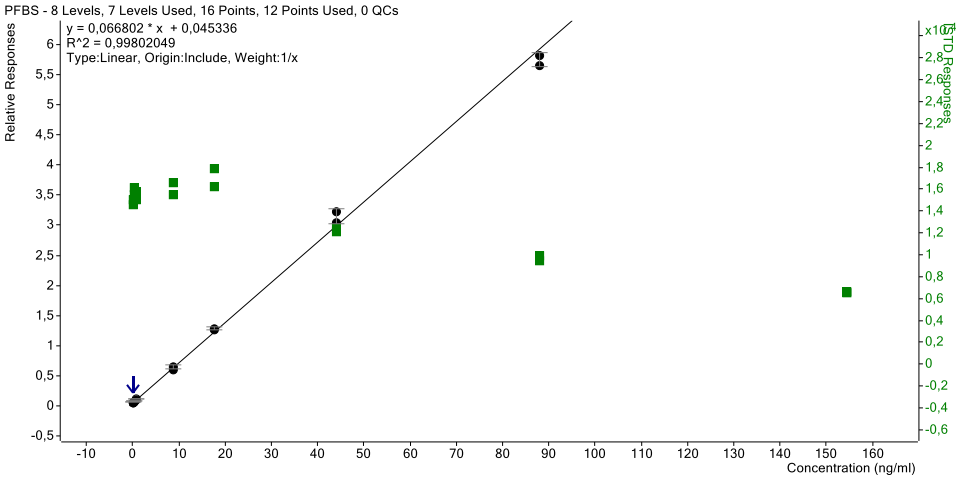


Figure D.8. Calibration curve for PFBS.

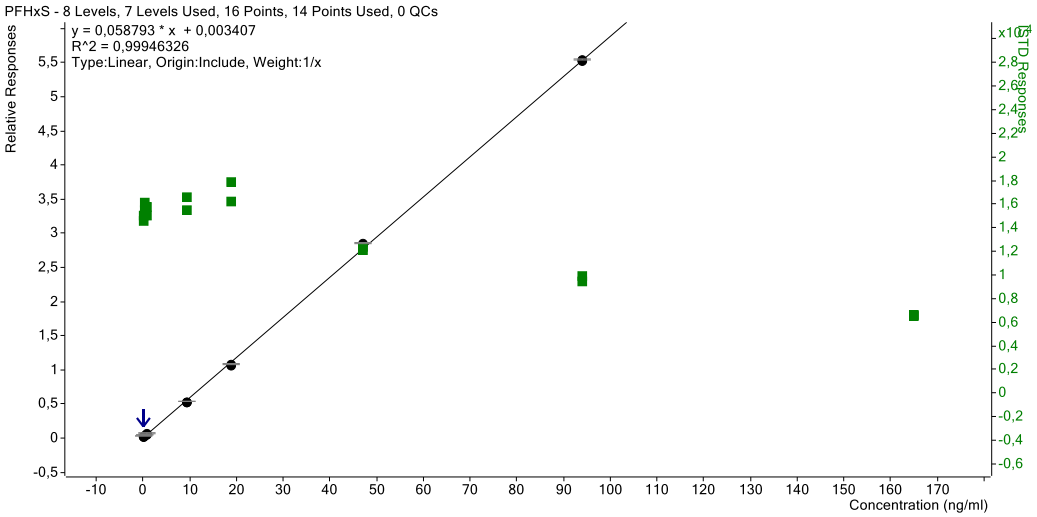


Figure D.9. Calibration curve for PFHxS.

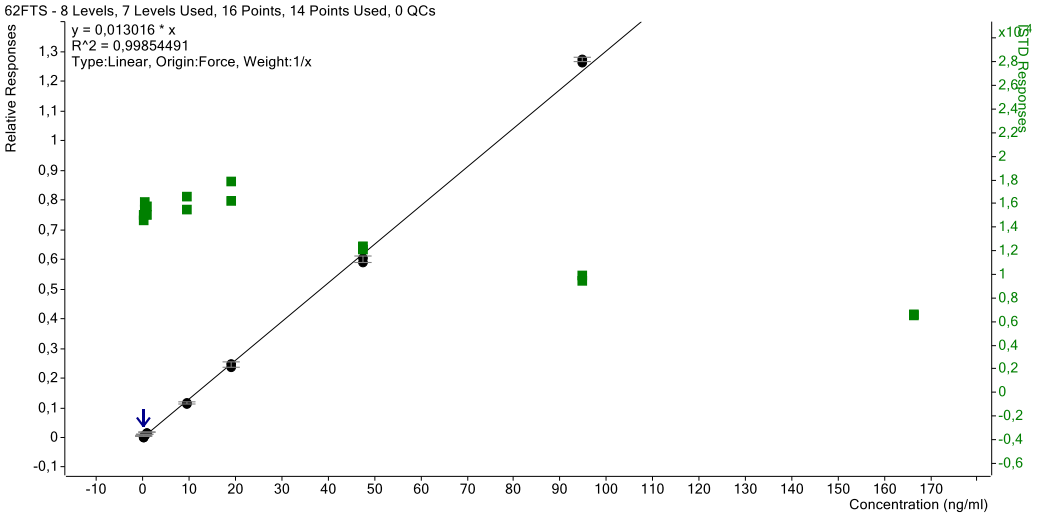


Figure D.10. Calibration curve for 6:2 FTSA.

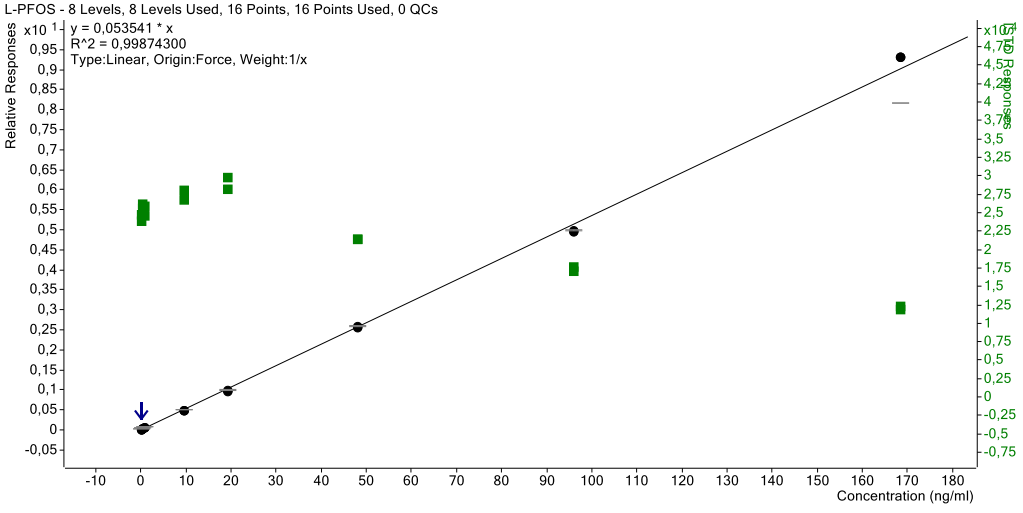


Figure D.11. Calibration curve for L-PFOS.

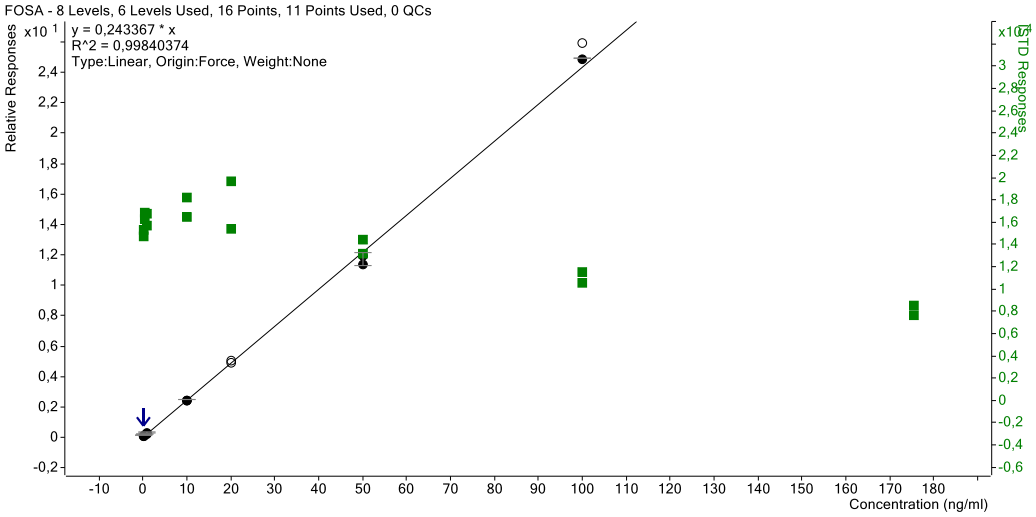


Figure D.12. Calibration curve for FOSA.

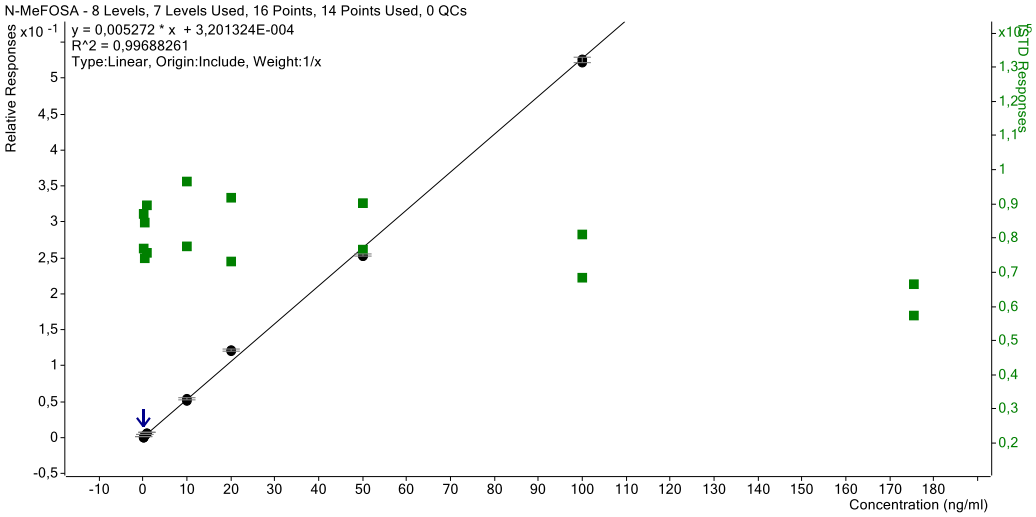


Figure D.13. Calibration curve for MeFOSA.

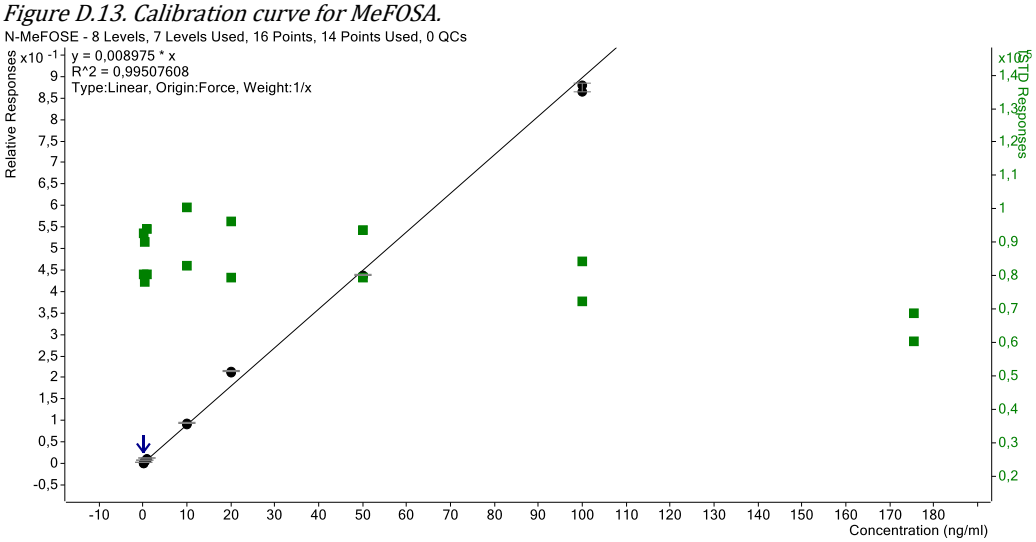


Figure D.14. Calibration curve for MeFOSE.

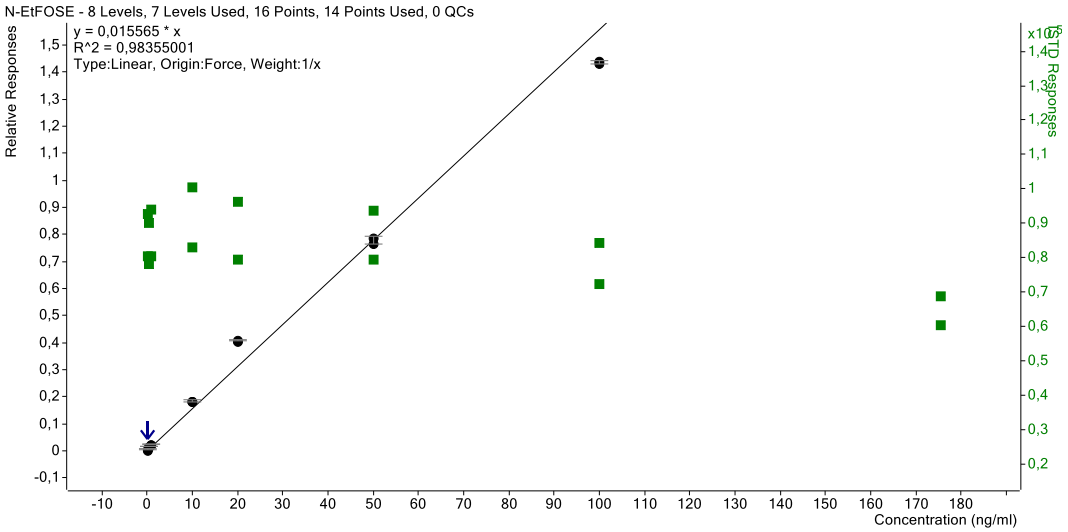


Figure D.15. Calibration curve for EtFOSE.

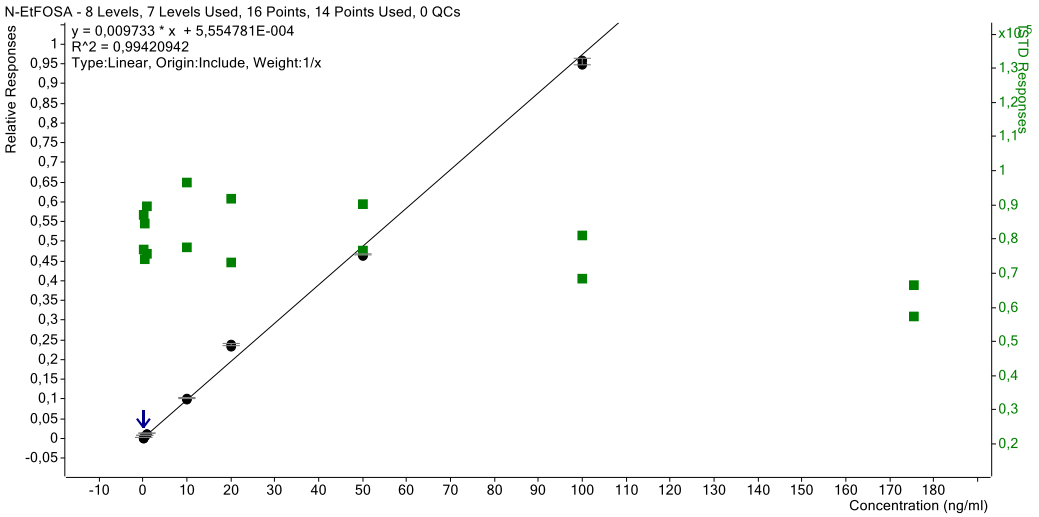


Figure D.16. Calibration curve for EtFOSA.

E QA and Analytical results

E.1 Sample and analytical protocol

Table E.1. Green = ISTD B added after extraction, and only used for quantification

Sample ID	Sample type	Sample name	Sampling date	Sampling time	Site identity	Position	Other info. (weather etc. during sampling, analytical or procedural info.)	Filtrated	Wt. Sample before filtrering [g]	Wt. Sample after filtrering [g]	Wt. Sample filtered [g]	Wt. Sample before extraction [g]	Wt. Sample after extraction [g]	Wt. extracted sample [g]	Vol. extracted sample [g]	Added ISTD A [uL]	Added ISTD B [µL]	Added RSTD Fr. 1 [uL]	Added RSTD Fr. 2 [uL]	LOT# WAX cartridge	Date exstracted	Concentrated F1	Concentrated F2	Date analysis FASA/FASE F1	Date analysis PFSA F2	Date analysis PFCA F2
PFC-JSS-001	Freshwater	Linnèvatnet	22.03.2014	18:00	L5	N 78°03.477' E 013°47.011 (78,05795N, 13,7835E)	Watersampling on Linnèvatnet, sampled by Jessica L. Bosch. Ice thickness 120 cm. Air temperature ca. -13°C. R. Kallenborn water PFAS analysis. Hole drilled in extension, next time stand on sled to drill hole. Great visibility. Seemed like uniform ice. Bottles were kept in the box of the scooter for 24 hours. Were driven trhoug barentsburg Stored in the small freezer in the chemistry lab C208 at UNIS until beginning of May, then moved to freezer in the logistics department at UNIS.	No	-	-	n.a.	2176,2	183,0	1993,2	**1,993**	50	50	50	50	002334080A	19.11.2014 - 22.11.2014	Adamstuen 24.08.15	Ås, 01.12.2014	16.10.2015	23.10.2015	30.10.2015
PFC-JSS-002	Freshwater	Linnèvatnet	22.03.2014	18:00	L5	N 78°03.477' E 013°47.011	Same conditions as PFC-JSS-001.	No	-	-	n.a.	1125,1	121,8	1003,3	**1,003**	50	50	50	50	002334080A	20.11.2014 - 23.11.2014	Adamstuen 24.08.15	Ås, 01.12.2014	16.10.2015	23.10.2015	30.10.2015
PFC-JSS-003	Freshwater	Linnèvatnet	22.03.2014	18:00	L5	N 78°03.477' E 013°47.011	Same conditions as PFC-JSS-001. Extract combined with PFC-JSS-002	No	-	-	n.a.	1036,4	126,2	910,2	**0,910**	0	0	0	0	002334080A	-	-	-	-	-	-
PFC-JSS-004	Blank	Feltblank	14.11.2014		A1	N 78°03.477' E 013°47.011	Approx. 250 mL WAX-water Exposed approx. 5 minutter during sampling in Småbåthavna. Extracted with PTFE-tubing. WAX cartridge by mistake conditioned with 1440 µL (4*360 µL) instead of 4 mL.	No	-	-	n.a.	368,9	123,2	245,7	**0,246**	50	50	50	50	002334080A	17.11.2014	Adamstuen 24.08.15	Ås, 01.12.2014	16.10.2015	23.10.2015	30.10.2015
PFC-JSS-005	Blank	Feltblank	14.11.2014		A1	N 78°03.477' E 013°47.011	Approx. 250 mL WAX-water Exposed approx. 5 minutter during sampling in Småbåthavna.	No	-	-	n.a.	369,0	124,7	244,3	**0,244**	50	50	50	50	002334080A	18.11.2014	Adamstuen 24.08.15		16.10.2015	23.10.2015	30.10.2015
PFC-JSS-006	Blank	Feltblank	14.11.2014		A1	N 78°03.477' E 013°47.011	Approx. 250 mL WAX-water Exposed approx. 5 minutter during sampling in Småbåthavna.	No	-	-	n.a.	369,1	124,5	244,6	**0,245**	50	50	50	50	002334080A	19.11.2014	Adamstuen 24.08.15	NMBU Ås, 01.12.2014	16.10.2015	23.10.2015	30.10.2015
PFC-JSS-007	Saltwater	Bukt småbåthavna 1A	14.11.2014	13:15	A1	78,2408N 15,5367E	Combined with PFC-JSS-008 for large enough sample. **Extracted with PTFE-tubing. WAX cartridge by mistake conditioned with 1440 µL (4*360 µL) instead of 4 mL.**	Yes	1107,4	126,0	981,4	3362,3	1320,2	2042,1	**1,988**	50	50	50	50	002334080A	17.11.2014 - 18.11.2014	Adamstuen 24.08.15	NMBU Ås, 01.12.2014	16.10.2015	23.10.2015	30.10.2015
PFC-JSS-008	Saltwater	Bukt småbåthavna 1B	14.11.2014	13:15	A1	78,2408N 15,5367E	Combined with PFC-JSS-007. **Extracted with PTFE-tubing.**	Yes	1162,8	124,5	1038,3	-	-	-	-	0	0	0	0	-	-	-	-	-	-	-
PFC-JSS-009	Saltwater	Bukt småbåthavna 2A	14.11.2014	13:15	A1	78,2408N 15,5367E	Combined with PFC-JSS-010 for large enough sample.	No	-	-	n.a.	1099,0	123,5	975,5	**0,950**	50	50	50	50	002334080A	18.11.2014	Adamstuen 24.08.15	NMBU Ås, 01.12.2014	16.10.2015	23.10.2015	30.10.2015
PFC-JSS-010	Saltwater	Bukt småbåthavna 2B	14.11.2014	13:15	A1	78,2408N 15,5367E	Combined with PFC-JSS-009	No	-	-	n.a.	1037,4	123,5	913,9	**0,890**	0	0	0	0	-	-	-	-	-	-	-

Sample ID	Sample type	Sample name	Sampling date	Sampling time	Site identity	Position	Other info. (weather etc. during sampling, analytical or procedural info.)	Filtrated	Wt. Sample before filtrering [g]	Wt. Sample after filtrering [g]	Wt. Sample filtered [g]	Wt. Sample before extraction [g]	Wt. Sample after extraction [g]	Wt. extracted sample [g]	Vol. extracted sample [g]	Added ISTD A [uL]	Added ISTD B [µL]	Added RSTD Fr. 1 [uL]	Added RSTD Fr. 2 [uL]	LOT# WAX cartridge	Date exstracted	Concentrated F1	Concentrated F2	Date analysis FASA/FASE F1	Date analysis PFSA F2	Date analysis PFCA F2
PFC-JSS-011	Saltwater	Bukt småbåthavna 3A	14.11.2014	13:15	A1	78,2408N 15,5367E	Combined with PFC-JSS-012 for large enough. F2-extract had a leak under transport. Remaining extract <0.2 mL kept with no concentration.	No	-	-	n.a.	1157,0	123,4	1033,6	**1,006**	50	50	50	50	002334080A	18.11.2014 - 20.11.2014	Adamstuen 24.08.15	Not concentrated*.	16.10.2015	24.10.2015	30.10.2015
PFC-JSS-012	Saltwater	Bukt småbåthavna 3B	14.11.2014	13:15	A1	78,2408N 15,5367E	Combined med PFC-JSS-011	No	-	-	n.a.	1177,4	132,1	1045,3	**1,018**	0	0	0	0	002334080A	-	-	-	-	-	-
PFC-JSS-013	Blank	0,1% NH3 i metanol	18.11.2014	-	C203	UNIS lab (C203)	Solvent/reagent blank, analyse for contamination.	No	-	-	n.a.	-	-	-	-	0	0	0	0	Ikke brukt	-	-	-	16.10.2015	24.10.2015	30.10.2015
PFC-JSS-014	Blank	0,1% NH3 i metanol	18.11.2014	-	C203	UNIS lab (C203)	Solvent/reagent blank, analyse for contamination.	No	-	-	n.a.	-	-	-	-	0	0	0	0	Ikke brukt	-	-	-	16.10.2015	24.10.2015	30.10.2015
PFC-JSS-015	Blank	Metanol, SupraSolv	18.11.2014	-	C203	UNIS lab (C203)	Solvent/reagent blank, analyse for contamination.	No	-	-	n.a.	-	-	-	-	0	0	0	0	Ikke brukt	-	-	-	16.10.2015	24.10.2015	30.10.2015
PFC-JSS-016	Blank	Metanol, SupraSolv	18.11.2014	-	C203	UNIS lab (C203)	Solvent/reagent blank, analyse for contamination.	No	-	-	n.a.	-	-	-	-	0	0	0	0	Ikke brukt	-	-	-	16.10.2015	24.10.2015	31.10.2015
PFC-JSS-017	Blank	Acetatbuffer	18.11.2014	-	C203	UNIS lab (C203)	Solvent/reagent blank, analyse for contamination.	No	-	-	n.a.	-	-	-	-	0	0	0	0	Ikke brukt	-	-	-	16.10.2015	24.10.2015	31.10.2015
PFC-JSS-018	Blank	Acetatbuffer	18.11.2014	-	C203	UNIS lab (C203)	Solvent/reagent blank, analyse for contamination.	No	-	-	n.a.	--	-	-	-	0	0	0	0	Ikke brukt	-	-	-	16.10.2015	24.10.2015	31.10.2015
PFC-JSS-019	Blank	Lablank	19.11.2014	09:00	C203	UNIS lab (C203)	Lab. blank. Fraksjon 2 oppkonsentrert på NMBU 01.12.2014.	No	-	-	n.a.	344,3	98,2	246,1	**0,246**	50	50	50	50	002334080A	20.11.2014 - 21.11.2014		NMBU Ås, 01.12.2014	16.10.2015	24.10.2015	31.10.2015
PFC-JSS-020	Blank	Metanol, LiChroSolv	21.11.2014	11:00	C203	UNIS lab (C203)	Solvent/reagent blank, analyse for contamination.	No	-	-	n.a.	-	-	-	-	50	0	0	0	Ikke brukt	-			16.10.2015	24.10.2015	31.10.2015
PFC-JSS-021	Blank	0.1 % NH3 i metanol LiChroSolv	21.11.2014	11:00	C203	UNIS lab (C203)	Solvent/reagent blank, analyse for contamination.	No	-	-	n.a.	-	-	-	-	0	0	0	0	Ikke brukt	-			16.10.2015	24.10.2015	31.10.2015
PFC-JSS-022	Blank	Fieldblank Linnèvatnet location 1	18.04.2015	12:00	L1	78.03420N 013.85450E	Snowing wind from east. Bottles filled approx. 15-20 cm below the surface. Ice-thickness reaching to fixing for drill-extender, approx. 140 cm. Ice-scoop of plastic used to remove ice from the hole. Samples stored outside (temperature approx. 0 til -10°C) from sampling until 21.04.15, then in freezer room at -18°C. **F2 concentrated almost dry, reconstituted in 0,5 mL metanol.**	No			n.a.	396,6	150,3	246,3	**0,246**	50	50	50	50	002535054A	04.06.2015	UNIS 27.06.2015	UNIS 21.06.2015	16.10.2015	24.10.2015	31.10.2015
PFC-JSS-023	Freshwater	Linnèvatnet Location 1	18.04.2015	12:00	L1	78.03420N 013.85450E	Sampling conditions as above.	No	-	-	n.a.	2322,6	151,6	2171,0	**2,171**	50	50	50	50	002535054A	04.06.2015	UNIS 27.06.2015	UNIS 21.06.2015	16.10.2015	24.10.2015	31.10.2015
PFC-JSS-024	Freshwater	Linnèvatnet Location 1	18.04.2015	12:00	L1	78.03420N 013.85450E	Sampling conditions as above. **F2 concentrated almost dry, reconstituted in 0,5 mL metanol.**	No	-	-	n.a.	2356,3	151,3	2205,0	**2,205**	50	50	50	50	002535054A	04.06.2015	UNIS 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-025 A/B	Freshwater	Linnèvatnet Location 1	18.04.2015	12:00	L1	78.03420N 013.85450E	Sampling conditions as above. **F2 concentrated almost dry, reconstituted in 0,5 mL metanol.**	No	-	-	n.a.	2244,2	254,6	1989,6	**1,990**	50	50	50	50	002334080A	04.06.15 - 05.06.15	UNIS 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015

Sample ID	Sample type	Sample name	Sampling date	Sampling time	Site identity	Position	Other info. (weather etc. during sampling, analytical or procedural info.)	Filtrated	Wt. Sample before filtrering [g]	Wt. Sample after filtrering [g]	Wt. Sample filtered [g]	Wt. Sample before extraction [g]	Wt. Sample after extraction [g]	Wt. extracted sample [g]	Vol. extracted sample [g]	Added ISTD A [uL]	Added ISTD B [µL]	Added RSTD Fr. 1 [uL]	Added RSTD Fr. 2 [uL]	LOT# WAX cartridge	Date exstracted	Concentrated F1	Concentrated F2	Date analysis FASA/FASE F1	Date analysis PFSA F2	Date analysis PFCA F2
PFC-JSS-026	Blank	Fieldblank Linnèvatnet Location 2	18.04.2015	15:30	L2	78.03976N 013.82748E	Sampling conditions as above. F2 concentrated almost dry, reconstituted in 0,5 mL metanol.	No	-	-	n.a.	399,8	151,3	248,5	**0,249**	50	50	50	50	002334080A	05.06.2015	UNIS 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-027	Freshwater	Linnèvatnet Location 2	18.04.2015	15:30	L2	78.03976N 013.82748E	Sampling conditions as above. F2 concentrated almost dry, reconstituted in 0,5 mL metanol.	No	-	-	n.a.	2398,9	151,2	2247,7	**2,248**	50	50	50	50	002334080A	05.06.2015	UNIS 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-028	Freshwater	Linnèvatnet Location 2	18.04.2015	15:30	L2	78.03976N 013.82748E	Sampling conditions as above.	No	-	-	n.a.	2385,8	150,4	2235,4	**2,235**	50	50	50	50	002334080A	05.06.2015	UNIS 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-029 A/B	Freshwater	Linnèvatnet Location 2	18.04.2015	15:30	L2	78.03976N 013.82748E	Sampling conditions as above.	No	-	-	n.a.	2274,21	258,42	2015,8	**2,016**	50	50	50	50	002334080A	05.06.2015	UNIS 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-030	Blank	Fieldblank Linnèvatnet Location 3	18.04.2015	16:30	L3	78.04803N 013.80151E	Sampling conditions as above.	No			n.a.	373,4	129,0	244,4	**0,244**	50	50	50	50	002334080A	06.06.2015	UNIS 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-031 A/B	Freshwater	Linnèvatnet Location 3	18.04.2015	16:30	L3	78.04803N 013.80151E	Sampling conditions as above.	No			n.a.	2242,9	249,8	1993,1	**1,993**	50	50	50	50	002334080A	06.06.2015	UNIS, 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-032 A/B	Freshwater	Linnèvatnet Location 3	18.04.2015	16:30	L3	78.04803N 013.80151E	Sampling conditions as above.	No			n.a.	2311,7	251,3	2060,4	**2,060**	50	50	50	50	002334080A	06.06.2015	UNIS, 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-033 A/B	Freshwater	Linnèvatnet Location 3	18.04.2015	16:30	L3	78.04803N 013.80151E	Sampling conditions as above.	No			n.a.	2239,3	250,7	1988,6	**1,989**	50	50	50	50	002334080A	06.06.2015	UNIS, 27.06.2015	UNIS 21.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-034	Blank	Fieldblank Linnèvatnet Location 4	18.04.2015	17:15	L4	78,06000N 013,77238E	Sampling conditions as above.	No			n.a.	367,0	125,4	241,6	**0,242**	50	50	50	50	002334080A	10.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-035 A/B	Freshwater	Linnèvatnet Location 4	18.04.2015	17:15	L4	78,06000N 013,77238E	Sampling conditions as above. (B not extracted). B-bottle trasported to NMBU. Analysed for pH, conductivity, alkalinity and major ions.**10.07.2015: pH = 8,00 @ 20,2°C (Mettler Toledo SevenCompact pH/ion, InLab Expert pro electrode (pH 0-14, T 0-100°C), , buffer pH 7,00 og 9,21.**	No			n.a.	1134,8	126,1	1008,7	**1,009**	50	50	50	50	002334080A	10.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-036 A/B	Freshwater	Linnèvatnet Location 4	18.04.2015	17:15	L4	78,06000N 013,77238E	Sampling conditions as above.	No			n.a.	2240,7	251,3	1989,3	**1,989**	50	50	50	50		10.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-037 A/B	Freshwater	Linnèvatnet Location 4	18.04.2015	17:15	L4	78,06000N 013,77238E	Sampling conditions as above.	No			n.a.	2266,3	255,7	2010,7	**2,011**	50	50	50	50		10.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-038	Blank	MilliQ water	03.06.2015	11:00	C208	UNIS lab (C208)	MilliQ-water extracted to make WAX water.	No			n.a.	2000.0	0.0	2000.0	**2,000**	50	50	50	50	002334080A	03.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-039	Blank	Field blank	05.06.2015	12:15	A1	78.24061N 015.53694E	Partly cloudy, 3.8°C, wind approx. 2 m/s from EAST.	No			n.a.	398,6	151,6	247,0	**0,247**	50	50	50	50	002535054A	11.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-040	Freshwater	Bukt småbåthavn	05.06.2015	12:15	A1	78.24061N 015.53694E	Sampling conditions as above.	Yes	2359.7	151,9	2207.8	2348.6	151,9	2196.7	**2,197**	50	50	50	50	002535054A	11.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-041	Freshwater	Bukt småbåthavn	05.06.2015	12:15	A1	78.24061N 015.53694E	Sampling conditions as above.	Yes	2407,2	154,9	2252.3	2119,6	152,2	1967,4	**1,967**	50	50	50	50	002535054A	11.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-042	Freshwater	Bukt småbåthavn	05.06.2015	12:15	A1	78.24061N 015.53694E	Sampling conditions as above. Filtered with GF/F filter, because no GF/C left.	Yes	2356.1	155,3	2200.9	2293.8	152.4	2141.4	**2,141**	50	50	50	50	002535054A	11.06.2015	UNIS, 27.06.2015	UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015

Sample ID	Sample type	Sample name	Sampling date	Sampling time	Site identity	Position	Other info. (weather etc. during sampling, analytical or procedural info.)	Filtrated	Wt. Sample before filtrering [g]	Wt. Sample after filtrering [g]	Wt. Sample filtered [g]	Wt. Sample before extraction [g]	Wt. Sample after extraction [g]	Wt. extracted sample [g]	Vol. extracted sample [g]	Added ISTD A [uL]	Added ISTD B [µL]	Added RSTD Fr. 1 [uL]	Added RSTD Fr. 2 [uL]	LOT# WAX cartridge	Date exstracted	Concentrated F1	Concentrated F2	Date analysis FASA/FASE F1	Date analysis PFSA F2	Date analysis PFCA F2
PFC-JSS-043	Blank	Fieldblank Linnèvatnet location 1	15.06.2015	13:45	L1	78.03420N 013.85453E	Sample bottles rinsed with 3 x 1/3 - 1/2 sample water before sampling. Applies to all samples collected in June at Kapp Linné.	No			n.a.	394,4	150.3	244,1	**0,244**	50	50	50	50	002535054A	20.06.2015		UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-044	Freshwater	Linnèvatnet Location 1	15.06.2015	13:45	L1	78.03420N 013.85453E	Drill/Auger 1 m lenght, diameter 200 mm, extender 45 cm, ice-axe 65 cm.	No			n.a.	2382,4	150,0	2232,4	**2,232**	50	50	50	50	002535054A	20.06.2015		UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-045	Freshwater	Linnèvatnet Location 1	15.06.2015	13:45	L1	78.03420N 013.85453E	Ice thickness 1 m (1 x ice-drill) at all sample sites in Lake Linnèvatnet.	No			n.a.	2397,2	152,2	2245,0	**2,245**	50	50	50	50	002535054A	20.06.2015		UNIS 23.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-046	Freshwater	Linnèvatnet Location 1	15.06.2015	13:45	L1	78.03420N 013.85453E	Depth = 18.5 x ice-axe = 12 m	No			n.a.	2376.5	150.8	2225.7	**2,226**	50	50	50	50	002535054A	20.06.2015		UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-047	Blank	Fieldblank Linnèvatnet Location 2	15.06.2015	15:35	L2	78.03978N 013.82747E	Depth = 49,3 ice-axe = 32 m	No			n.a.	397,1	151,4	245,7	**0,246**	50	50	50	50	002535054A	20.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-048	Freshwater	Linnèvatnet Location 2	15.06.2015	15:35	L2	78.03978N 013.82747E		No			n.a.	2425,4	153,0	2272,4	**2,272**	50	50	50	50	002535054A	20.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-049	Freshwater	Linnèvatnet Location 2	15.06.2015	15:35	L2	78.03978N 013.82747E		No			n.a.	2380,3	153,6	2226,7	**2,227**	50	50	50	50	002535054A	20.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-050	Freshwater	Linnèvatnet Location 2	15.06.2015	15:35	L2	78.03978N 013.82747E	Sample bottle broken before analysis.	No	-	-	n.a.	-	-	-	-	-		-	50	-	-	-	-	-	-	-
PFC-JSS-051	Blank	Fieldblank Linnèvatnet Location 3	16.06.2015	12:00	L3	78,04803N 013.80148E	Depth = 54 x ice-axe (+ some cm) = 35 m	No			n.a.	399,7	153,0	246,7	**0,247**	50	50	50	50	002535054A	22.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-052	Freshwater	Linnèvatnet Location 3	16.06.2015	12:00	L3	78,04803N 013.80148E		No			n.a.	2377,7	152,9	2224,8	**2,225**	50	50	50	50	002535054A	22.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-053	Freshwater	Linnèvatnet Location 3	16.06.2015	12:00	L3	78,04803N 013.80148E	SPE "dry" over night, but whole sample loaded.	No			n.a.	2369,6	152,2	2217,4	**2,217**	50	50	50	50	002535054A	22.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-054	Freshwater	Linnèvatnet Location 3	16.06.2015	12:00	L3	78,04803N 013.80148E	SPE "dry" over night, but whole sample loaded.	No			n.a.	2380,7	151,7	2229,0	**2,229**	50	50	50	50	002535054A	22.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-055	Blank	Fieldblank Linnèvatnet Location 4	16.06.2015	14:30	L4	78,06000N 013,77238E	Depth = 41 ice-axe = 27 m	No			n.a.	397,2	151,1	246,1	**0,246**	50	50	50	50	002535054A	22.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-056	Freshwater	Linnèvatnet Location 4	16.06.2015	14:30	L4	78,06000N 013,77238E	SPE "dry" over night, but whole sample loaded.	No			n.a.	2379,9	150,5	2229,5	**2,229**	50	50	50	50	002535054A	22.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-057	Freshwater	Linnèvatnet Location 4	16.06.2015	14:30	L4	78,06000N 013,77238E		No			n.a.	2368,4	150,7	2217,7	**2,218**	50	50	50	50	002535054A	22.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-058	Freshwater	Linnèvatnet Location 4	16.06.2015	14:30	L4	78,06000N 013,77238E	09.10.15: ISTD possibly forgotten, added 50 µL ISTD A in F1 and F2, 50 µL av ISTD B in F2.	No			n.a.	2372,3	150,6	2221,7	**2,222**	50	50	50	50	002535054A	22.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-059	Quality control	Spike location 4	16.06.2015	14:30	L4	78,06000N 013,77238E	Divided in two sub-samples(2 x 1 L). Part 2 is PCF-JSS-076. Added 50 µL native spike-mix. Examine matrix-effect/recovery.	No			n.a.	1394,9	151,0	1244,0	**1,244**	50	50	50	50	002535054A	26.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015
PFC-JSS-060	Quality control	Spike location 4	16.06.2015	14:30	L4	78,06000N 013,77238E	Divided in two sub-samples(2 x 1 L). Part 2 is PCF-JSS-077. Added 50 µL native spike-mix. Examine matrix-effect/recovery.	No			n.a.	1392,8	150,3	1242,5	**1,243**	50	50	50	50	002535054A	26.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	24.10.2015	31.10.2015

Sample ID	Sample type	Sample name	Sampling date	Sampling time	Site identity	Position	Other info. (weather etc. during sampling, analytical or procedural info.)	Filtrated	Wt. Sample before filtrering [g]	Wt. Sample after filtrering [g]	Wt. Sample filtered [g]	Wt. Sample before extraction [g]	Wt. Sample after extraction [g]	Wt. extracted sample [g]	Vol. extracted sample [g]	Added ISTD A [uL]	Added ISTD B [uL]	Added RSTD Fr. 1 [uL]	Added RSTD Fr. 2 [uL]	LOT# WAX cartridge	Date exstracted	Concentrated F1	Concentrated F2	Date analysis FASA/FASE F1	Date analysis PFSA F2	Date analysis PFCA F2
PFC-JSS-061	Freshwater	Inflow Linnevatnet	15.06.2015	11:14	I	78.02846N 013.86180E		Yes	2432.5	153.7	2278.8	2431.8	152.9	2278,9	**2,279**	50	50	50	50	002535054A	26.-27.06.15	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	31.10.2015
PFC-JSS-062	Freshwater	Smeltewater 1	16.06.2015	11:40	M1	N78.03306 E13.79750	Some sample leaked out in refrigirator at Isfjord Radio because of loose cap. **F2 extract spilled in fume hood at Adamsttuen. Attemted to be collected and recovered, but likely contaminated. Compare with Ahrens results.**	No			n.a.	2442.5	151.0	2291.5	**2,291**	50	50	50	50	002535054A	26.-28.06.2015	Adamstuen, 24.08.15	Adamstuen, 24.08.15	17.10.2015	25.10.2016	31.10.2015
PFC-JSS-063	Freshwater	Snow sample 1	13.06.2015	17:00	S1	N78.03153 E13.79294	First snowsample. Some sediment. but not filtrated. Used 3 WAX-cartridges because of particles plugging it.	No			n.a.	2051.5		2051.5	**2,052**	50	50	50	50	002535054A	26.06.2015	Adamstuen, 24.08.15	Adamstuen, 24.08.15	17.10.2015	25.10.2016	31.10.2015
PFC-JSS-064	Freshwater	Outflow Linnevatnet	14.06.2015	11:50	O	N78.06665 E13.78019		No			n.a.	2487.9		2487.9	**2,488**	50	50	50	50	002535054A	26.06.2015	Adamstuen, 24.08.15	Adamstuen, 24.08.15	17.10.2015	25.10.2016	31.10.2015
PFC-JSS-065	Freshwater	Smeltewater 2	16.06.2015	12:45	M2	N78.03883 E13.86175	Some sediment/particles, but not filtratedt. Two WAX cartridges used. WAX#2 LOT nr: 002334148A	No			n.a.	2306.6		2306.6	**2,307**	50	50	50	50	002535054A	26.06.2015	Adamstuen, 24.08.15	Adamstuen, 24.08.15	17.10.2015	25.10.2016	31.10.2015
PFC-JSS-066	Freshwater	Snow sample 2	15.06.2015	16:00	S2	N78.04001 E13.86818	15-W-14	Yes	2461.4	145.3	2316.2	2461.3	145.2	2316.0	**2,316**	50	50	50	50	002535054A	26.-27.06.15	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	31.10.2015
PFC-JSS-067	Quality control	Blank recovery 1	21.06.2015	09:30		UNIS Lab C208	50 µL of native spike-mix	No			n.a.	2281.8	151.3	2130.5	**2,131**	50	50	50	50	002535054A	21.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	01.11.2015
PFC-JSS-068	Quality control	Breakthrough 1	21.06.2015	09:30		UNIS Lab C208		No			n.a.	-	-	-	-	0	0	50	50	002535054A	21.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	01.11.2015
PFC-JSS-069	Quality control	Blank recovery 2	21.06.2015	09:30		UNIS Lab C208	50 µL of native spike-mix	No			n.a.	2230.3	150.7	2079.6	**2,080**	50	50	50	50	002535054A	21.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	01.11.2015
PFC-JSS-070	Quality control	Breakthrough 2	21.06.2015	09:30		UNIS Lab C208		No			n.a.	-	-	-	-	0	0	50	50	002535054A	21.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	01.11.2015
PFC-JSS-071	Quality control	Blank recovery 3	21.06.2015	09:30		UNIS Lab C208	50 µL of native spike-mix	No			n.a.	2252.8	145.5	2107.3	**2,107**	50	50	50	50	002535054A	21.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	01.11.2015
PFC-JSS-072	Quality control	Breakthrough 3	21.06.2015	09:30		UNIS Lab C208		No			n.a.	-		-	-	0	0	50	50	002535054A	21.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	01.11.2015
PFC-JSS-073	Blank	Lab blank June 2015 - 1	21.06.2015	16:00		UNIS Lab C208	250 g WAX- Water in 250 mL PE-bottle cleaned 3x4 mL methanol and 3x4 mL WAX-water. F1 possibly eluted with 0.1% NH3/Metanol	No			n.a.	284.9	34.3	250.6	**0,251**	50	50	50	50	002535054A	26.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	01.11.2015
PFC-JSS-074	Blank	Lab blank June 2015 - 2	21.06.2015	16:00		UNIS Lab C208	250 g WAX- Water in 250 mL PE-bottle cleaned 3x4 mL methanol and 3x4 mL WAX-water. (NB! Paper clip fell into the blank!!). F1 possibly eluted with 0.1% NH3/Metanol	No			n.a.	283.8	33.4	250.4	**0,250**	50	50	50	50	002535054A	26.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	17.10.2015	25.10.2016	01.11.2015
PFC-JSS-075	Blank	Lab blank June 2015 - 3	21.06.2015	16:00		UNIS Lab C208	250 g WAX- Water in 250 mL PE-bottle cleaned 3x4 mL methanol and 3x4 mL WAX-water	No			n.a.	284.4	34.2	250.2	**0,250**	50	50	50	50	002334148A	27.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	18.10.2015	25.10.2016	01.11.2015

Sample ID	Sample type	Sample name	Sampling date	Sampling time	Site identity	Position	Other info. (weather etc. during sampling, analytical or procedural info.)	Filtrated	Wt. Sample before filtrering [g]	Wt. Sample after filtrering [g]	Wt. Sample filtered [g]	Wt. Sample before extraction [g]	Wt. Sample after extraction [g]	Wt. extracted sample [g]	Vol. extracted sample [g]	Added ISTD A [uL]	Added ISTD B [µL]	Added RSTD Fr. 1 [uL]	Added RSTD Fr. 2 [uL]	LOT# WAX cartridge	Date exstracted	Concentrated F1	Concentrated F2	Date analysis FASA/FASE F1	Date analysis PFSA F2	Date analysis PFCA F2
PFC-JSS-076	Quality control	Spike location 4	16.06.2015	14:30	L4	78,06000N 013,77238E	Sub-sample two (2 x 1 L). Part 1 is PCF-JSS-059. Added 50 µL of native spike-mix. Examine matic-effect/recovery.	No			n.a.	1097,9	125,9	972,0	**0,972**	50	50	50	50	002535054A	26.-28.06.2015	Adamstuen, 24.08.15	Adamstuen 24.08.15	18.10.2015	25.10.2016	01.11.2015
PFC-JSS-077	Quality control	Spike location 4	16.06.2015	14:30	L4	78,06000N 013,77238E	Sub-sample two (2 x 1 L). Part 1 is PCF-JSS-060. Added 50 µL of native spike-mix. Examine matic-effect/recovery.	No			n.a.	1080,4	126,6	953,8	**0,954**	50	50	50	50	002535054A	26.-27.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	18.10.2015	25.10.2016	01.11.2015
PFC-JSS-078	Blank	Filtration blank	26.06.2015	21:00		UNIS Lab C208		Yes	397,0	150,2	246,9	397,5	150,2	247,3	**0,247**	50	50	50	50	002334148A	27.06.2015	Adamstuen, 24.08.15	UNIS 27.06.2015	18.10.2015	25.10.2016	01.11.2015
PFC-JSS-079	Blank	Lab blank Adamstuen.	25.08.2015	11:00		H-116 Miljøtokslab Adamstuen	4 mL VWR methanol HiPerSolv in methanol-cleaned 15 mL PP-rør, concentrated to 0,5 mL	No			n.a.	-	-	-	-	50	50	50	-	Ikke brukt	25.08.2015	Adamstuen 25.08.15	-	18.10.2015	25.10.2016	01.11.2015
SPE vask1		SPE rinse 1	13.11.2014			UNIS	Vasket SPE ventiler med 3x1mL metanol. Brukes til å sjekke kontaminering.				0,0			0,0	**0,000**	50				-	-	Adamstuen 25.08.15	Adamstuen 25.08.15	18.10.2015	25.10.2016	01.11.2015
SPE vask2		SPE rinse 2	13.11.2014			UNIS	Vasket SPE ventiler med 3x1mL metanol. Brukes til å sjekke kontaminering.				0,0			0,0	**0,000**	50				-	-	Adamstuen 25.08.15	Adamstuen 25.08.15	18.10.2015	25.10.2016	01.11.2015
SPE vask3		SPE rinse 3	13.11.2014			UNIS	Vasket SPE ventiler med 3x1mL metanol. Brukes til å sjekke kontaminering.				0,0			0,0	**0,000**	50				-	-	Adamstuen 25.08.15	Adamstuen 25.08.15	18.10.2015	25.10.2016	01.11.2015
PFC-JSS-083		PTFE cap-liner	13.11.2014			UNIS	PTFE innlegg fra kork i metanolflaskeble lagt i et 50 mL pp-rør med 10 mL metanol.				0,0			0,0	**0,000**	50				-	-	Adamstuen 25.08.15	Adamstuen 25.08.15	18.10.2015	25.10.2016	01.11.2015

E.2 QA results

Table E.2. Blue = ISTD B added after extraction, used only for quantification
Green dots mark acceptable recoveries, red dots are recoveries <40 % or >120 %.

Sample ID	Sample Type	ISTD 1 [ng]	ISTD 2 [ng]	RSTD [ng]	$^{13}C_8$PFOA Recovery	$^{13}C_4$PFBA Recovery	$^{13}C_5$PFHxA Recovery	$^{13}C_4$PFHpA Recovery	$^{13}C_4$PFOA Recovery	$^{13}C_5$PFNA Recovery	$^{13}C_2$PFDA Recovery	$^{13}C_2$PFUdA Recovery	$^{13}C_2$PFDoDA Recovery	$^{18}O_2$PFHxS Recovery	$^{13}C_4$PFOS Recovery
PFC-JSS-001	Sample	10	10	9,8	86,0 %	106,4 %	141,1 %	97,0 %	180,1 %	163,1 %	43,4 %	17,5 %	227,0 %	239,0 %	
PFC-JSS-002-003	Sample	10	10	9,8	76,6 %	77,4 %	94,3 %	104,8 %	129,2 %	111,1 %	90,3 %	55,7 %	95,0 %	97,8 %	
PFC-JSS-004	MatrixBlank	10	10	9,8	114,6 %	40,9 %	53,0 %	101,5 %	136,8 %	105,9 %	101,8 %	100,7 %	99,4 %	98,2 %	
PFC-JSS-005	MatrixBlank	10	10	9,8	102,0 %	23,0 %	31,3 %	101,3 %	131,6 %	100,8 %	97,8 %	93,4 %	97,8 %	97,7 %	
PFC-JSS-006	MatrixBlank	10	10	9,8	125,0 %	64,9 %	84,3 %	102,0 %	142,4 %	108,4 %	112,5 %	112,0 %	95,5 %	95,0 %	
PFC-JSS-007-8	Sample	10	10	9,8	87,6 %	38,2 %	50,8 %	99,5 %	155,8 %	128,4 %	125,1 %	126,7 %	98,8 %	100,0 %	
PFC-JSS-009-10	Sample	10	10	9,8	70,9 %	54,2 %	70,4 %	96,1 %	133,3 %	111,2 %	121,0 %	122,7 %	89,4 %	91,5 %	
PFC-JSS-011-12	Sample	10	10	9,8	92,9 %	2,8 %	3,6 %	103,1 %	111,6 %	97,7 %	94,2 %	93,1 %	100,5 %	99,1 %	
PFC-JSS-019	MatrixBlank	10	10	9,8	89,6 %	27,8 %	36,7 %	92,5 %	97,5 %	92,9 %	86,3 %	83,1 %	89,4 %	87,8 %	
PFC-JSS-022	MatrixBlank	10	10	9,8	103,5 %	62,8 %	64,4 %	96,9 %	111,5 %	91,8 %	102,2 %	94,8 %	57,5 %	93,5 %	
PFC-JSS-023	Sample	10	10	9,8	77,1 %	77,0 %	89,9 %	98,0 %	121,0 %	108,3 %	98,9 %	94,5 %	81,6 %	96,2 %	
PFC-JSS-024	Sample	10	10	9,8	80,9 %	79,3 %	89,4 %	102,5 %	120,1 %	105,9 %	90,3 %	88,4 %	78,8 %	99,1 %	
PFC-JSS-025	Sample	10	10	9,8	88,9 %	95,0 %	106,1 %	103,6 %	132,8 %	122,7 %	100,0 %	100,8 %	116,5 %	118,7 %	
PFC-JSS-026	MatrixBlank	10	10	9,8	115,0 %	74,6 %	74,4 %	100,7 %	110,3 %	105,1 %	113,3 %	113,9 %	62,0 %	97,1 %	
PFC-JSS-027	Sample	10	10	9,8	67,4 %	74,0 %	91,5 %	102,0 %	116,1 %	104,5 %	76,8 %	75,1 %	83,8 %	95,6 %	
PFC-JSS-028	Sample	10	10	9,8	65,1 %	74,0 %	89,2 %	96,3 %	110,8 %	99,3 %	77,1 %	79,9 %	82,4 %	90,9 %	
PFC-JSS-029	Sample	10	10	9,8	78,8 %	87,8 %	98,4 %	97,2 %	125,8 %	112,0 %	91,1 %	96,3 %	107,5 %	109,0 %	
PFC-JSS-030	MatrixBlank	10	10	9,8	125,5 %	85,7 %	74,1 %	100,2 %	131,1 %	112,7 %	121,0 %	116,7 %	60,8 %	98,6 %	
PFC-JSS-031	Sample	10	10	9,8	47,0 %	73,5 %	91,0 %	102,9 %	123,9 %	118,6 %	117,5 %	105,3 %	116,1 %	125,4 %	
PFC-JSS-032	Sample	10	10	9,8	39,0 %	65,2 %	81,7 %	93,6 %	109,6 %	97,2 %	101,8 %	105,7 %	110,1 %	117,4 %	
PFC-JSS-033	Sample	10	10	9,8	53,3 %	73,7 %	83,0 %	96,4 %	114,3 %	110,1 %	107,6 %	106,7 %	111,6 %	118,0 %	
PFC-JSS-034	MatrixBlank	10	10	9,8	129,5 %	60,9 %	88,3 %	101,5 %	94,5 %	115,8 %	127,8 %	123,3 %	105,8 %	101,3 %	
PFC-JSS-035	Sample	10	10	9,8	94,1 %	78,6 %	86,2 %	100,4 %	121,6 %	109,2 %	111,6 %	96,7 %	111,3 %	109,4 %	
PFC-JSS-036	Sample	10	10	9,8	88,7 %	94,9 %	80,8 %	102,1 %	115,4 %	93,7 %	94,9 %	93,5 %	120,0 %	117,3 %	
PFC-JSS-037	Sample	10	10	9,8	1249,6 %	0,0 %	0,1 %	87,6 %	1,9 %	2,1 %	0,0 %	0,0 %	0,0 %	1,8 %	
PFC-JSS-038	MatrixBlank	10	10	9,8	99,3 %	67,9 %	80,3 %	101,4 %	117,9 %	96,3 %	101,2 %	97,4 %	88,0 %	95,7 %	
PFC-JSS-039	MatrixBlank	10	10	9,8	102,1 %	62,0 %	94,4 %	100,6 %	104,7 %	97,2 %	103,2 %	100,7 %	93,9 %	92,2 %	
PFC-JSS-040	Sample	10	10	9,8	15,0 %	47,1 %	81,0 %	96,2 %	101,3 %	111,3 %	152,4 %	174,3 %	80,0 %	82,4 %	
PFC-JSS-041	Sample	10	10	9,8	15,4 %	43,2 %	74,4 %	98,6 %	101,3 %	130,2 %	142,8 %	154,2 %	78,4 %	85,7 %	
PFC-JSS-042	Sample	10	10	9,8	16,4 %	46,5 %	78,6 %	100,0 %	106,6 %	134,0 %	155,1 %	164,6 %	78,0 %	87,9 %	
PFC-JSS-043	MatrixBlank	10	20	9,8	84,7 %	53,7 %	91,7 %	85,2 %	80,1 %	77,8 %	80,3 %	69,3 %	80,9 %	74,1 %	
PFC-JSS-044	Sample	10	20	9,8	75,7 %	69,8 %	89,6 %	88,8 %	90,0 %	83,8 %	87,0 %	75,6 %	79,1 %	81,1 %	
PFC-JSS-045	Sample	10	20	9,8	76,9 %	69,4 %	89,8 %	90,2 %	86,3 %	84,4 %	90,1 %	76,7 %	79,9 %	83,9 %	
PFC-JSS-046	Sample	10	20	9,8	75,3 %	64,0 %	83,2 %	87,9 %	84,0 %	82,8 %	83,2 %	70,7 %	78,4 %	79,7 %	
PFC-JSS-047	MatrixBlank	10	10	9,8	92,9 %	56,3 %	95,6 %	88,4 %	91,5 %	85,3 %	79,5 %	44,9 %	80,5 %	75,5 %	
PFC-JSS-048	Sample	10	10	9,8	79,5 %	71,9 %	94,0 %	92,7 %	89,8 %	82,4 %	60,5 %	55,9 %	77,8 %	80,9 %	
PFC-JSS-049	Sample	10	10	9,8	77,5 %	70,8 %	94,3 %	91,9 %	93,5 %	82,1 %	63,2 %	49,8 %	69,8 %	79,8 %	
PFC-JSS-051	MatrixBlank	10	10	9,8	84,5 %	44,7 %	89,9 %	78,4 %	76,9 %	80,5 %	77,4 %	56,6 %	74,3 %	63,3 %	
PFC-JSS-052	Sample	10	10	9,8	67,4 %	70,5 %	90,6 %	87,0 %	90,3 %	81,2 %	64,1 %	40,9 %	73,2 %	77,2 %	
PFC-JSS-053	Sample	10	10	9,8	67,0 %	72,7 %	91,4 %	87,2 %	99,2 %	84,3 %	72,0 %	46,1 %	78,3 %	84,1 %	
PFC-JSS-054	Sample	10	10	9,8	74,3 %	74,5 %	95,1 %	87,7 %	94,0 %	88,2 %	71,9 %	44,2 %	67,6 %	81,7 %	
PFC-JSS-055	MatrixBlank	10	10	9,8	97,1 %	50,7 %	97,3 %	90,5 %	90,3 %	86,8 %	77,7 %	47,0 %	84,6 %	73,6 %	
PFC-JSS-056	Sample	10	10	9,8	76,3 %	73,6 %	98,1 %	90,8 %	93,9 %	82,8 %	70,5 %	49,6 %	78,8 %	82,0 %	
PFC-JSS-057	Sample	10	10	9,8	79,7 %	69,5 %	87,8 %	92,9 %	96,9 %	89,0 %	85,0 %	57,5 %	78,1 %	83,9 %	
PFC-JSS-058	Sample	20	20	9,8	83,3 %	87,0 %	100,9 %	97,5 %	95,9 %	82,4 %	105,8 %	86,1 %	80,6 %	79,0 %	
PFC-JSS-059	Sample	10	10	9,8	89,5 %	71,5 %	88,3 %	93,4 %	103,0 %	93,3 %	93,3 %	70,8 %	93,1 %	95,1 %	
PFC-JSS-060	Sample	10	10	9,8	87,5 %	79,0 %	99,9 %	94,4 %	102,5 %	96,3 %	92,8 %	68,9 %	93,6 %	95,2 %	
PFC-JSS-061	Sample	10	10	9,8	59,7 %	76,6 %	99,1 %	89,2 %	101,9 %	100,7 %	95,7 %	74,1 %	79,1 %	93,1 %	
PFC-JSS-062	Sample	10	10	9,8	14,9 %	17,9 %	22,8 %	22,6 %	24,1 %	18,8 %	14,6 %	10,2 %	18,0 %	17,1 %	
PFC-JSS-063	Sample	10	10	9,8	100,9 %	87,2 %	112,2 %	95,7 %	116,2 %	104,8 %	98,9 %	66,7 %	80,9 %	85,2 %	
PFC-JSS-064	Sample	10	10	9,8	60,5 %	73,4 %	83,6 %	90,0 %	104,8 %	96,9 %	72,0 %	41,6 %	67,0 %	92,6 %	
PFC-JSS-065	Sample	10	10	9,8	51,6 %	70,7 %	90,8 %	92,0 %	100,1 %	95,8 %	80,2 %	57,8 %	79,1 %	88,3 %	
PFC-JSS-066	Sample	10	10	9,8	108,7 %	89,7 %	113,8 %	91,3 %	102,7 %	104,4 %	112,2 %	79,1 %	83,5 %	88,0 %	
PFC-JSS-067	Sample	10	10	9,8	84,2 %	70,6 %	84,6 %	80,9 %	93,3 %	86,8 %	90,8 %	71,8 %	70,9 %	80,7 %	
PFC-JSS-069	Sample	10	10	9,8	93,3 %	79,9 %	95,8 %	89,8 %	103,4 %	94,3 %	104,0 %	83,7 %	85,9 %	95,2 %	
PFC-JSS-071	Sample	10	10	9,8	121,9 %	62,4 %	102,5 %	89,0 %	97,0 %	117,1 %	126,4 %	96,2 %	79,2 %	81,6 %	
PFC-JSS-073	MatrixBlank	10	10	9,8	90,5 %	70,3 %	90,3 %	90,3 %	100,8 %	95,6 %	94,5 %	75,4 %	88,3 %	86,8 %	
PFC-JSS-074	MatrixBlank	10	10	9,8	91,8 %	75,2 %	99,4 %	92,8 %	104,8 %	89,6 %	93,4 %	77,3 %	86,0 %	82,8 %	
PFC-JSS-075	MatrixBlank	10	10	9,8	79,5 %	64,1 %	87,8 %	80,4 %	92,2 %	84,0 %	81,6 %	64,0 %	79,3 %	77,9 %	
PFC-JSS-076	Sample	10	10	9,8	84,1 %	74,8 %	94,3 %	89,8 %	96,9 %	84,1 %	80,2 %	46,2 %	87,5 %	87,9 %	
PFC-JSS-077	Sample	10	10	9,8	94,6 %	88,0 %	107,0 %	92,8 %	108,9 %	99,6 %	104,9 %	78,6 %	91,6 %	96,7 %	
PFC-JSS-078	MatrixBlank	10	10	9,8	86,8 %	70,7 %	99,7 %	86,5 %	96,3 %	82,8 %	79,6 %	50,0 %	88,5 %	80,8 %	
PFC-JSS-079	MatrixBlank	10	10	9,8	78,4 %	82,6 %	94,5 %	86,3 %	91,8 %	85,1 %	86,5 %	80,3 %	85,6 %	82,8 %	

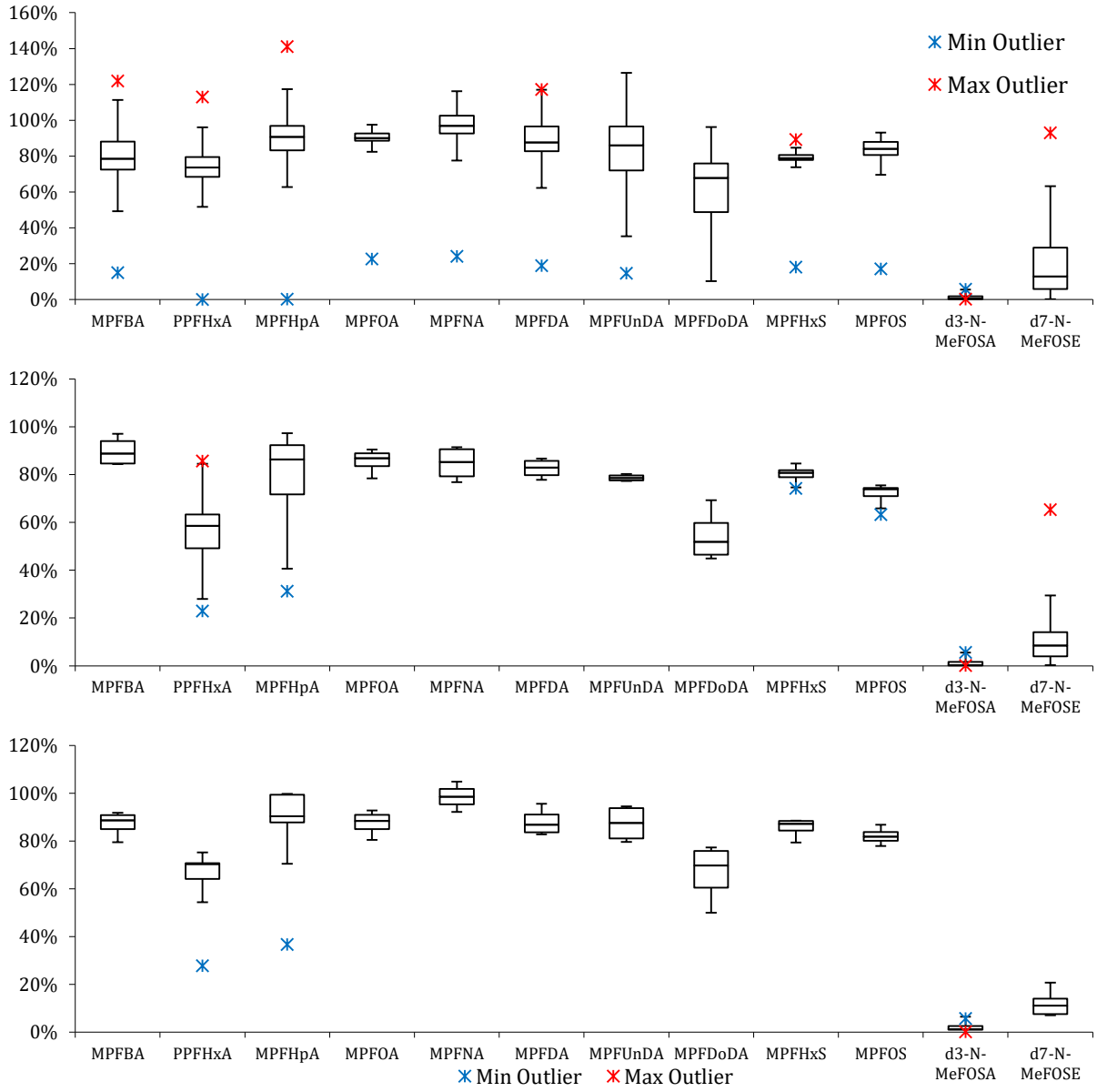


Figure E.1. Recoveries of internal standards
Upper is in samples, middle is in field blanks and lower is in lab. blanks.

Table E.3. S/N ratios, retention times (min.) and qualifier/quantifier ratios
for each single sample and matrix blank (PFBA-PFHpA, PFC-JSS-001-045). Green is acceptable values, yellow is >LOD and <LOQ and red is unacceptable or <LOD.

Sample		PFBA results		PFPeA Results		PFHxA results		Qualifier (313,0 -> 119,0)		PFHpA results		Qualifier (363,0 -> 169,0)	
Name	Type	S/N	RT	S/N	RT	S/N	RT	Ratio		S/N	RT	Ratio	
PFC-JSS-001	Sample	22,1	8,9	5,7	9,62	45,9	10,14	3,8	82,4 %	39,5	10,69	14,0	105,8 %
PFC-JSS-002-003	Sample	33,7	8,9	4,7	9,61	12,3	10,17	4,8	104,8 %	14,0	10,72	13,6	103,3 %
PFC-JSS-004	MatrixBlank	11,0	9,1	5,4	9,66	12,2	10,24	3,6	77,6 %	23,2	10,79	10,4	79,1 %
PFC-JSS-005	MatrixBlank	8,9	9,1	5,5	9,67	4,5	10,22	3,2	69,6 %	1,8	10,76	18,3	138,7 %
PFC-JSS-006	MatrixBlank	10,7	9,1	10,9	9,69	6,3	10,21	0,9	18,5 %	2,6	10,74	1,2	9,3 %
PFC-JSS-007-8	Sample	9,2	9,0	84,1	9,71	236,6	10,24	4,3	93,9 %	15,5	10,77	11,1	84,0 %
PFC-JSS-009-10	Sample	11,0	9,0	52,9	9,72	196,4	10,26	3,9	83,8 %	23,3	10,79	11,9	90,0 %
PFC-JSS-011-12	Sample	43,1	9,0	12,2	9,71	12,9	10,22	3,7	81,3 %	6,2	10,79	8,3	62,5 %
PFC-JSS-019	MatrixBlank	11,0	9,3	5,3	9,82	7,5	10,27	2,3	50,4 %	3,5	10,77	7,4	56,2 %
PFC-JSS-022	MatrixBlank	32,5	9,3	9,9	9,86	5,1	10,37	1,2	26,8 %	3,5	10,77	8,5	64,4 %
PFC-JSS-026	MatrixBlank	27,0	9,3	6,2	9,87	20,3	10,39	2,5	53,7 %	4,8	10,81	17,6	133,6 %
PFC-JSS-027	Sample	22,1	9,3	3,9	9,92	4,5	10,37	2,4	52,8 %	6,9	10,84	12,3	93,5 %
PFC-JSS-028	Sample	39,8	9,2	5,4	9,89	6,2	10,41	2,1	46,5 %	19,5	10,84	14,1	107,1 %
PFC-JSS-029	Sample	227,8	9,3	3,3	9,94	16,5	10,41	4,4	95,0 %	6,7	10,86	12,1	91,8 %
PFC-JSS-030	MatrixBlank	14,1	9,4	10,3	9,94	7,5	10,39	4,4	95,3 %	3,4	10,81	13,0	98,5 %
PFC-JSS-031	Sample	43,9	9,3	8,0	9,92	16,9	10,41	3,7	80,8 %	27,8	10,87	13,6	102,9 %
PFC-JSS-032	Sample	42,2	9,3	13,6	9,94	15,3	10,44	4,3	93,5 %	22,2	10,87	12,5	94,8 %
PFC-JSS-033	Sample	39,1	9,3	7,8	9,94	11,8	10,42	4,6	100,5 %	12,0	10,89	13,6	103,0 %
PFC-JSS-034	MatrixBlank	∞	9,4	5,7	9,96	3,1	10,54	3,7	81,5 %	3,7	10,86	7,9	59,6 %
PFC-JSS-035	Sample	25,0	9,3	3,8	9,92	7,7	10,44	4,1	89,1 %	4,9	10,91	5,6	42,2 %
PFC-JSS-036	Sample	28,6	9,3	5,7	9,99	6,4	10,42	3,7	79,4 %	8,9	10,84	7,5	57,1 %
PFC-JSS-037	Sample	21,7	9,5	4,2	9,99	4,7	10,46			3,2	10,86	3,1	23,3 %
PFC-JSS-038	MatrixBlank	32,1	9,5	5,9	9,99	7,5	10,46	2,4	51,7 %	1,5	10,91	6,4	48,4 %
PFC-JSS-039	MatrixBlank	30,6	9,5	4,7	9,99	5,8	10,46	3,9	85,4 %	3,1	10,87	9,5	72,2 %
PFC-JSS-040	Sample	9,0	9,3	25,0	9,94	98,4	10,42	3,8	82,5 %	86,1	10,87	14,2	107,2 %
PFC-JSS-041	Sample	13,0	9,3	17,2	9,94	70,2	10,44	3,9	83,7 %	47,2	10,91	12,9	97,4 %
PFC-JSS-042	Sample	9,3	9,3	20,7	9,96	99,2	10,44	3,9	85,8 %	50,5	10,89	13,6	103,0 %
PFC-JSS-043	MatrixBlank	27,2	9,5	4,1	9,99	4,0	10,44	1,3	27,5 %	19,8	10,91	14,2	108,0 %
PFC-JSS-044	Sample	26,7	9,3	1,5	9,21	11,0	10,47	5,3	115,3 %	17,2	10,92	4,8	36,2 %
PFC-JSS-045	Sample	23,4	9,3	1,8	9,97	6,4	10,49	5,3	115,5 %	13,3	10,91	15,2	115,1 %

Table E.4. S/N ratios, retention times (min.) and qualifier/quantifier ratios for each single sample and matrix blank (PFBA-PFHpA, PFC-JSS-046-079). Green is acceptable values, yellow is >LOD and <LOQ and red is unacceptable or <LOD.

Sample		PFBA results		PFPeA Results		PFHxA results		Qualifier (313,0 -> 119,0)		PFHpA results		Qualifier (363,0 -> 169,0)	
Name	Type	S/N	RT	S/N	RT	S/N	RT	Ratio		S/N	RT	Ratio	
PFC-JSS-046	Sample	30,0	9,3	1,3	9,96	6,0	10,44	4,8	103,5 %	4,8	10,92	10,5	79,9 %
PFC-JSS-047	MatrixBlank	7,4	9,5	4,6	9,99	4,2	10,46	5,3	115,0 %	3,6	10,96	13,7	103,9 %
PFC-JSS-048	Sample	34,3	9,3	5,6	10,01	16,8	10,47	4,0	86,4 %	7,3	10,94	16,1	121,9 %
PFC-JSS-049	Sample	15,0	9,3	10,0	10,01	13,8	10,49	5,0	109,0 %	5,7	10,92	9,6	72,6 %
PFC-JSS-051	MatrixBlank	15,4	9,4	4,5	9,97	2,5	10,51	10,8	234,1 %	4,0	10,92	14,0	106,1 %
PFC-JSS-052	Sample	29,9	9,3	3,4	9,96	11,5	10,47	3,4	73,9 %	7,3	10,91	12,6	95,8 %
PFC-JSS-053	Sample	39,4	9,3	3,1	9,97	6,5	10,42	5,2	113,9 %	8,1	10,94	14,9	112,7 %
PFC-JSS-054	Sample	35,5	9,3	2,7	9,96	36,9	10,47	4,0	87,5 %	6,8	10,92	11,5	87,3 %
PFC-JSS-055	MatrixBlank	11,4	9,4	4,2	10,01	2,3	10,51	6,4	139,5 %	4,4	10,96	1,8	13,6 %
PFC-JSS-056	Sample	49,8	9,3	18,1	9,96	9,1	10,47	4,2	91,0 %	16,6	10,92	11,5	86,8 %
PFC-JSS-057	Sample	36,9	9,3	28,7	9,99	9,2	10,47	5,0	107,6 %	11,4	10,92	12,8	97,2 %
PFC-JSS-058	Sample	19,2	9,5	5,6	9,99	4,4	10,53	2,5	53,8 %	3,2	10,99	14,3	108,0 %
PFC-JSS-059	Sample	114,3	9,3	243,9	9,99	351,2	10,49	4,0	86,7 %	321,0	10,94	13,3	100,7 %
PFC-JSS-060	Sample	304,7	9,3	250,3	9,99	1123,7	10,47	4,4	94,9 %	464,9	10,94	5,9	44,9 %
PFC-JSS-061	Sample	57,6	9,3	3,5	9,97	10,2	10,47	5,2	113,3 %	10,9	10,96	14,7	111,1 %
PFC-JSS-062	Sample	∞	9,3	4,1	9,94	10,4	10,46	3,2	69,1 %	14,0	10,91	10,2	77,6 %
PFC-JSS-063	Sample	29,1	9,3	6,1	9,96	14,5	10,47	4,6	99,4 %	4,3	10,94	4,2	31,6 %
PFC-JSS-064	Sample	20,8	9,3	3,8	9,97	11,6	10,46	5,3	115,4 %	19,1	10,91	13,3	101,1 %
PFC-JSS-065	Sample	78,6	9,3	3,5	9,94	62,1	10,44	4,1	89,4 %	16,1	10,91	11,8	89,8 %
PFC-JSS-066	Sample	10,3	9,3	6,2	9,96	1,4	10,42	3,2	69,5 %	13,4	10,92	8,6	65,1 %
PFC-JSS-067	Sample	285,1	9,3	358,9	9,96	375,5	10,46	4,3	94,3 %	185,2	10,91	12,8	96,8 %
PFC-JSS-068	Sample	50,8	9,3	3,1	9,96	5,1	10,49	2,2	47,3 %	2,4	10,92	7,3	55,6 %
PFC-JSS-069	Sample	588,7	9,3	253,7	9,97	1170,8	10,46	4,4	94,7 %	318,7	10,94	13,3	100,7 %
PFC-JSS-070	Sample	27,3	9,3	3,7	9,96	6,8	10,42	5,4	117,9 %	2,0	10,84	1,0	7,5 %
PFC-JSS-071	Sample	396,8	9,3	309,1	9,97	391,9	10,49	4,6	99,2 %	216,8	10,94	13,3	100,7 %
PFC-JSS-072	Sample	33,6	9,3	2,7	9,96	3,0	10,47	0,7	14,6 %	1,5	10,64	4,0	30,6 %
PFC-JSS-073	MatrixBlank	4,7	9,3	12,4	9,96	4,4	10,46	1,1	24,4 %	3,9	10,97	4,2	32,1 %
PFC-JSS-074	MatrixBlank	18,4	9,4	6,4	9,92	4,2	10,46	7,7	167,1 %	4,1	10,94	10,0	75,8 %
PFC-JSS-075	MatrixBlank	18,2	9,4	4,4	9,96	3,6	10,49	0,4	7,7 %	1,5	10,92	7,9	59,9 %
PFC-JSS-076	Sample	221,0	9,3	253,8	9,96	293,0	10,44	4,1	90,1 %	295,7	10,92	13,2	99,9 %
PFC-JSS-077	Sample	250,3	9,3	229,8	9,92	255,2	10,44	4,2	90,7 %	271,8	10,89	13,0	98,3 %
PFC-JSS-078	MatrixBlank	14,1	9,4	5,3	9,92	4,2	10,42	0,9	19,6 %	3,6	10,92	3,1	23,3 %
PFC-JSS-079	MatrixBlank	8,0	9,4	7,9	9,94	2,8	10,44	1,9	42,0 %	2,1	10,92	3,8	28,6 %

Table E.5. S/N ratios, retention times (min.) and qualifier/quantifier ratios
for each single sample and matrix blank (PFOA-PFDoDA, PFC-JSS-001-045). Green is acceptable values, yellow is >LOD and <LOQ and red is unacceptable or <LOD.

Sample		PFOA Results		Qualifier (413,0 -> 169,0)		PFNA Results		Qualifier (463,0 -> 219,0)		PFDA Results		Qualifier (513,0 -> 219,0)		PFUdA Results		PFDoDA Results	
Name	Type	S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	S/N	RT
PFC-JSS-001	Sample	115,0	11,31	28,9	95,9 %	44,2	11,96	8,3	84,0 %	552,8	12,61	13,1	101,6 %	32,7	13,11	91,0	13,79
PFC-JSS-002-003	Sample	95,7	11,29	29,1	96,7 %	35,4	11,94	8,6	86,5 %	319,1	12,61	12,4	96,3 %	54,7	13,24	25,1	13,84
PFC-JSS-004	MatrixBlank	9,2	11,34	28,9	96,2 %	5,2	12,06	10,6	107,2 %	2,6	12,68	10,0	77,8 %	3,4	13,38	1,2	12,66
PFC-JSS-005	MatrixBlank	4,2	11,31	26,9	89,3 %	4,9	12,01	11,1	112,4 %	5,1	12,61	10,2	78,9 %	4,7	13,34	1,2	12,62
PFC-JSS-006	MatrixBlank	5,5	11,32	34,2	113,5 %	5,8	11,99	9,6	96,7 %	2,4	12,64	1,2	9,2 %	4,9	13,28	1,3	12,62
PFC-JSS-007-8	Sample	23,2	11,32	28,4	94,2 %	5,4	11,97	8,5	86,2 %	5,7	12,59	6,9	53,4 %	5,6	13,31	1,3	12,64
PFC-JSS-009-10	Sample	13,6	11,36	22,5	74,9 %	14,9	11,97	9,3	93,7 %	2,2	12,64	16,3	126,5 %	4,4	13,28	1,2	12,61
PFC-JSS-011-12	Sample	3,8	11,31	34,4	114,2 %	7,7	11,96	11,3	113,8 %	3,5	12,63	7,7	60,1 %	7,7	13,24	1,3	12,59
PFC-JSS-019	MatrixBlank	2,9	11,31	27,7	92,0 %	3,9	11,87	8,5	86,1 %	3,9	12,42	18,5	143,5 %	4,0	13,01	1,5	12,42
PFC-JSS-022	MatrixBlank	12,8	11,27	30,3	100,5 %	10,9	11,89	8,4	84,8 %	3,2	12,41	13,9	107,6 %	18,6	12,96	7,0	13,49
PFC-JSS-026	MatrixBlank	8,0	11,31	29,8	99,0 %	6,0	11,87	5,5	55,3 %	6,1	12,34	13,2	102,2 %	8,1	12,91	1,8	12,32
PFC-JSS-027	Sample	16,3	11,31	28,8	95,7 %	40,4	11,82	10,2	103,2 %	∞	12,36	13,9	107,6 %	15,8	12,83	33,9	13,29
PFC-JSS-028	Sample	13,2	11,32	30,1	99,9 %	14,8	11,82	9,1	91,9 %	∞	12,32	11,8	91,8 %	23,3	12,83	18,2	13,28
PFC-JSS-029	Sample	40,1	11,32	26,4	87,8 %	9,4	11,86	6,3	63,8 %	17,8	12,34	11,4	88,6 %	8,5	12,84	∞	13,34
PFC-JSS-030	MatrixBlank	7,8	11,31	28,3	94,1 %	4,1	11,84	9,0	91,1 %	5,2	12,31	14,1	108,9 %	12,8	12,81	2,0	12,32
PFC-JSS-031	Sample	118,1	11,31	28,6	95,1 %	18,6	11,79	8,7	88,0 %	13,2	12,29	11,9	92,0 %	8,4	12,78	3,7	13,28
PFC-JSS-032	Sample	70,5	11,31	29,4	97,7 %	23,5	11,82	11,6	116,7 %	∞	12,31	12,8	99,2 %	5,4	12,79	2,2	12,30
PFC-JSS-033	Sample	77,9	11,32	28,0	93,0 %	23,2	11,79	11,7	118,0 %	5,0	12,29	12,7	98,2 %	10,0	12,78	4,8	15,97
PFC-JSS-034	MatrixBlank	5,2	11,32	37,3	123,9 %	2,8	11,86	13,3	134,8 %	5,2	12,31	6,8	52,5 %	10,2	12,81	2,0	12,32
PFC-JSS-035	Sample	21,7	11,32	31,2	103,7 %	4,9	11,82	10,4	104,7 %	7,6	12,29	6,8	52,4 %	11,3	12,81	5,4	15,95
PFC-JSS-036	Sample	46,1	11,31	21,9	72,6 %	8,5	11,81	10,3	103,8 %	9,4	12,31	9,0	70,0 %	17,2	12,76	2,6	13,26
PFC-JSS-037	Sample	2,3	11,37	49,1	163,2 %	6,9	11,81	7,1	71,4 %	0,9	12,93			1,0	12,96	1,5	14,23
PFC-JSS-038	MatrixBlank	4,6	11,34	32,9	109,2 %	2,5	11,87	8,5	85,9 %	2,8	12,36	11,8	91,3 %	6,0	12,83	1,8	12,30
PFC-JSS-039	MatrixBlank	3,0	11,34	28,9	96,1 %	5,2	11,84	10,0	101,2 %	5,2	12,36	12,9	100,1 %	8,9	12,81	2,0	12,32
PFC-JSS-040	Sample	76,5	11,36	30,9	102,7 %	29,4	11,82	11,8	119,2 %	22,7	12,34	12,6	98,0 %	17,2	12,84	6,1	13,33
PFC-JSS-041	Sample	168,6	11,34	29,4	97,5 %	36,9	11,84	9,8	98,9 %	61,6	12,34	11,8	91,5 %	14,3	12,84	16,6	13,29
PFC-JSS-042	Sample	165,7	11,36	27,8	92,5 %	39,4	11,86	10,9	110,0 %	24,3	12,37	12,1	93,6 %	7,8	12,86	6,0	13,36
PFC-JSS-043	MatrixBlank	3,8	11,39	32,2	107,1 %	7,7	11,86	8,5	86,1 %	5,2	12,36	12,9	100,4 %	22,8	12,86	1,8	12,37
PFC-JSS-044	Sample	30,7	11,34	29,4	97,8 %	18,3	11,84	9,9	100,4 %	71,5	12,32	14,8	114,9 %	19,3	12,84	12,2	13,36
PFC-JSS-045	Sample	17,9	11,36	28,2	93,7 %	15,5	11,87	10,1	102,4 %	19,6	12,37	13,2	102,1 %	∞	12,89	2,9	13,39

Table E.6. S/N ratios, retention times (min.) and qualifier/quantifier ratios for each single sample and matrix blank (PFOA-PFDoDA, PFC-JSS-046-079). Green is acceptable values, yellow is >LOD and <LOQ and red is unacceptable or <LOD.

Sample		PFOA Results		Qualifier (413,0 -> 169,0)		PFNA Results		Qualifier (463,0 -> 219,0)		PFDA Results		Qualifier (513,0 -> 219,0)		PFUdA Results		PFDoDA Results	
Name	Type	S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	S/N	RT
PFC-JSS-046	Sample	11,0	11,34	34,3	113,9 %	22,0	11,86	10,6	107,3 %	15,3	12,32	11,7	90,3 %	12,0	12,83	30,3	13,31
PFC-JSS-047	MatrixBlank	3,8	11,34	27,8	92,2 %	8,4	11,89	9,7	98,3 %	5,8	12,37	13,9	107,9 %	22,9	12,91	1,6	12,35
PFC-JSS-048	Sample	25,4	11,37	34,0	113,0 %	17,2	11,87	10,4	104,7 %	75,4	12,37	9,9	76,8 %	10,4	12,84	16,2	13,29
PFC-JSS-049	Sample	18,1	11,39	31,7	105,2 %	38,7	11,86	8,8	88,6 %	16,2	12,39	13,1	101,2 %	14,3	12,88	32,5	13,38
PFC-JSS-051	MatrixBlank	1,8	11,41	37,9	125,9 %	5,3	11,91	10,8	108,7 %	10,7	12,42	12,8	99,1 %	27,9	12,88	3,8	13,39
PFC-JSS-052	Sample	18,5	11,39	31,9	105,8 %	18,5	11,89	9,9	100,3 %	13,7	12,39	10,8	83,9 %	6,8	12,91	4,8	13,41
PFC-JSS-053	Sample	11,1	11,39	31,8	105,6 %	39,1	11,89	11,2	113,4 %	14,8	12,44	14,0	108,5 %	6,4	12,89	6,4	13,41
PFC-JSS-054	Sample	18,6	11,37	29,0	96,3 %	17,3	11,87	8,5	86,4 %	12,8	12,42	12,9	99,7 %	6,5	12,93	7,2	13,41
PFC-JSS-055	MatrixBlank	2,4	11,41	37,7	125,2 %	3,5	11,89	10,2	103,0 %	6,4	12,44	9,5	73,3 %	8,5	12,93	1,5	12,39
PFC-JSS-056	Sample	34,5	11,37	31,4	104,3 %	17,2	11,89	8,2	83,2 %	12,9	12,39	16,0	123,7 %	7,1	12,89	13,2	13,41
PFC-JSS-057	Sample	34,5	11,41	30,2	100,3 %	35,0	11,92	9,3	93,5 %	32,7	12,48	13,4	103,6 %	25,2	12,96	28,3	13,46
PFC-JSS-058	Sample	4,0	11,41	28,1	93,2 %	3,8	11,94	8,4	85,1 %	3,1	12,42	12,2	94,4 %	56,5	12,96	1,7	14,40
PFC-JSS-059	Sample	183,6	11,41	28,6	94,9 %	241,2	11,91	10,2	103,2 %	1016,8	12,41	12,9	100,3 %	9,7	12,94	8,5	13,49
PFC-JSS-060	Sample	176,5	11,41	29,1	96,8 %	337,9	11,94	10,7	107,9 %	559,2	12,46	13,1	101,9 %	11,1	12,94	6,2	13,48
PFC-JSS-061	Sample	20,8	11,43	29,7	98,8 %	41,5	11,91	10,3	104,4 %	15,3	12,48	12,0	93,2 %	5,7	12,96	6,8	13,54
PFC-JSS-062	Sample	21,3	11,39	28,2	93,8 %	22,6	11,92	10,3	104,3 %	6,0	12,48	15,7	121,7 %	5,6	12,98	8,9	13,38
PFC-JSS-063	Sample	30,5	11,41	33,4	110,9 %	140,4	11,92	10,4	105,3 %	37,5	12,44	13,2	102,1 %	37,1	12,96	3,7	13,49
PFC-JSS-064	Sample	24,2	11,39	30,5	101,5 %	30,8	11,91	10,7	107,9 %	38,8	12,46	12,5	97,0 %	8,3	13,01	14,0	13,49
PFC-JSS-065	Sample	30,6	11,41	27,6	91,6 %	46,8	11,91	9,4	95,1 %	11,0	12,44	11,4	88,1 %	20,3	13,01	1,6	12,47
PFC-JSS-066	Sample	11,9	11,41	28,0	93,0 %	147,5	11,91	9,2	92,9 %	30,5	12,42	13,4	104,2 %	88,8	12,98	119,6	13,53
PFC-JSS-067	Sample	137,2	11,37	29,9	99,2 %	180,6	11,91	10,1	102,3 %	450,6	12,44	13,5	104,6 %	7,2	13,03	1,5	12,44
PFC-JSS-068	Sample	4,5	11,36	21,9	72,8 %	4,2	11,94	10,4	105,2 %	1,6	12,46	3,5	27,1 %	1,9	13,21	2,3	13,88
PFC-JSS-069	Sample	159,8	11,43	28,2	93,6 %	432,7	11,94	10,6	106,8 %	1155,1	12,46	12,6	98,1 %	10,5	13,01	1,5	12,46
PFC-JSS-070	Sample	2,9	11,41	22,3	74,0 %	4,1	11,94	6,4	65,0 %	2,3	12,48	7,2	55,9 %	0,8	13,04	1,6	13,91
PFC-JSS-071	Sample	230,5	11,41	30,0	99,7 %	586,4	11,92	10,5	105,8 %	637,2	12,48	12,5	97,1 %	7,4	12,99	1,5	12,47
PFC-JSS-072	Sample	1,8	11,36	29,8	99,1 %	3,9	11,94	12,2	122,8 %	1,9	12,54	8,0	61,8 %	0,9	13,58	1,1	14,28
PFC-JSS-073	MatrixBlank	2,4	11,39	29,6	98,4 %	10,3	11,99	3,2	32,3 %	4,1	12,46	12,0	93,0 %	13,2	12,99	1,4	12,47
PFC-JSS-074	MatrixBlank	3,6	11,39	44,6	148,1 %	2,8	11,94	5,7	57,2 %	2,3	12,46	16,1	125,2 %	7,7	12,98	1,5	12,46
PFC-JSS-075	MatrixBlank	4,3	11,39	34,3	113,8 %	2,8	11,96	5,5	55,1 %	4,1	12,51	12,2	94,2 %	6,1	12,99	1,5	12,47
PFC-JSS-076	Sample	156,4	11,39	29,4	97,6 %	189,7	11,92	10,3	104,0 %	395,7	12,48	12,9	100,4 %	15,4	13,01	1,5	12,46
PFC-JSS-077	Sample	159,4	11,37	28,2	93,8 %	336,6	11,91	10,2	103,1 %	602,4	12,44	13,0	100,5 %	19,8	12,99	6,0	13,49
PFC-JSS-078	MatrixBlank	9,5	11,37	32,6	108,4 %	3,1	11,92	12,8	129,4 %	3,2	12,41	10,5	81,6 %	4,5	12,98	1,5	12,44
PFC-JSS-079	MatrixBlank	3,7	11,43	33,0	109,7 %	4,9	11,99	5,5	55,6 %	3,3	12,56	11,2	86,9 %	6,8	13,06	1,7	14,50

Table E.7 . S/N ratios, retention times (min.) and qualifier/quantifier ratios
for each single sample and matrix blank (PFBS-PFOS, PFC-JSS-001-045). Green is acceptable values, yellow is >LOD and <LOQ and red is unacceptable or <LOD.

Sample		PFBS Results		Qualifier (298,9 -> 99,0)		PFHxS Results		Qualifier (398,9 -> 99,0)		6:2 FTSA Results		Qualifier (427,0 -> 81,0)		Br-PFOS Results		Qualifier (498,9 -> 99,0)		L-PFOS Results		Qualifier (498,9 -> 99,0)	
Sample ID	Type	S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	Ratio	
PFC-JSS-001	Sample	49,2	8,52	43,9	109,9 %	9,8	9,67	57,1	109,7 %	9,7	10,34	3,2	22,6 %	29,1	10,75	14,7	87,9 %	35,5	10,95	54,1	117,0 %
PFC-JSS-002-003	Sample	19,2	8,54	41,4	103,8 %	6,0	9,71	48,4	92,8 %	44,0	10,42	3,8	26,5 %	13,0	10,72	18,9	113,4 %	27,9	10,93	48,1	104,1 %
PFC-JSS-004	MatrixBlank	90,0	8,52	42,0	105,2 %	5,8	9,71	78,0	149,6 %	1,4	10,37	18,5	129,5 %	1,7	10,68			3,2	11,00	28,5	61,8 %
PFC-JSS-005	MatrixBlank	29,2	8,52	39,8	99,7 %	19,2	9,69	50,3	96,6 %	10,2	10,35	91,8	642,0 %	7,1	10,75			10,0	10,95	36,4	78,9 %
PFC-JSS-006	MatrixBlank	26,9	8,52	36,5	91,6 %	7,8	9,66	32,0	61,3 %	2,0	10,75	218,2	1525,7 %	2,7	10,50	54,0	323,2 %	2,3	10,98	21,9	47,3 %
PFC-JSS-007-8	Sample	52,8	8,49	44,5	111,6 %	410,1	9,66	53,1	101,9 %	77,4	10,32			47,8	10,73	17,9	107,2 %	58,6	10,93	48,8	105,6 %
PFC-JSS-009-10	Sample	154,3	8,51	43,4	108,8 %	54,0	9,66	48,6	93,2 %	58,0	10,35			257,6	10,70	21,0	125,7 %	64,3	10,93	47,9	103,6 %
PFC-JSS-011-12	Sample	53,4	8,49	35,0	87,6 %	14,0	9,69	43,3	83,2 %	90,9	10,59		0,0 %	4,2	10,67	12,7	75,8 %	6,2	10,92	66,9	144,9 %
PFC-JSS-019	MatrixBlank	20,7	8,52	45,7	114,6 %	17,1	9,64	38,1	73,2 %	68,5	9,48		0,0 %				0,0 %	2,8	10,92	60,6	131,1 %
PFC-JSS-022	MatrixBlank	43,1	8,51	42,3	106,1 %	17,6	9,67	101,3	194,4 %	4,7	10,52	135,6	948,0 %	9,5	10,97	21,5	128,7 %	9,2	10,97	22,6	48,8 %
PFC-JSS-023	Sample	12,9	8,51	38,7	97,0 %	4,8	9,67	58,3	111,9 %	51,6	10,35		0,0 %	11,0	10,72	20,2	120,8 %	11,6	10,93	44,1	95,5 %
PFC-JSS-024	Sample	16,0	8,49	43,9	110,0 %	8,3	9,67	73,4	140,9 %	70,6	10,35		0,0 %	10,9	10,70	25,5	152,7 %	8,3	10,93	58,9	127,5 %
PFC-JSS-025	Sample	7,8	8,52	34,1	85,5 %	5,1	9,64	45,4	87,1 %	5,7	10,35	17,4	121,9 %	15,1	10,70	17,8	106,8 %	18,8	10,93	48,4	104,8 %
PFC-JSS-026	MatrixBlank	∞	8,51	33,4	83,8 %	32,0	9,69	65,9	126,6 %	41,1	10,64		0,0 %	1,9	10,67	29,9	179,1 %	5,7	10,92	68,2	147,7 %
PFC-JSS-027	Sample	13,0	8,51	42,2	105,7 %	4,7	9,69	47,1	90,5 %	6,0	10,37	22,1	154,3 %	10,1	10,72	21,5	128,8 %	9,3	10,95	53,1	114,9 %
PFC-JSS-028	Sample	24,8	8,52	41,1	103,0 %	4,6	9,64	64,1	123,1 %	8,1	10,39	10,0	69,9 %	16,9	10,72	19,2	114,9 %	6,5	10,88	38,5	83,3 %
PFC-JSS-029	Sample	15,6	8,56	42,1	105,6 %	10,4	9,67	55,4	106,2 %	8,4	10,30	7,5	52,2 %	7,2	10,65	15,4	92,0 %	4,7	10,92	51,3	111,0 %
PFC-JSS-030	MatrixBlank	21,3	8,51	35,2	88,3 %	4,1	9,64	69,1	132,6 %	62,7	10,64			3,2	10,72	55,0	329,1 %	3,1	10,98		
PFC-JSS-031	Sample	3,3	8,54	46,1	115,6 %	50,2	9,69	46,1	88,4 %	5,7	10,37	22,1	154,7 %	20,6	10,68	13,3	79,8 %	9,5	10,90	53,4	115,6 %
PFC-JSS-032	Sample	7,7	8,56	45,3	113,4 %	19,5	9,69	49,9	95,7 %	3,4	10,35	27,6	192,7 %	20,3	10,70	20,8	124,6 %	9,9	10,90	59,7	129,2 %
PFC-JSS-033	Sample	11,5	8,51	37,9	94,9 %	15,0	9,71	46,5	89,3 %	4,0	10,39	11,9	83,5 %	16,8	10,68	17,4	104,1 %	10,5	10,92	45,7	99,0 %
PFC-JSS-034	MatrixBlank	233,1	8,54	32,3	80,8 %	59,0	9,69	77,7	149,1 %	67,8	10,35		0,0 %	4,4	10,87	20,2	120,8 %	5,9	10,95	92,1	199,3 %
PFC-JSS-035	Sample	14,8	8,54	40,6	101,8 %	5,1	9,69	127,8	245,2 %	99,6	10,37			6,2	10,77	14,8	88,6 %	10,0	10,92	31,4	67,9 %
PFC-JSS-036	Sample	9,3	8,54	52,2	130,7 %	15,8	9,67	69,2	132,7 %	22,7	10,39		0,0 %	7,0	10,67	20,9	125,0 %	19,1	10,92	51,4	111,3 %
PFC-JSS-037	Sample	13,1	8,56	43,4	108,9 %	1,5	9,74	3603,0	6915,6 %	38,8	10,27		0,0 %	1,2	10,83			1,2	10,83	222,1	480,7 %
PFC-JSS-038	MatrixBlank	∞	8,54	42,3	105,9 %	35,3	9,67	134,4	258,0 %	3,1	10,37	19,9	139,5 %	2,8	10,68	94,9	568,1 %	6,1	10,97	141,6	306,5 %
PFC-JSS-039	MatrixBlank	37,5	8,54	37,6	94,2 %	94,9	9,69	92,0	176,5 %	2,9	10,37	47,9	334,7 %	7,4	10,67	8,4	50,4 %	8,5	10,87	51,0	110,3 %
PFC-JSS-040	Sample	60,7	8,51	44,8	112,2 %	437,4	9,67	49,1	94,2 %	124,9	10,34	13,8	96,7 %	1255,0	10,68	17,2	102,9 %	45,1	10,92	50,1	108,4 %
PFC-JSS-041	Sample	89,4	8,52	43,6	109,2 %	469,0	9,67	49,5	95,0 %	1136,0	10,34	15,3	106,7 %	1177,8	10,70	16,6	99,2 %	44,5	10,92	50,0	108,3 %
PFC-JSS-042	Sample	93,6	8,52	44,1	110,6 %	691,6	9,69	50,1	96,2 %	130,8	10,35	14,3	99,9 %	∞	10,68	16,5	98,7 %	41,7	10,92	51,2	110,9 %
PFC-JSS-043	MatrixBlank	52,4	8,57	37,9	95,1 %	43,1	9,71	84,2	161,6 %	35,4	10,34		0,0 %	6,5	10,70			8,9	10,92	45,7	98,9 %
PFC-JSS-044	Sample	27,9	8,57	41,0	102,7 %	6,8	9,72	62,3	119,6 %	29,3	10,34	6,8	47,5 %	18,6	10,73	22,4	134,2 %	9,9	10,95	47,2	102,2 %
PFC-JSS-045	Sample	10,1	8,54	46,4	116,2 %	17,5	9,69	62,4	119,8 %	3,5	10,37	1,5	10,3 %	26,5	10,72	13,7	82,2 %	13,1	10,92	45,8	99,2 %

Table E.8. S/N ratios, retention times (min.) and qualifier/quantifier ratios
for each single sample and matrix blank (PFBS-PFOS, PFC-JSS-046-079). Green is acceptable values, yellow is >LOD and <LOQ and red is unacceptable or <LOD.

Sample		PFBS Results		Qualifier (298,9 -> 99,0)		PFHxS Results		Qualifier (398,9 -> 99,0)		6:2 FTSA Results		Qualifier (427,0 -> 81,0)		Br-PFOS Results		Qualifier (498,9 -> 99,0)		L-PFOS Results		Qualifier (498,9 -> 99,0)	
Sample ID	Type	S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	Ratio		S/N	RT	Ratio	
PFC-JSS-046	Sample	19,1	8,56	48,5	121,7 %	10,4	9,69	66,0	126,7 %	2,6	10,32	10,8	75,3 %	22,2	10,70	18,3	109,9 %	10,0	10,93	45,8	99,2 %
PFC-JSS-047	MatrixBlank	∞	8,57	36,8	92,3 %	7,8	9,74	92,0	176,5 %	27,8	10,40		0,0 %	2,3	10,73			7,0	10,92	48,3	104,5 %
PFC-JSS-048	Sample	8,1	8,56	32,7	81,9 %	10,0	9,69	81,1	155,7 %	24,7	10,40	12,5	87,2 %	24,6	10,68	20,7	123,9 %	6,0	10,92	59,7	129,2 %
PFC-JSS-049	Sample	13,3	8,54	38,9	97,6 %	8,2	9,74	49,8	95,5 %	5,3	10,35	8,8	61,7 %	14,6	10,72			12,1	10,92	59,6	129,1 %
PFC-JSS-051	MatrixBlank	36,2	8,57	45,0	112,8 %	22,8	9,67	56,2	107,9 %	6,2	10,37	15,4	107,7 %	3,8	10,68	95,4	571,2 %	3,5	10,92	33,0	71,5 %
PFC-JSS-052	Sample	62,5	8,56	37,4	93,8 %	6,7	9,71	96,2	184,6 %	400,0	10,34	4,6	31,9 %	42,0	10,70	23,7	142,1 %	18,0	10,93	47,5	102,9 %
PFC-JSS-053	Sample	14,3	8,57	36,7	92,0 %	7,3	9,71	65,4	125,6 %	2,3	10,30	14,9	103,9 %	23,1	10,73	17,8	106,8 %	11,6	10,93	48,6	105,1 %
PFC-JSS-054	Sample	22,7	8,56	40,1	100,4 %	10,0	9,71	80,5	154,5 %	6,2	10,40	2,5	17,6 %	30,2	10,73	19,2	114,7 %	11,8	10,92	53,3	115,3 %
PFC-JSS-055	MatrixBlank	83,1	8,57	39,7	99,4 %	9,9	9,72	57,3	110,0 %	3,8	10,89	141,3	988,1 %	2,5	10,67	100,3	600,8 %	5,5	10,95	37,5	81,2 %
PFC-JSS-056	Sample	13,2	8,56	39,2	98,2 %	8,7	9,72	61,3	117,7 %	7,8	10,39	0,9	6,2 %	16,6	10,72	21,7	130,1 %	31,7	10,92	54,4	117,7 %
PFC-JSS-057	Sample	9,4	8,61	40,5	101,5 %	6,2	9,72	82,8	158,9 %	3,8	10,40			17,1	10,72	21,3	127,7 %	29,1	10,92	55,9	120,9 %
PFC-JSS-058	Sample	217,1	8,61	44,7	112,1 %	14,6	9,71	51,5	98,8 %	5,5	10,40	15,7	109,7 %	42,0	10,68	19,2	115,1 %	118,7	10,90	53,7	116,2 %
PFC-JSS-059	MatrixSpike	627,7	8,57	40,2	100,8 %	721,7	9,71	50,6	97,1 %	8174,7	10,34	14,4	100,6 %	8,7	10,67			680,9	10,90	46,7	101,1 %
PFC-JSS-060	MatrixSpike	958,6	8,57	39,4	98,8 %	1244,8	9,71	52,6	101,0 %	∞	10,37	14,4	101,0 %	8,6	10,72			474,3	10,92	46,5	100,6 %
PFC-JSS-061	Sample	4,7	8,56	44,4	111,2 %	8,3	9,69	56,0	107,5 %	4,3	10,37	39,4	275,6 %	17,5	10,72	22,4	134,1 %	15,9	10,92	54,0	116,8 %
PFC-JSS-062	Sample	9,5	8,57	28,2	70,6 %	9,0	9,72	62,6	120,1 %	24,0	10,02		0,0 %	7,4	10,70	21,5	128,9 %	9,4	10,92	54,1	117,1 %
PFC-JSS-063	Sample	21,2	8,59	35,4	88,7 %	9,8	9,72	43,6	83,7 %	6,1	10,37	14,2	99,6 %	25,3	10,72	14,9	89,3 %	30,0	10,90	47,8	103,5 %
PFC-JSS-064	Sample	6,8	8,59	44,8	112,2 %	9,3	9,74	49,1	94,3 %	44,6	10,49		0,0 %	10,0	10,65	20,5	122,9 %	13,5	10,90	53,3	115,4 %
PFC-JSS-065	Sample	8,2	8,61	40,3	101,0 %	14,2	9,76	62,2	119,5 %	42,6	10,35		0,0 %	35,8	10,67	15,8	94,9 %	27,3	10,92	47,1	102,0 %
PFC-JSS-066	Sample	15,1	8,59	36,8	92,2 %	17,2	9,72	52,8	101,3 %	5,9	10,42	13,2	92,4 %	45,7	10,70	18,9	113,4 %	36,6	10,90	46,7	101,1 %
PFC-JSS-067	QC	1902,3	8,59	39,9	100,0 %	5340,9	9,71	52,4	100,6 %	507,1	10,35	14,5	101,3 %	960,2	10,87	46,4	277,9 %	960,1	10,87	46,2	100,0 %
PFC-JSS-068	QC	144,7	8,61	42,1	105,4 %	1,8	9,74			50,2	10,35			1,7	10,68	64,5	386,3 %	2,5	10,97	76,1	164,8 %
PFC-JSS-069	QC	3020,9	8,59	40,8	102,3 %	∞	9,72	51,4	98,7 %	1451,0	10,39	14,9	104,1 %				0,0 %	1006,4	10,90	47,3	102,3 %
PFC-JSS-070	QC	376,3	8,59	42,4	106,3 %	4,0	9,74	51,6	99,0 %	4,3	10,44	187,3	1309,7 %	1,0	10,88			1,6	10,93	461,6	999,2 %
PFC-JSS-071	QC	954,5	8,59	40,6	101,8 %	702,1	9,71	51,6	99,0 %	10358,7	10,40	14,8	103,2 %				0,0 %	1276,5	10,92	46,6	100,9 %
PFC-JSS-072	QC	29,0	8,61	44,5	111,5 %	1,8	9,94	44,1	84,7 %	43,3	10,45		0,0 %	3,8	10,72	27,9	167,4 %	2,2	10,98	57,3	124,0 %
PFC-JSS-073	MatrixBlank	69,9	8,61	41,4	103,8 %	20,0	9,77	91,9	176,4 %	45,6	10,40			1,2	10,72	29,5	176,9 %	4,2	10,87	64,6	139,9 %
PFC-JSS-074	MatrixBlank	26,6	8,59	37,6	94,3 %	137,9	9,71	47,7	91,6 %	21,9	9,99		0,0 %	18,1	10,75	15,4	92,4 %	48,1	10,87	33,2	71,9 %
PFC-JSS-075	MatrixBlank	45,3	8,62	33,3	83,4 %	10,6	9,74	41,0	78,7 %	71,7	10,22		0,0 %	2,7	10,82	17,9	107,0 %	2,9	10,95	50,6	109,6 %
PFC-JSS-076	MatrixSpike	827,9	8,61	40,1	100,6 %	627,7	9,74	52,5	100,7 %	9549,6	10,40	14,3	100,3 %				0,0 %	405,5	10,93	46,6	100,8 %
PFC-JSS-077	MatrixSpike	605,1	8,62	40,9	102,5 %	1542,7	9,72	51,5	98,8 %	2290,2	10,39	14,5	101,4 %				0,0 %	333,2	10,90	46,0	99,6 %
PFC-JSS-078	MatrixBlank	11,0	8,57	39,4	98,8 %	15,0	9,74	50,8	97,5 %	98,6	10,47			1,1	10,68			5,8	10,95		
PFC-JSS-079	MatrixBlank	127,8	8,61	41,6	104,2 %	36,1	9,74	36,2	69,5 %	60,9	10,42			2,5	10,73	50,3	301,5 %	7,1	10,88	51,8	112,2 %

E.3 Sample results

Table E.9. PFAS result for the individual samples in ng L^{-} . Further remarks explaining symbols used is supplied on the next page.

Sample ID	Loc. ID	PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnDA	PFDoDA	PFBS	PFHxS	Br-PFOS	L-PFOS	Σ-PFOS	6:2 FTSA	Σ-PFCA	Σ-PFSA	Σ-PFAS
PFC-JSS-001	L5	<0.69	<0.10	0.41	0.32[c]	2.66	0.32[c]	0.92[c]	<0.13	0.22[d]	<0.025	0.022[c]	0.12[c]	0.14[c]	0.27	<0.14[c]	4.8	0.29	5.1
PFC-JSS-002-003	L5	1.09	<0.10	0.34	0.26	1.78	0.24[c]	0.61	<0.13	0.16	<0.026	0.023	0.083	0.11	0.19	<0.14[a]	4.5	0.21	4.7
PFC-JSS-007-008	A1	ND	1.29[b]	2.66[b]	0.57	0.31	<0.085[c]	ND[c]	<0.13[c]	ND[c]	0.035	0.21	0.088	0.10	0.19	ND	4.8	0.43	5.3
PFC-JSS-009-010	A1	ND	1.55	3.02	0.40	0.36[a]	<0.092[c]	ND	<0.14[c]	ND[c]	0.14	0.43	0.20	0.24	0.44	ND	5.3	1.01	6.3
PFC-JSS-011-012[e]	A1	*	(2.16)[d]	(2.65)[d]	(0.81)[ad]	*	*	*	*	*	*	*	*	*	*	*	5.6	0.014	5.6
PFC-JSS-023	L1	0.99	<0.092	0.15	0.17	0.47	0.16[c]	0.11	<0.12	0.033	<0.023	0.010	0.038	0.042	0.079	ND	2.1	0.090	2.2
PFC-JSS-024	L1	0.86	<0.090	0.11	0.14	0.39	0.16[c]	0.12	<0.11	0.047	<0.023	<0.06[a]	0.035	0.033	0.068	ND	1.8	0.068	1.9
PFC-JSS-025	L1	0.93	<0.100	0.14	0.15	0.45	0.16[c]	0.11	<0.13	0.029	<0.025	0.015	0.041	0.041	0.082	<0.14[a]	2.0	0.10	2.1
PFC-JSS-027	L2	1.15	<0.089[a]	<0.080	0.14	0.24	0.12	0.050	<0.11	0.019	<0.022	0.012[a]	0.029	0.024	0.053	<0.12[a]	1.7	0.065	1.8
PFC-JSS-028	L2	1.01	<0.089[a]	<0.081	0.13	0.25	0.12	0.061	<0.11	0.015	<0.022	0.007	0.028	0.027	0.055	<0.12[a]	1.6	0.062	1.6
PFC-JSS-029	L2	1.08	<0.099	<0.089	0.14	0.26	0.14[a]	0.043	<0.12	<0.016	<0.025	0.014	0.032	0.024	0.056	<0.14[a]	1.7	0.070	1.7
PFC-JSS-031	L3	4.63	0.21	0.34	0.50	1.36	0.32[c]	0.041	<0.13	ND	<0.025	0.17	0.11[c]	0.069[c]	0.18	<0.14[a]	7.4	0.35	7.7
PFC-JSS-032	L3	5.23[b]	0.21	0.38	0.53	1.28	0.30	<0.034	<0.12	ND	<0.024	0.16	0.10	0.060	0.16	<0.13[a]	8.0	0.32	8.3
PFC-JSS-033	L3	2.81	0.14	0.21	0.31	0.84	0.21	<0.036	<0.13	ND	<0.025	0.10	0.077	0.051	0.13	<0.14	4.5	0.22	4.7
PFC-JSS-035	L4	1.37	ND	<0.18	0.42	<0.27	<0.17[c]	<0.070[a]	<0.25	ND	<0.050	0.007	<0.038	0.044	0.044	ND	1.8	0.05	1.8
PFC-JSS-036	L4	1.23	<0.10	0.10	0.24	0.18[a]	0.10	0.041	<0.13	<0.016	ND	0.010[a]	0.034	0.025	0.059	ND	1.9	0.07	2.0
PFC-JSS-037[e]	L4	*	*	*	*	0.22[a]	*	*	*	*	*	*	*	*	*	*	0.22	*	0.22
PFC-JSS-040	A1	(3.99)[d]	3.16	14.8	4.07	5.53	0.85	0.19	0.13[c]	<0.015[c]	2.40	14.8	27.0	41.2	68.3	4.25	33	90	122
PFC-JSS-041	A1	(3.92)[d]	3.86	16.5	4.48	5.35	0.86	0.17[c]	<0.13[c]	<0.016[c]	2.41	14.8	26.0	38.6	64.5	4.17	35	86	121
PFC-JSS-042	A1	(4.07)[d]	3.07	15.2	4.32	5.62	0.87	0.15[c]	<0.12[c]	<0.015[c]	2.33	14.8	24.7	37.2	61.9	4.35	33	83	117
PFC-JSS-044	L1	ND	ND	0.12	0.15	0.16	0.14	0.052	<0.11	0.017	<0.022	0.010	0.085[a]	0.087	0.17	<0.12[a]	0.63	0.18	0.82
PFC-JSS-045	L1	ND	ND	0.10	0.13	0.14	0.13	0.048	<0.11	<0.014	<0.022	ND	0.095	0.085	0.18	<0.12[a]	0.55	0.18	0.73
PFC-JSS-046	L1	ND	ND	0.13	0.14	0.13	0.11	0.049	<0.11	0.015	ND	<0.06[a]	0.073	0.079	0.15	<0.12	0.57	0.15	0.73
PFC-JSS-048	L2	ND	ND	<0.079	<0.078[a]	0.16	0.11	0.071[a]	<0.11	0.021	<0.022	0.007	0.056	0.054	0.11	<0.12[a]	0.37	0.12	0.49
PFC-JSS-049	L2	ND	ND	<0.081	<0.080[a]	0.15	0.14	0.061	<0.11	0.014	<0.022	0.008	0.060	0.057	0.12	<0.12[a]	0.36	0.13	0.49
PFC-JSS-052	L3	0.89	<0.089	<0.081[a]	0.11	0.20	0.16	0.076	<0.11	0.024	<0.022	0.016a	0.080[a]	0.11	0.19	<0.12[a]	1.5	0.20	1.7
PFC-JSS-053	L3	0.70	ND	<0.081[a]	0.087	0.14	0.14	0.054	<0.11	0.016	<0.023	0.013a	0.068	0.091	0.16	<0.12	1.1	0.17	1.3
PFC-JSS-054	L3	0.68	ND	<0.081[a]	<0.080	0.16	0.14	0.048	<0.11	0.021	<0.022	0.011a	0.071	0.084	0.15	<0.12[a]	1.0	0.17	1.2
PFC-JSS-056	L4	0.77	<0.089	<0.081[a]	<0.080	0.30	0.14	0.086[a]	<0.11	0.026	<0.022	0.016	0.086	0.14	0.23	<0.12[a]	1.3	0.24	1.6
PFC-JSS-057	L4	<0.62	<0.090	<0.081[a]	<0.080	0.21	0.11	0.083	<0.11	0.025	<0.023	0.011	0.077[a]	0.15	0.23	<0.12[a]	0.42	0.24	0.66
PFC-JSS-058[e]	L4	ND	ND	ND	ND	ND	ND	ND	<0.11	ND	<0.023	ND	0.035	0.083	0.12	<0.12	<0.11	0.12	0.12
PFC-JSS-061	I	1.50	0.24	0.11	0.19	0.29	0.20	0.036	<0.11	<0.014	<0.022	0.022	0.066	0.057	0.12	<0.12[a]	2.6	0.15	2.7
PFC-JSS-062[f]	M1	(2.85)[d]	(0.15)[d]	(0.25)[ad]	(0.46)[d]	0.54[b]	0.61[b]	(0.10)[ad]	<0.11[d]	ND[d]	ND[d]	(0.041)[d]	(0.15)[d]	(0.16)[d]	(0.31)[d]	ND	5.0	0.35	5.3
PFC-JSS-063	S1	ND	ND	<0.088	ND	0.41	0.94	0.17	0.13	0.017	<0.024	0.007	0.21	0.23	0.45	<0.13	1.7	0.45	2.1
PFC-JSS-064	O	1.34	<0.080	0.15	0.19	0.26	0.15	0.035	<0.10	0.030	<0.020	0.021	0.051	0.066	0.12	ND	2.2	0.14	2.3
PFC-JSS-065	M2	2.65	<0.086	0.59	0.25	0.41	0.20	<0.031	<0.11	ND	<0.022	0.020	0.057	0.058	0.12	ND	4.1	0.14	4.2
PFC-JSS-066	S2	ND	ND	ND	ND	<0.12	0.66	0.12	0.17	0.035	<0.022	ND	0.092	0.13	0.22	<0.12	0.98	0.22	1.2

Remarks to Sample results

Table E.9:

a. Qualifier transition ratio outside the ±20 % uncertainty
b. ISTD recovery less than 40 %.
c. ISTD recovery higher than 120 %.
d. ISTD recovery less than 20 %.
e. Sample rejected
f. Extract spilled and was attempted to be recovered.
   * = not analysed
   ND = not detected.
   <"value" = detected below the quantification limit

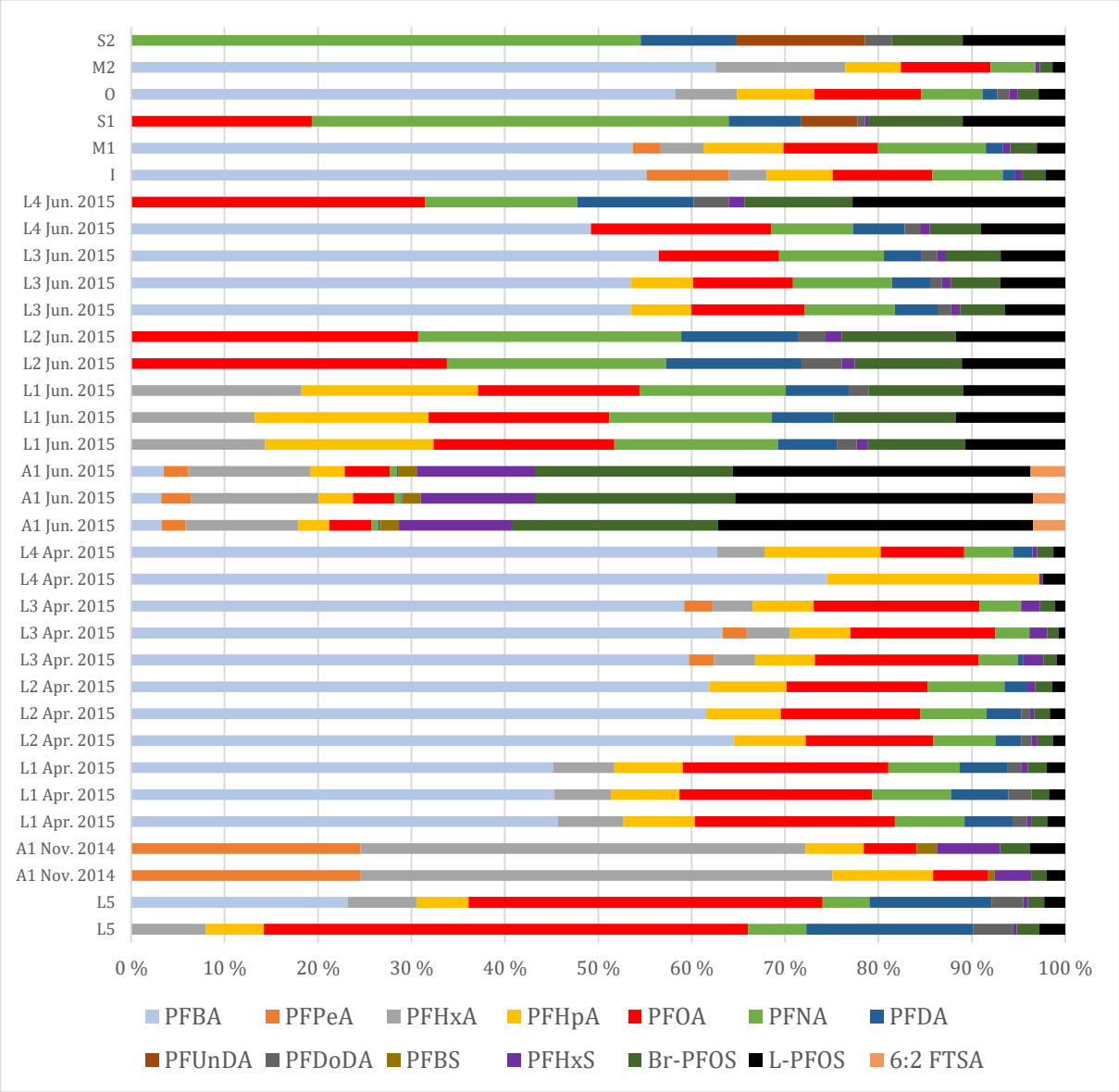


Figure E.2. PFAS composition profiles for all sample sites in this study.
All results >MDLs are included. Results <MDL are included as ½MDL
.

Table E.10. Overview of calculated congener ratios.

	ΣPFCA			ΣPFSA			ΣPFAS			Br-PFOS (%)			PFOA/L-PFOS			PFOA/PFNA			ΣPFCA/ΣPFSA		
Location	Mean	SD	n	Mean	SD	n	Mean	SD	n	Mean	SD	n	Mean	SD	n	Mean	SD	n	Mean	SD	n
A1 Nov. 14	5,3	0,40	3	0,5	0,50	3	5,7	0,54	3	45,4 %	0,31 %	2	2	1,1	2	NA	NA		8	4,1	2
A1 Jun. 15	34	1,3	3	86	3,2	3	120	3,0	3	39,9 %	0,31 %	3	0,141	0,0089	3	6,4	0,15	3	0,39	0,024	3
L5	4,7	0,25	2	0,25	0,055	2	4,9	0,31	2	45 %	1,5 %	2	18	1,2	2	7,9	0,49	2	19	3,1	2
L1 Apr. 15	2,0	0,13	3	0,085	0,015	3	2,0	0,14	3	50 %	2,2 %	3	11,3	0,45	3	2,7	0,25	3	23	3,3	3
L2 Apr. 15	1,66	0,066	3	0,0657	0,0042	3	1,71	0,058	3	54 %	3,1 %	3	10,1	0,87	3	2,0	0,14	3	25	1,4	3
L3 Apr. 15	7	1,8	3	0,30	0,066	3	7	1,9	3	62 %	1,5 %	3	19	2,6	3	4,1	0,13	3	22	2,7	3
L4 Apr. 15	1,83	0,075	2	0,060	0,012	2	1,89	0,087	2	58 %	NA	1	7,0	NA	1	1,7	NA	1	31	5,1	2
L1 Jun. 15	0,58	0,046	3	0,17	0,016	3	0,76	0,053	3	50 %	2,4 %	3	1,7	0,12	3	1,107	0,0030	3	3,4	0,36	3
L2 Jun. 15	0,367	0,0057	2	0,121	0,006	2	0,4880	0,00044	2	51,0 %	0,23 %	2	2,8	0,30	2	1,3	0,25	2	3,0	0,20	2
L3 Jun. 15	1,2	0,22	3	0,18	0,020	3	1,4	0,24	3	44 %	1,8 %	3	1,8	0,20	3	1,1	0,12	3	6,7	0,46	3
L4 Jun. 15	0,9	0,63	2	0,241	0,0022	2	1,1	0,63	2	34 %	4,1 %	3	1,8	0,54	2	2,1	0,19	2	4	2,6	2
I	2,6	NA	1	0,15	NA	1	2,7	NA	1	54 %	NA	1	5,0	NA	1	1,4	NA	1	18	NA	1
O	2,2	NA	1	0,14	NA	1	2,3	NA	1	44 %	NA	1	4,0	NA	1	1,7	NA	1	16	NA	1
M1	5,0	NA	1	0,35	NA	1	5,3	NA	1	48 %	NA	1	3,3	NA	1	0,88	NA	1	14	NA	1
M2	4,1	NA	1	0,14	NA	1	4,2	NA	1	50 %	NA	1	7,0	NA	1	2,0	NA	1	30	NA	1
S1	1,7	NA	1	0,45	NA	1	2,1	NA	1	48 %	NA	1	1,8	NA	1	0,43	NA	1	3,7	NA	1
S2	0,98	NA	1	0,22	NA	1	1,2	NA	1	41 %	NA	1	NA	NA	1	NA	NA	1	4,4	NA	1
Linnèv. March 2014	4,7	0,25	2	0,25	0,055	2	4,9	0,31	2	45 %	1,5 %	2	18	1,2	2	7,9	0,49	2	19	3,1	2
Linnèv. April 2015	3	2,4	11	0,1	0,11	11	3	2,5	11	55 %	5,3 %	10	13	4,7	10	2,8	0,98	10	25	4,2	11
Linnèv. June 2015	0,8	0,41	10	0,18	0,042	10	0,89	0,48	11	44 %	7,6 %	11	2,0	0,52	10	1,3	0,41	10	4	1,9	10
All sites (except A1)	2	2,0	31	0,2	0,10	31	2	2,1	31	49 %	7,6 %	30	7,6	6,4	27	2	1,9	26	15	10,2	29
A1 (June only)	34	1,3	3	86	3,2	3	120	3,0	3	39,9 %	0,31 %	3	0,141	0,0089	3	6,4	0,15	3	0,39	0,024	3
Grønfjorden a)	1,3	0,61	5	0,08	0,031	5	1,3	0,62	5	NA			7	4,5	5	NA			18	7,7	5
Adventfjorden b)	0,3	0,10	3	0,05	0,020	3	0,3	0,11	3	NA			11	6,2	3	NA			5	1,9	3

a) Sample sites W3, W4, W5, W6 and W7 (Rakovic et al. 2016 (in prep.))

b) Sample sites W15, W17and W20 (Rakovic et al. 2016 (in prep.))

E.4 Blank results

Table E.11 Field blanks

		PFBA		PFPeA		PFHxA		PFHpA		PFOA		PFNA		PFDA		PFUnDA		PFDoDA	
Location	Sample ID	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N
A1	PFC-JSS-004	202,5	11,0	69,9	5,4	**215,4**	12,2	**303,9**	23,2	**227,4**	9,2	16,6	5,2	ND	2,6	28,2	3,4	ND	1,2
A1	PFC-JSS-005	432,7	8,9	72,0	5,5	88,1	4,5	ND	1,8	63,8	4,2	24,7	4,9	0,0	5,1	13,0	4,7	ND	1,2
A1	PFC-JSS-006	350,1	10,7	0,0	10,9	35,0	6,3	ND	2,6	62,4	5,5	29,0	5,8	ND	2,4	24,0	4,9	ND	1,3
L1	PFC-JSS-022	599,7	32,5	<5,6	9,9	17,5	5,1	39,9	3,5	121,8	12,8	75,1	10,9	19,3	3,2	70,0	18,6	ND	7,0
L2	PFC-JSS-026	359,5	27,0	0,0	6,2	27,5	20,3	29,8	4,8	107,0	8,0	49,9	6,0	20,3	6,1	50,7	8,1	ND	1,8
L3	PFC-JSS-030	617,4	14,1	1,0	10,3	44,6	7,5	53,3	3,4	105,7	7,8	60,4	4,1	26,9	5,2	58,1	12,8	ND	2,0
L4	PFC-JSS-034	566,3	∞	0,0	5,7	66,7	3,1	80,6	3,7	18,3	5,2	ND	2,8	16,4	5,2	56,3	10,2	ND	2,0
A1	PFC-JSS-039	612,7	30,6	0,0	4,7	58,1	5,8	38,4	3,1	32,8	3,0	53,3	5,2	21,9	5,2	53,3	8,9	ND	2,0
L1	PFC-JSS-043	0,0	27,2	91,3	4,1	64,6	4,0	105,8	19,8	0,0	3,8	63,6	7,7	32,4	5,2	141,2	22,8	ND	1,8
L2	PFC-JSS-047	450,7	7,4	15,4	4,6	2,7	4,2	61,5	3,6	34,6	3,8	72,6	8,4	33,7	5,8	109,5	22,9	ND	1,6
L3	PFC-JSS-051	551,7	15,4	33,6	4,5	ND	2,5	62,1	4,0	ND	1,8	91,1	5,3	30,0	10,7	95,0	27,9	27,7	3,8
L4	PFC-JSS-055	485,4	11,4	21,4	4,2	ND	2,3	39,5	4,4	ND	2,4	65,0	3,5	24,2	6,4	73,1	8,5	ND	1,5
Average		**435,7**	**17,8**	**27,7**	**6,3**	**45,0**	**6,5**	**56,8**	**6,5**	**60,7**	**5,6**	**54,7**	**5,8**	**22,5**	**5,3**	**64,4**	**12,8**	**27,7**	**2,3**
SD		**186,3**	**9,5**	**34,4**	**2,5**	**27,0**	**5,1**	**24,2**	**7,1**	**43,1**	**3,3**	**23,0**	**2,2**	**9,8**	**2,2**	**36,9**	**8,2**		**1,6**

		PFBS		PFHxS		Br-PFOS		L-PFOS		6:2 FTSA		FOSA	
Location	Sample ID	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N
A1	PFC-JSS-004	<50	90,0	<1,7	5,8	ND	1,7	10,9	3,2	ND	1,4	11,4	3,5
A1	PFC-JSS-005	<50	29,2	<1,7	19,2	4,5	7,1	17,7	10,0	2,5	10,2	7,6	41,1
A1	PFC-JSS-006	<50	26,9	2,9	7,8	ND	2,7	ND	2,3	ND	2,0	-	-
L1	PFC-JSS-022	<50	43,1	<1,7	17,6	6,9	9,5	7,0	9,2	2,8	4,7	10,8	13,0
L2	PFC-JSS-026	<50	∞	<1,7	32,0	ND	1,9	5,5	5,7	ND	-	11,0	28,0
L3	PFC-JSS-030	<50	21,3	<1,7	4,1	0,6	3,2	0,9	3,1	ND	-	-	-
L4	PFC-JSS-034	<50	233,1	4,2	59,0	3,1	4,4	2,9	5,9	ND	-	4,7	13,9
A1	PFC-JSS-039	<50	37,5	6,7	94,9	10,8	7,4	20,7	8,5	ND	2,9	1,8	4,8
L1	PFC-JSS-043	<50	52,4	<1,7	43,1	4,1	6,5	12,3	8,9	ND	-	10,2	17,7
L2	PFC-JSS-047	<50	∞	<1,7	7,8	ND	2,3	11,6	7,0	ND	-	7,2	8,3
L3	PFC-JSS-051	<50	36,2	3,3	22,8	2,7	3,8	9,8	3,5	100,9	6,2	-	-
L4	PFC-JSS-055	<50	83,1	2,4	9,9	ND	2,5	5,1	5,5	1,6	3,8	71,4	37,7
Average		**<50**	**65,3**	**3,9**	**27,0**	**4,7**	**4,4**	**9,5**	**6,1**	**27**	**4,4**	**15,1**	**18,7**
SD		**0**	**63,3**	**1,7**	**27,1**	**3,3**	**2,6**	**6,0**	**2,7**	**49**	**3,0**	**21,3**	**13,9**

Table E.12 Lab blanks.

Location	Sample ID	PFBS Amount [pg]	PFBS S/N	PFHxS Amount [pg]	PFHxS S/N	Br-PFOS Amount [pg]	Br-PFOS S/N	L-PFOS Amount [pg]	L-PFOS S/N	6:2 FTSA Amount [pg]	FOSA Amount [pg]	FOSA S/N
UNIS C203	PFC-JSS-019	<50	20,7	5,2	17,1	ND		ND	2,8	ND	7,9	4,3
UNIS C208	PFC-JSS-073	<50	69,9	<1,7	20,0	ND	1,2	7,7	4,2	ND	14,1	37,4
UNIS C208	PFC-JSS-074	<50	26,6	1,1	137,9	2,3	18,1	12,2	48,1	ND	18,2	41,2
UNIS C208	PFC-JSS-075	<50	45,3	7,2	10,6	ND	2,7	ND	2,9	ND	28,8	57,8
UNIS C208 (filtered)	PFC-JSS-078	<50	11,0	<1,7	15,0	ND	1,1	0,9	5,8	ND	19,1	62,1
Average		**<50**	**34,7**	**4,5**	**40,1**	**2,3**	**5,8**	**6,9**	**12,7**	**ND**	**17,6**	**40,6**
SD			**23,3**	**3,1**	**54,8**		**8,2**	**5,7**	**19,8**		**7,6**	**22,8**

Sample ID	PFBA Amount [pg]	PFBA S/N	PFPeA Amount [pg]	PFPeA S/N	PFHxA Amount [pg]	PFHxA S/N	PFHpA Amount [pg]	PFHpA S/N	PFOA Amount [pg]	PFOA S/N	PFNA Amount [pg]	PFNA S/N	PFDA Amount [pg]	PFDA S/N	PFUnDA Amount [pg]	PFUnDA S/N	PFDoDA Amount [pg]	PFDoDA S/N
PFC-JSS-019	**269,4**	11,0	0,0	10,9	64,0	7,5	52,8	3,5	ND	2,9	26,0	3,9	3,9	3,9	13,2	4,0	ND	1,5
PFC-JSS-073		4,7	0,0	12,4	4,1	4,4	17,8	3,9	ND	2,4	17,5	10,3	5,9	4,1	16,8	13,2	ND	1,4
PFC-JSS-074	640,1	18,4	0,0	6,4	0,8	4,2	16,5	4,1	1,7	3,6	ND	2,8	ND	2,3	30,1	7,7	ND	1,5
PFC-JSS-075	659,7	18,2	0,0	4,4	20,3	3,6	21,5	1,5	93,1	4,3	ND	2,8	12,1	4,1	23,8	6,1	ND	1,5
PFC-JSS-078	572,7	14,1	0,0	5,3	19,8	4,2	11,3	3,6	143,4	9,5	27,6	3,1	10,6	3,2	22,0	4,5	ND	1,5
Average	**624,2**	**13,3**	**0,0**	**7,9**	**21,8**	**4,8**	**24,0**	**3,3**	**79,4**	**4,5**	**23,7**	**4,6**	**8,1**	**3,5**	**21,2**	**7,1**	**ND**	**1,5**
SD	**45,6**	**5,7**	**0,0**	**3,6**	**25,2**	**1,5**	**16,5**	**1,0**	**71,8**	**2,9**	**5,5**	**3,2**	**3,9**	**0,8**	**6,5**	**3,7**		**0,0**

Table E.13 Reagent blanks.

Description	Date	Sample ID	PFBS Amount [pg]	PFBS S/N	PFHxS Amount [pg]	PFHxS S/N	Br-PFOS Amount [pg]	Br-PFOS S/N	L-PFOS Amount [pg]	L-PFOS S/N	6:2 FTSA Amount [pg]	6:2 FTSA S/N	FOSA Amount [pg]	FOSA S/N
0,1 NH3 i metanol 18.11.2014	18.11.2014	PFC-JSS-013	<50	71,9	ND	1,6	ND	1,6	ND	3,1	ND	1,4	ND	1,5
0,1 NH3 i metanol (SupraSolv) 18.11.2014	18.11.2014	PFC-JSS-014	<50	15,6	ND	1,0	ND	1,3	n.q.	4,7	ND	1,1	ND	1,1
Metanol, SupraSolv	18.11.2014	PFC-JSS-015	<50	5,8	ND	1,8	ND	1,2	n.q.	4,5	ND	1,4	n.q.	8,9
Metanol, SupraSolv	18.11.2014	PFC-JSS-016	<50	7,4	ND	2,1	ND	0,7	ND	1,5	ND	2,5	ND	0,8
Acetatbuffer	18.11.2014	PFC-JSS-017	<50	8,0	ND	0,7	ND	1,8	ND	0,8	ND	1,2	n.q.	3,1
Acetatbuffer	18.11.2014	PFC-JSS-018	<50	6,3	ND	1,9	ND	2,0	ND	1,9	ND	1,9	ND	0,9
Metanol, LiChroSolv	21.11.2014	PFC-JSS-020	<50	11,9	ND	2,2	n.q.	5,5	n.q.	7,6	ND		n.q.	6,3
0.1 NH3 i metanol LiChroSolv	21.11.2014	PFC-JSS-021	<50	3,3	n.q.	5,6	ND		n.q.	15,0	ND	1,3	ND	1,1
MilliQ water (2 L extracted)	03.06.2015	PFC-JSS-038	<50	∞	2,0	35,3	ND	2,8	2,1	6,1	17,4	3,1	8,5	23,3

Sample ID	PFBA Amount [pg]	PFBA S/N	PFPeA Amount [pg]	PFPeA S/N	PFHxA Amount [pg]	PFHxA S/N	PFHpA Amount [pg]	PFHpA S/N	PFOA Amount [pg]	PFOA S/N	PFNA Amount [pg]	PFNA S/N	PFDA Amount [pg]	PFDA S/N	PFUnDA Amount [pg]	PFUnDA S/N	PFDoDA Amount [pg]	PFDoDA S/N
PFC-JSS-013		8,4	ND	4,5		3,9		2,2		3,4		8,1		1,0		1,4		1,1
PFC-JSS-014		8,8	ND	3,3		3,0		3,2		1,3		6,1		0,8		2,6		2,4
PFC-JSS-015		7,0	ND	4,8		4,4		2,6		1,8		5,6		1,4		3,4		0,8
PFC-JSS-016		8,2	ND	2,7		2,8		1,5		1,1		3,9		2,1		2,0		1,2
PFC-JSS-017		12,0	ND	5,9		7,3		1,3		2,0		17,7		2,2		1,7		1,9
PFC-JSS-018		15,3	ND	2,8		5,5		1,4		1,3		7,6		0,9		1,1		0,7
PFC-JSS-020		8,1	ND	2,9		3,2		1,8		1,9		4,6		1,1		1,1		1,3
PFC-JSS-021		9,8	ND	5,1		4,1		2,4		3,6		4,8		0,8		1,2		2,5
PFC-JSS-038	517,3	32,1	0,0	5,9	5,4	7,5	ND	1,5	103,3	4,6	ND	2,5	ND	2,8	27,3	6,0	ND	1,8

Table E.14 Evaporation blank

Location	Sample ID	PFBS Amount [pg]	PFBS S/N	PFHxS Amount [pg]	PFHxS S/N	Br-PFOS Amount [pg]	Br-PFOS S/N	L-PFOS Amount [pg]	L-PFOS S/N	6:2 FTSA Amount [pg]	FOSA Amount [pg]	FOSA S/N
Adamstuen H-116	PFC-JSS-079	<50	127,8	8,1	36,1	n.d.	2,5	7,7	7,1	n.d.	38,6	68,8

Sample ID	PFBA Amount [pg]	PFBA S/N	PFPeA Amount [pg]	PFPeA S/N	PFHxA Amount [pg]	PFHxA S/N	PFHpA Amount [pg]	PFHpA S/N	PFOA Amount [pg]	PFOA S/N	PFNA Amount [pg]	PFNA S/N	PFDA Amount [pg]	PFDA S/N	PFUnDA Amount [pg]	PFUnDA S/N	PFDoDA Amount [pg]	PFDoDA S/N
PFC-JSS-079	208,4	8,0	0,0	7,9	n.d.	2,8	n.d.	2,1	6,9	3,7	24,4	4,9	10,1	3,3	21,4	6,8	n.d.	1,7

Table E.15 Other blanks.

Description	Sample ID	PFBS		PFHxS		Br-PFOS		L-PFOS		6:2 FTSA		FOSA	
		Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N
SPE valve 1	PFC-JSS-080	<50	∞	<1,7	17,6	135,8	27,9	340,0	69,8	1052,7	66,5	22,9	12,8
SPE valve 2	PFC-JSS-081	<50	21,0	<1,7	10,2	152,7	52,4	332,9	148,6	1116,2	29,6	30,6	152,8
SPE valve 3	PFC-JSS-082	<50	63,8	<1,7	14,0	141,4	50,3	344,3	629,5	273,3	14,0	27,2	11,2
Methanol bottle PTFE cap-liner	PFC-JSS-083	<50	129,8	<1,7	6,6	140,9	48,6	335,5	186,4	ND		31,1	63,2

Description	Sample ID	PFBA		PFPeA		PFHxA		PFHpA		PFOA		PFNA		PFDA		PFUnDA		PFDoDA	
		Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N	Amount [pg]	S/N
SPE valve 1	PFC-JSS-080	322,3	12,4	821,4	39,0	155,5	13,0	254,1	9,6	254,1	12,3	33,4	3,5	5,1	4,9	ND	2,6	ND	1,9
SPE valve 2	PFC-JSS-081	591,2	19,4	3514,3	160,0	65,3	9,1	111,0	13,3	253,8	12,0	ND	2,9	12,9	4,1	24,5	11,3	ND	1,8
SPE valve 3	PFC-JSS-082	706,6	10,5	312,8	10,0	48,9	12,5	61,3	5,2	99,5	3,5	46,1	4,2	8,1	3,0	22,7	4,2	ND	1,8
Methanol bottle PTFE cap-liner	PFC-JSS-083	477,6	9,6	39,0	8,5	64,3	3,5	ND	2,2	ND	1,9	34,0	3,2	ND	1,3	22,2	6,9	ND	1,9

SPE valve 1 – 3: methanol was collected of each cleaning-step initially high amounts found, emphasize the importance of methanol rinsing before use.

F Water characterization analyses

F.1 pH

Measurements were done according to NS-EN ISO 10523:2012. For pH measurements, a Metrohm 867 pH Module connected to a computer with Tiamo version 2.3 software and a Metrohm Unitrode pH-electrode with Pt-1000 temperature sensor was used. Calibration was performed at room temperature with buffers at pH 7.00 and 9.01 (VWR Chemicals), slope was 98.0 and pH(0) was 6.783. As a control of the calibration, a second buffer at pH 10.00±0.05 (Merck KGaA, Darmstadt, Germany) was measured at same temperature as the calibration, the result was pH 10.03.

A subsample was transferred to a 100 mL PP-beaker with lid and left to be tempered to room temperature (measured at calibration temperature ±1.0°C). A magnetic stirrer was used during measurement, and the result was recorded when no signal drift was noticeable.

F.2 Alkalinity

Alkalinity was measured according to NS-EN ISO 9963-1. Alkalinity was determined by potentiometric titration with 10 mmol/L Hydrochloric acid (Merck KGaA, Darmstadt, Germany). The equivalence point for total alkalinity was determined by a pH-electrode (Metrohm AG, Herisau, Switzerland).

An auto-titrator system from Metrohm connected to a computer with Metrohm Tiamo 2.3 software was used.

A titer was determined to verify HCl concentration. A 19.82 mmol/L Sodium carbonate solution was prepared by weighing 2.1005 g Na_2CO_3 (Merck KGaA, Darmstadt, Germany, dried at 300 °C for 2 hours) and dissolving it in 1000 mL of Millipore water purged with nitrogen (5.5, Air Liquide, Bergen, Norway) for 30 minutes. Three replicates of 2.5 mL of the Na_2CO_3-solition was titrated, the titer was determined to 1.005 ± 0.0021.

To determine total alkalinity, 10 mL of sample was titrated. Consumed volume of HCl at equivalence point #2 of the titration curve (pH approx. 4.5) was used to calculate alkaline equivalent.

F.3 Conductivity

Conductivity was measured in compliance with NS-ISO 7888:1993 by a Metrohm 856 Conductivity Module and a 5-ring conductivity measuring cell ($c = 1.0\ cm^{-1}$) with Pt1000 temperature sensor connected to a computer with Metrohm Tiamo 2.3 software. Conductivity was measured at room temperature, and corrected to conductivity at 25 °C. To assure the accuracy of the cell constant, a conductivity standard at 100.0±1.0 µS/cm at 25 °C (VWR Prolabo) was measured as a control, the result was 99,7 µS/cm.

A subsample was transferred to a 20 mL glass vial with lid, and left to be tempered to room temperature. The measuring cell was lowered into the sample, avoiding any air bubbles. The sample was stirred by magnetic stirrer for 30 seconds before measurement, the result was recorded when no signal drift was noticeable.

F.4 Ion composition

Anions and cations analysed according to NS-EN ISO 14911:1999 and ISO 10304-1:2007. Samples were filtered by a 0.45 µm syringe filter (Sartorius, Göttingen, Germany). An aliquot of each sample was diluted by a factor of 10 using MilliQ water to get within the linear range for sulfate. The samples were analysed undiluted for the rest of the analytes. To verify that magnesium was within the linear range, a standard at 40 mg L^{-1} was prepared and analysed along with the samples. Calibration standards were diluted from 1000 mg/L standards traceable to SRM from NIST (Merck Certipur®) in MilliQ-water.

Metrohm 940 Professional IC Vario ion chromatograpgh system(Metrohm AG, Herisau, Switzerland). Column for anions Metrohm A SUPP 4 250/4.0 and A SUPP 4 Guard. The mobile phase for anions contained 1.7 mmol/L sodium bicarbonate and 1.8 mmol/L sodium carbonate in MilliQ-water purged with nitrogen (5.5, Air Liquide, Bergen, Norway) for 30 minutes. The flowrate of the mobile phase was 1.00 mL/min. Detection was done by conductivity detector afterpassing an MCS CO_2-supressor (Metrohm AG, Herisau, Switzerland) to lower background conductivity. Peak integrations and quantifications done by Methohm MagicICnet version 3.1. An external calibration 6-point curve for each ion was used for quantification.

- Chloride 1 – 50 mg/L
- Nitrate-N 0,18 – 9,05 mg/L
- Sulfate 1 – 50 mg/L

The Cation column used was Metrosep C 4 – 150 and C4 guard. The mobile phase for cations contained 2.0 mmol/L nitric acid, 0.1 mmol/L pyridin-2.6-dicarboksylic acid and 3.0 mmol/L ascorbic acid in MilliQ-water purged with nitrogen (5.5, Air Liquide, Bergen, Norway) for 30 minutes. The flowrate of the mobile phase was 0.900 mL/min. Detection was done by directly by conductivity detector. Peak integrations and quantifications done by Methohm MagicICnet version 3.1. An external calibration 6-point curve for each ion was used for quantification.

- Sodium 5,00 – 500 mg/L
- Potassium 0,5 – 25 mg/L
- Magnesium 0,25 – 12,5 mg/L
- 0,25 – 12,5 mg/L

F.5 Results

Parameter	Result	±SD	unit	Measurement T [°C]	[meq/L]	±SD
pH	7,97	0,01	-	22,4		
Total alkalinity	1,003	0,0083	meq/L			
Conductivity at 25°C	305,7	0,65	µS/cm	22,6		
Sodium	4,42	0,010	mg/L		0,1923	0,00044
Potassium	0,34	0,014	mg/L		0,0086	0,00036
Magnesium	9,8	0,15	mg/L		0,81	0,012
Calcium	41	1,1	mg/L		2,04	0,057
Chloride	5,79	0,033	mg/L		0,1633	0,00093
Nitrate	0,543	0,0026	mg/L		0,00876	4,1E-05
Sulphate	98	1,5	mg/L		2,04	0,032
Bicarbonate*	61,2	0,50	mg/L		1,003	0,0083
Sum cations	55,5		mg/L		3,050	
Sum anions	165,5		mg/L		3,214	
Total dissolved solids (TDS)	220,9		mg/L			
Ion balance	-2,6		-			

a. Calculated by assuming that mainly bicarbonate contribute to the alkalinity.

G Chromatograms

Example MRM chromatograms from selected standards, samples and blanks. Chromatograms were exported from MassHunter Workstation Qualitative analysis software.

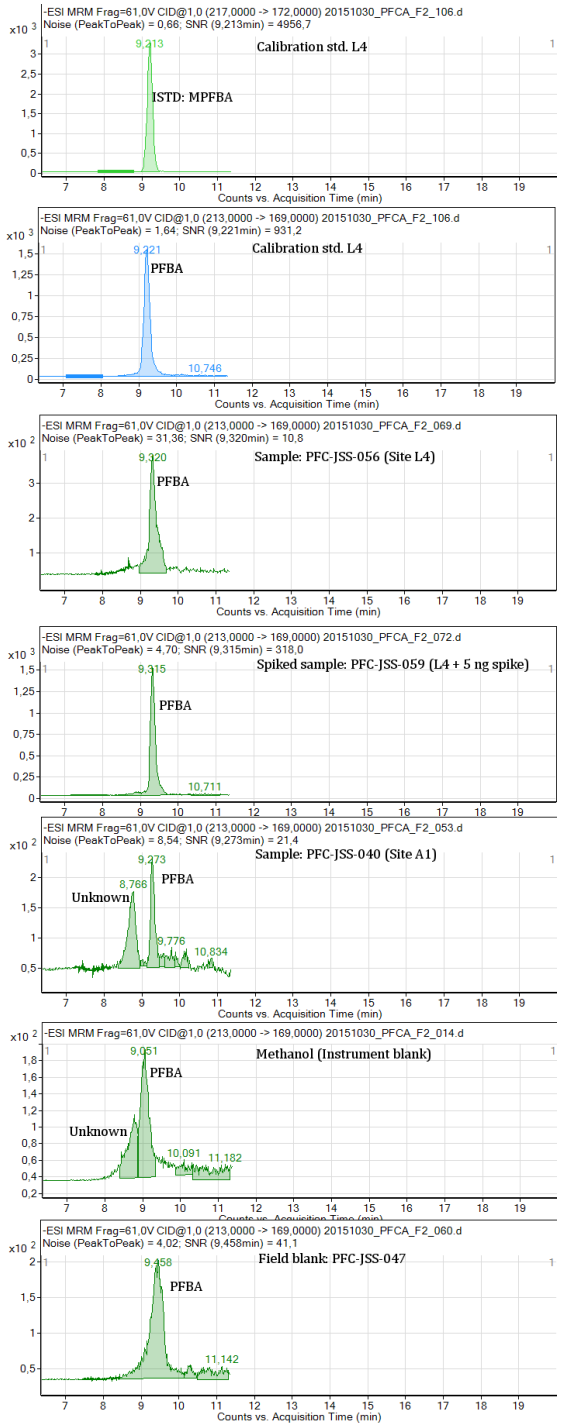


Figure G.1. MRM Chromatograms PFBA.

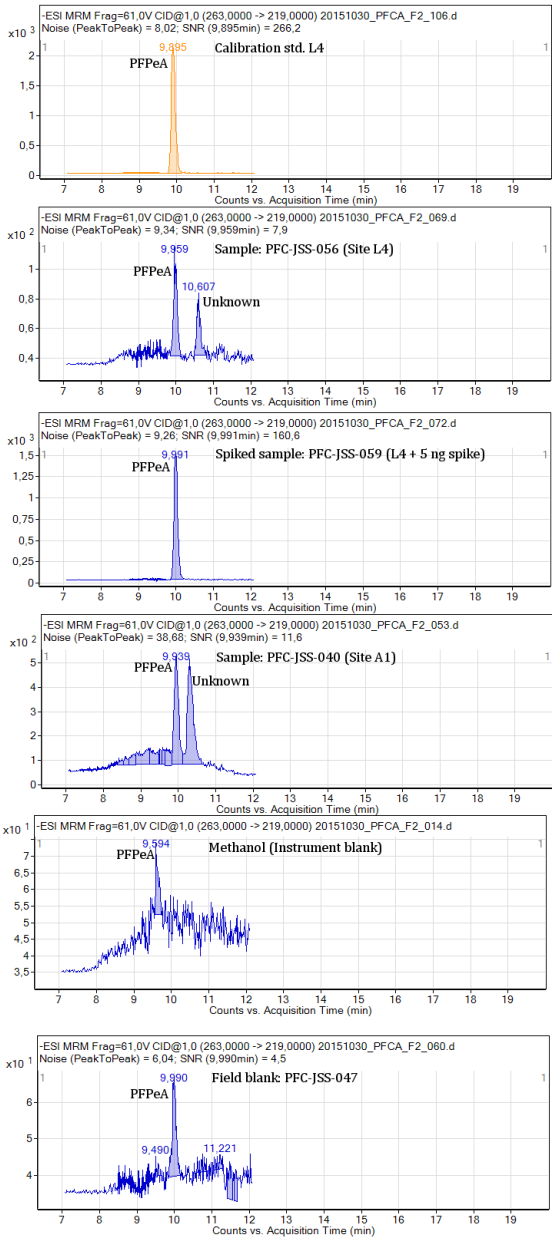


Figure G.2. MRM Chromatograms PFPeA.

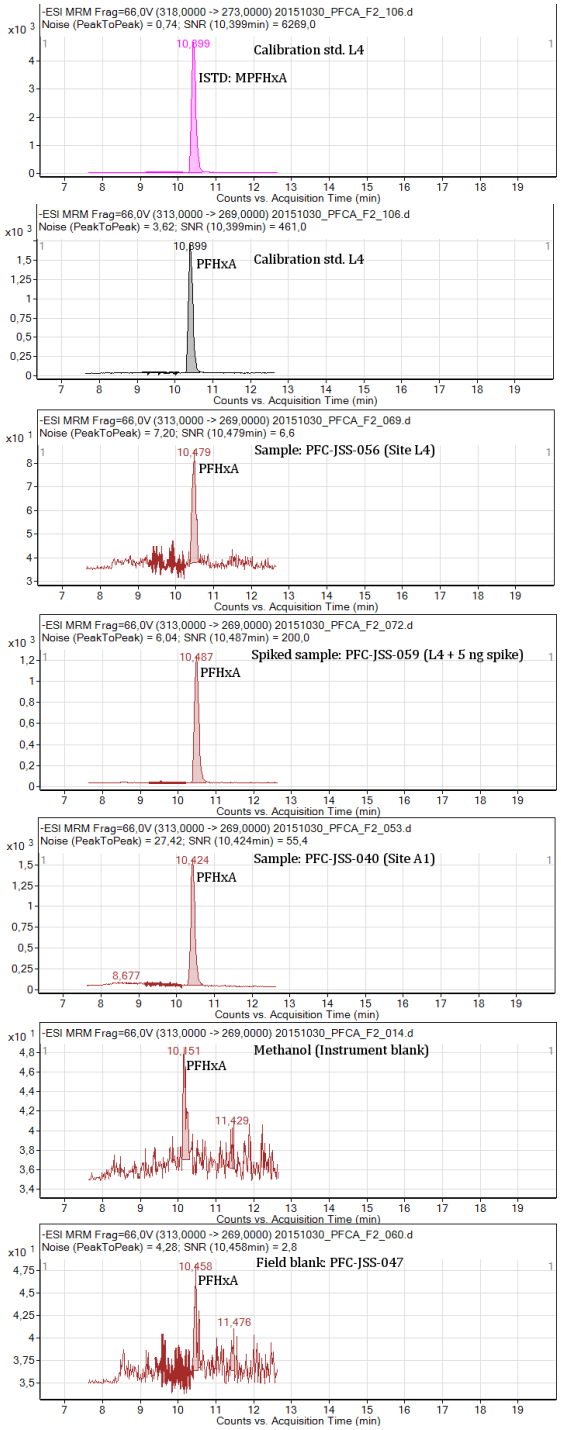


Figure G.3. MRM Chromatograms PFHxA.

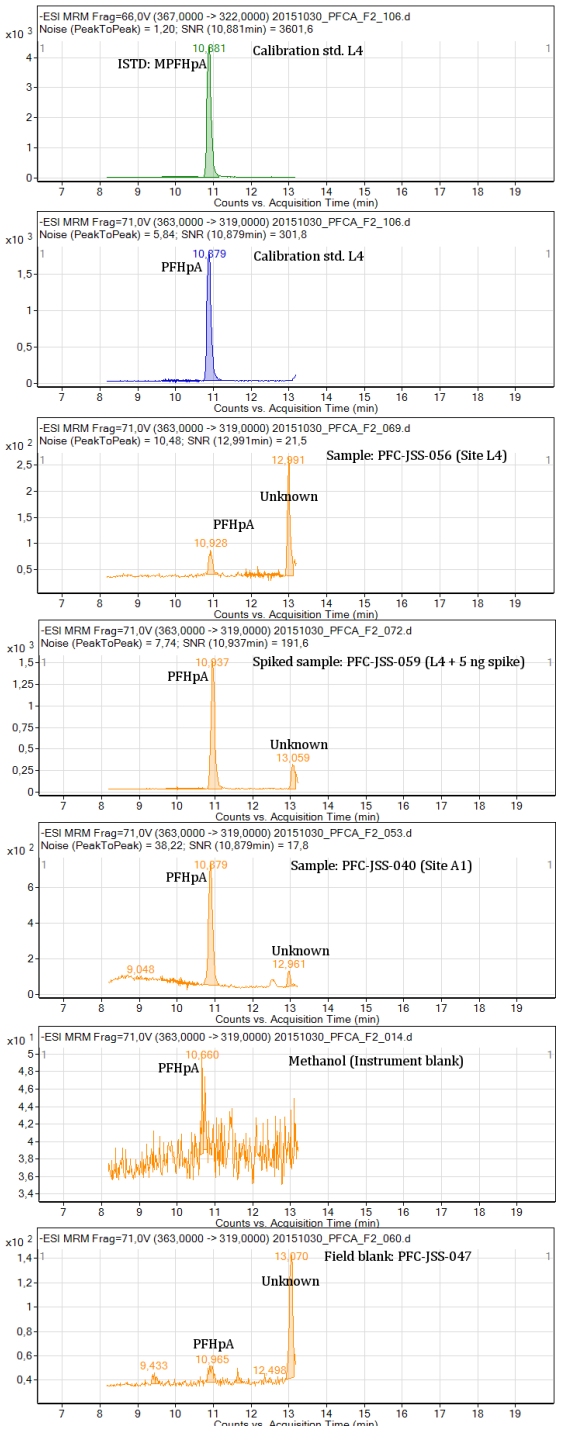


Figure G.4. MRM Chromatograms PFHpA.

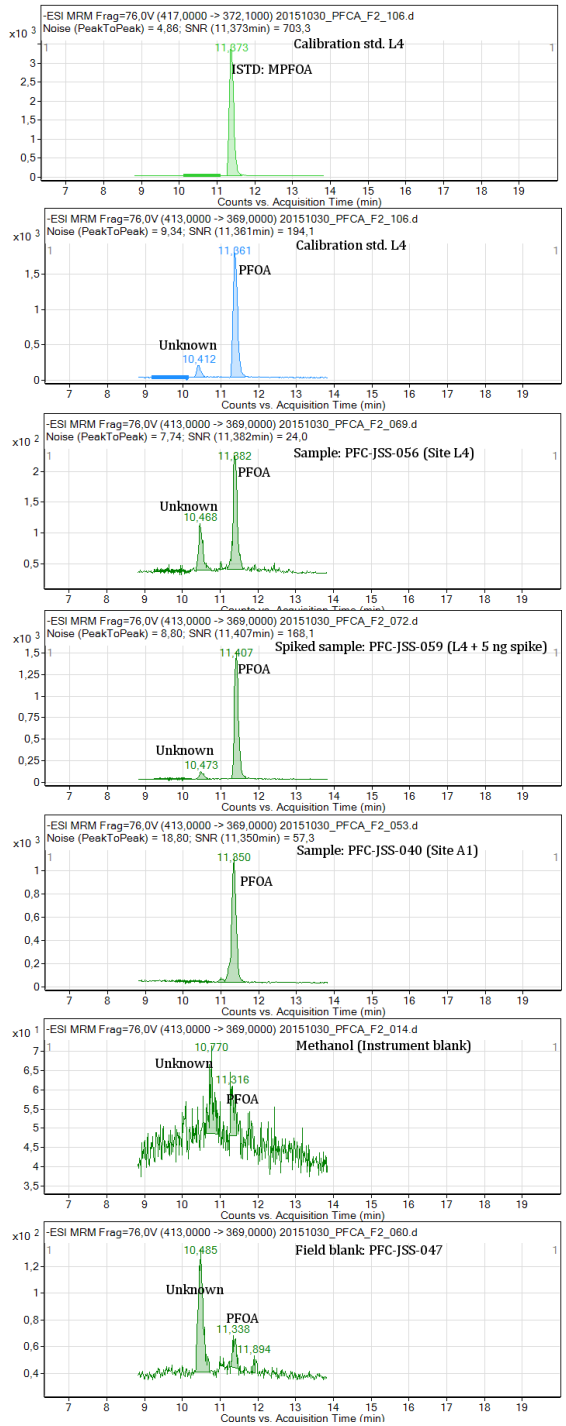


Figure G.5. MRM Chromatograms PFOA.

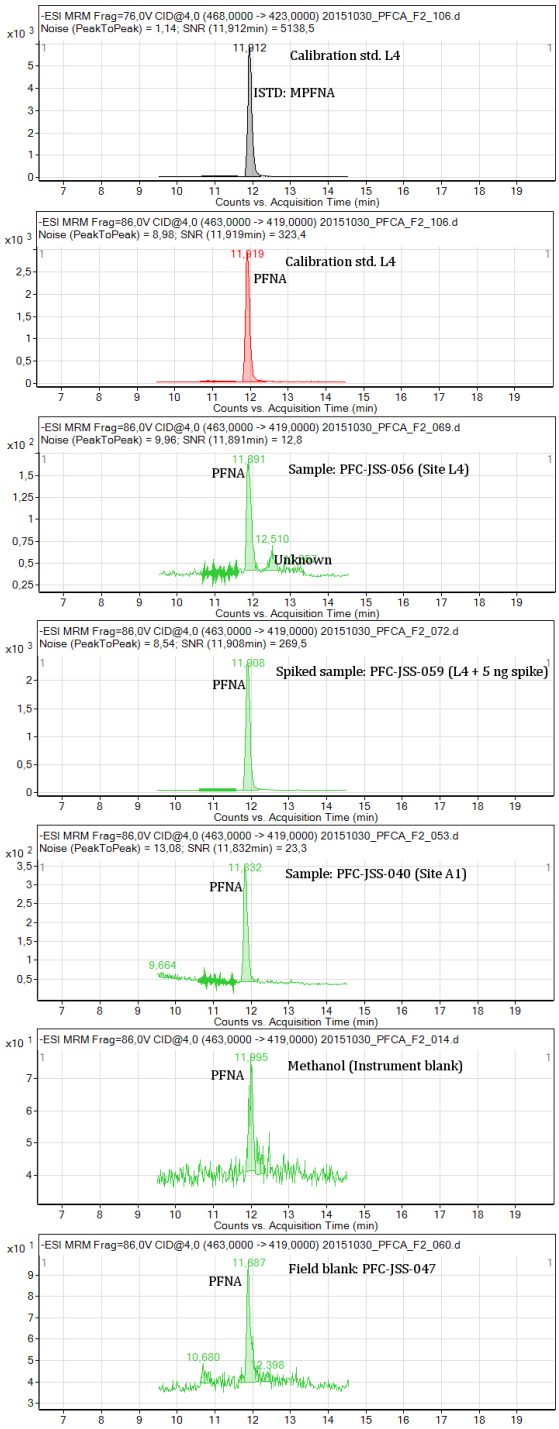


Figure G.6. MRM Chromatograms PFNA.

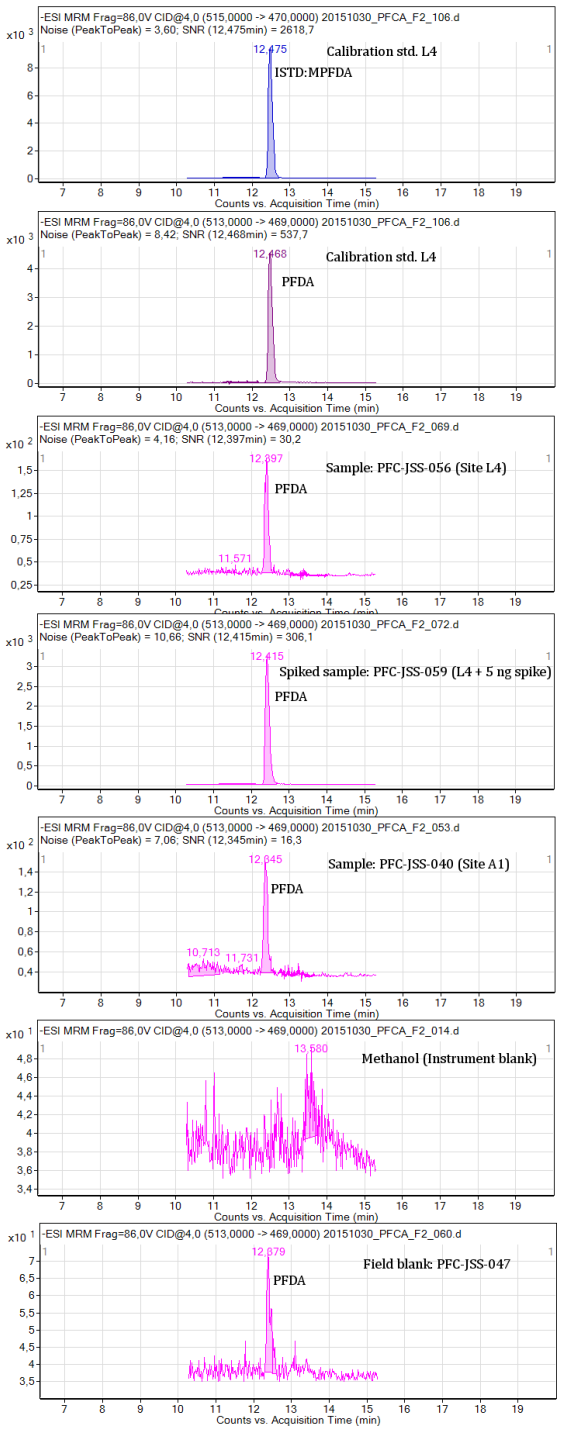


Figure G.7. MRM Chromatograms PFDA.

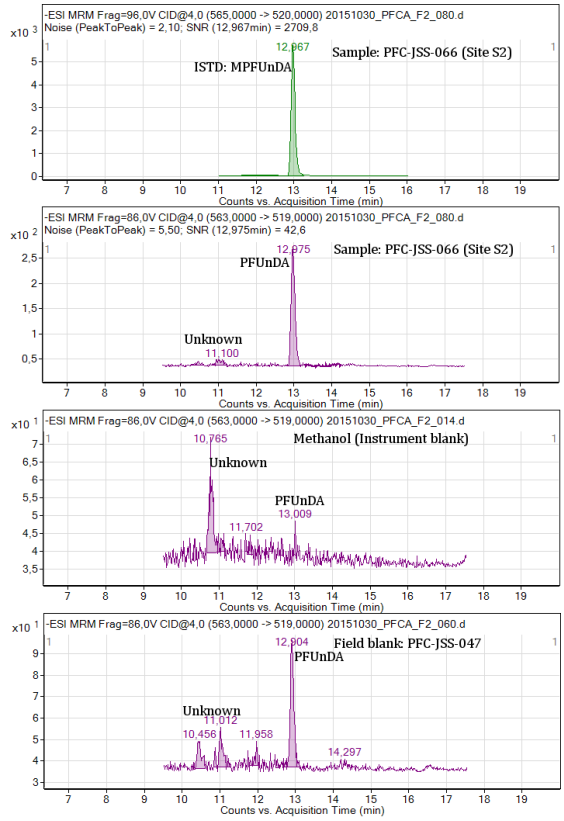


Figure G.8 MRM Chromatograms PFUnA.

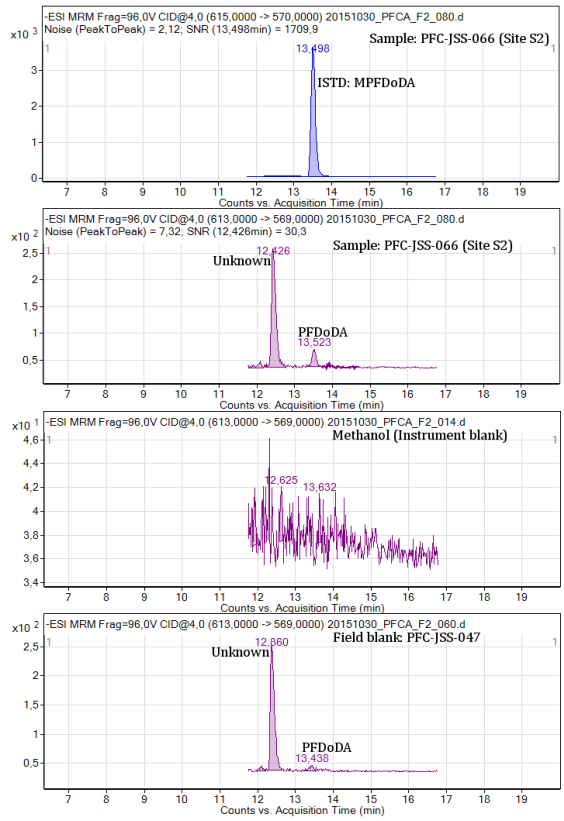


Figure G.9. MRM Chromatograms PFDoA.

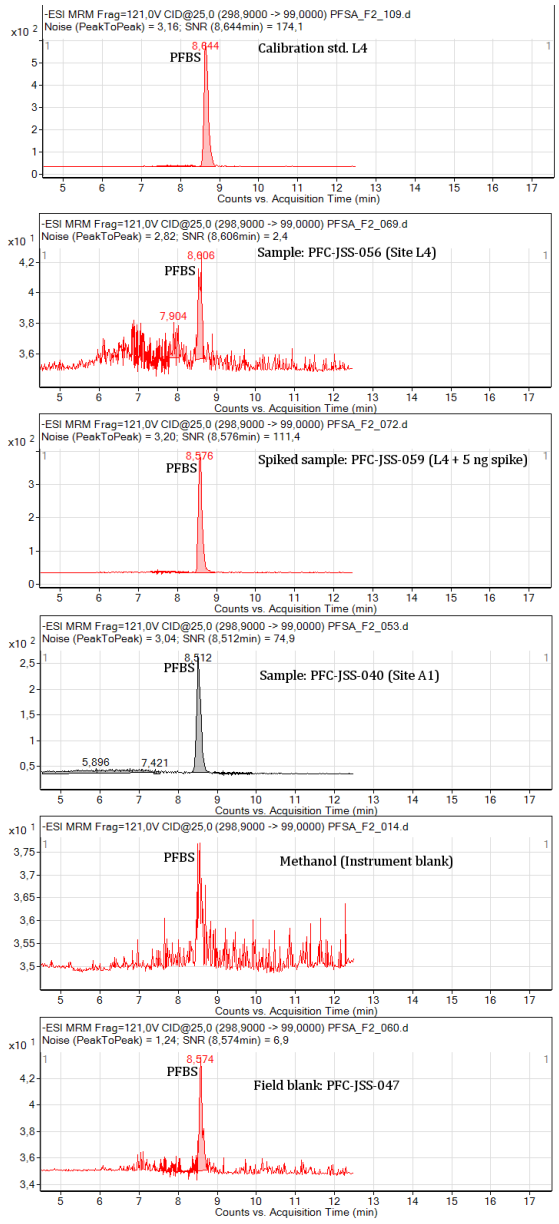


Figure G.10. MRM Chromatograms PFBS.

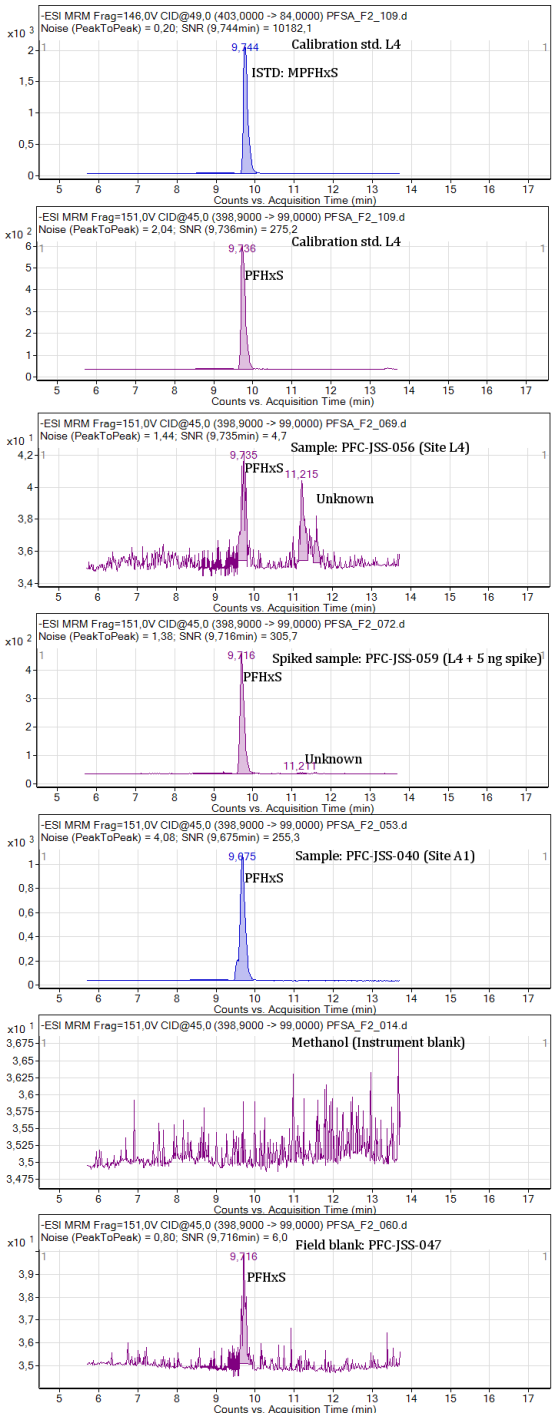


Figure G.11. MRM Chromatograms PFHxS.

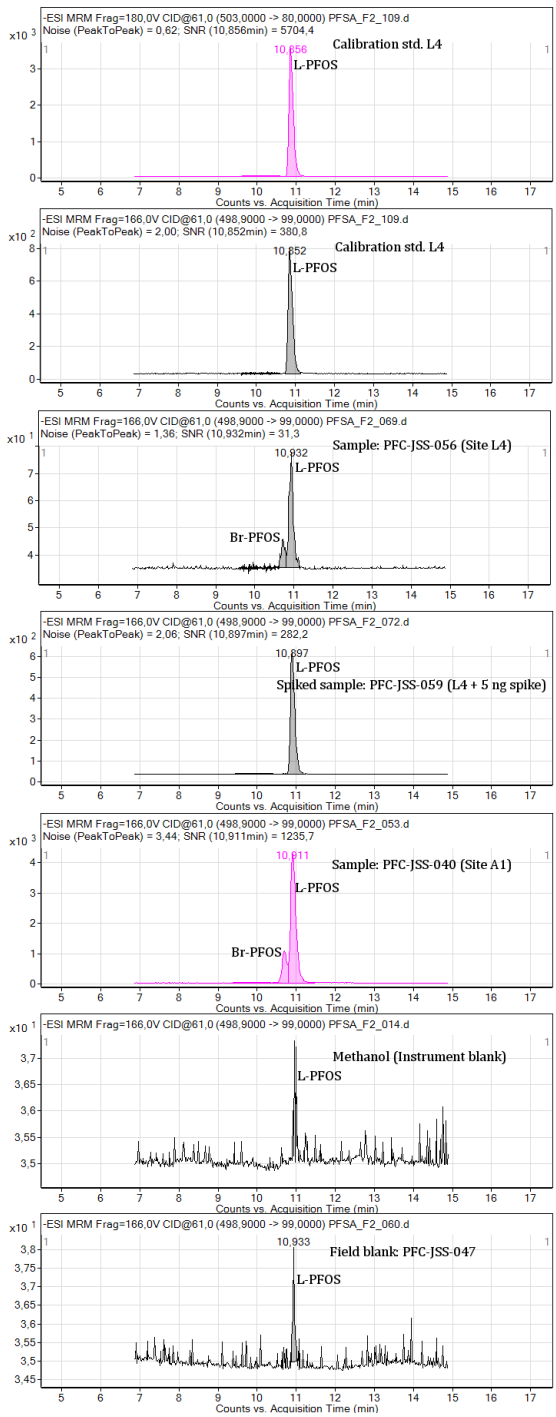


Figure G.12. MRM Chromatograms PFOS.

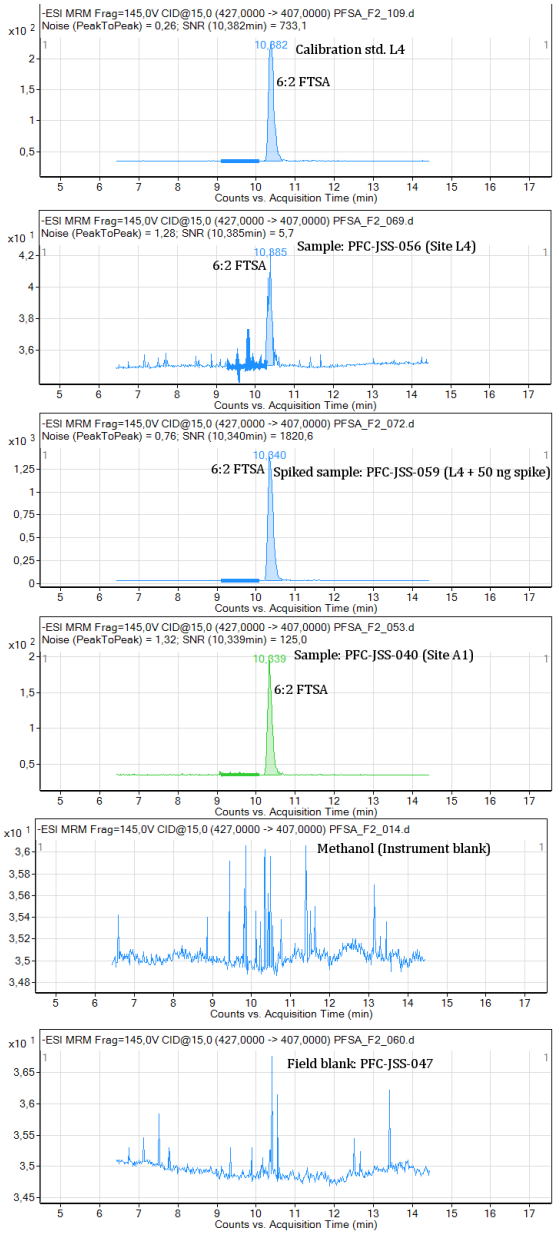


Figure G.13. MRM Chromatograms 6:2 FTSA.

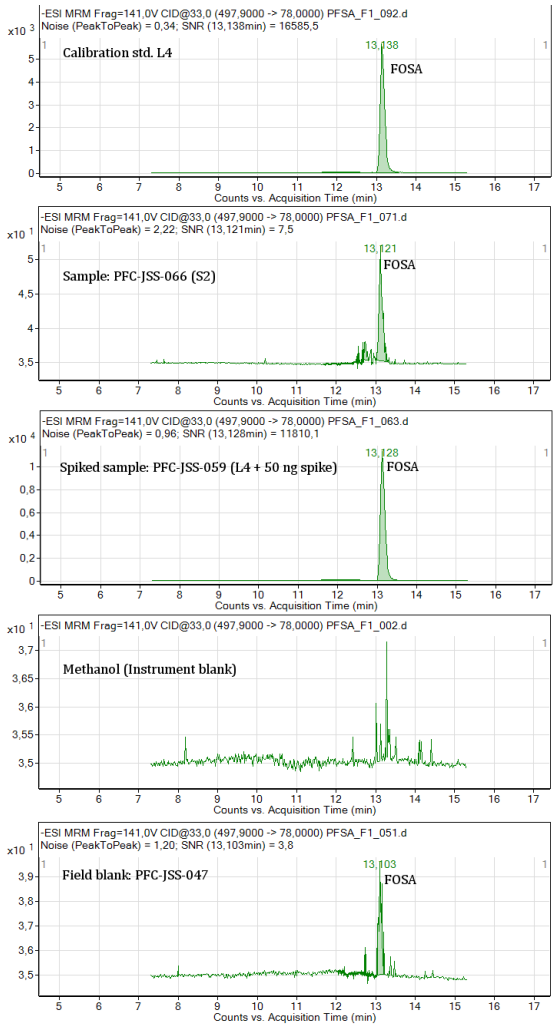


Figure G.14. MRM Chromatograms FOSA.

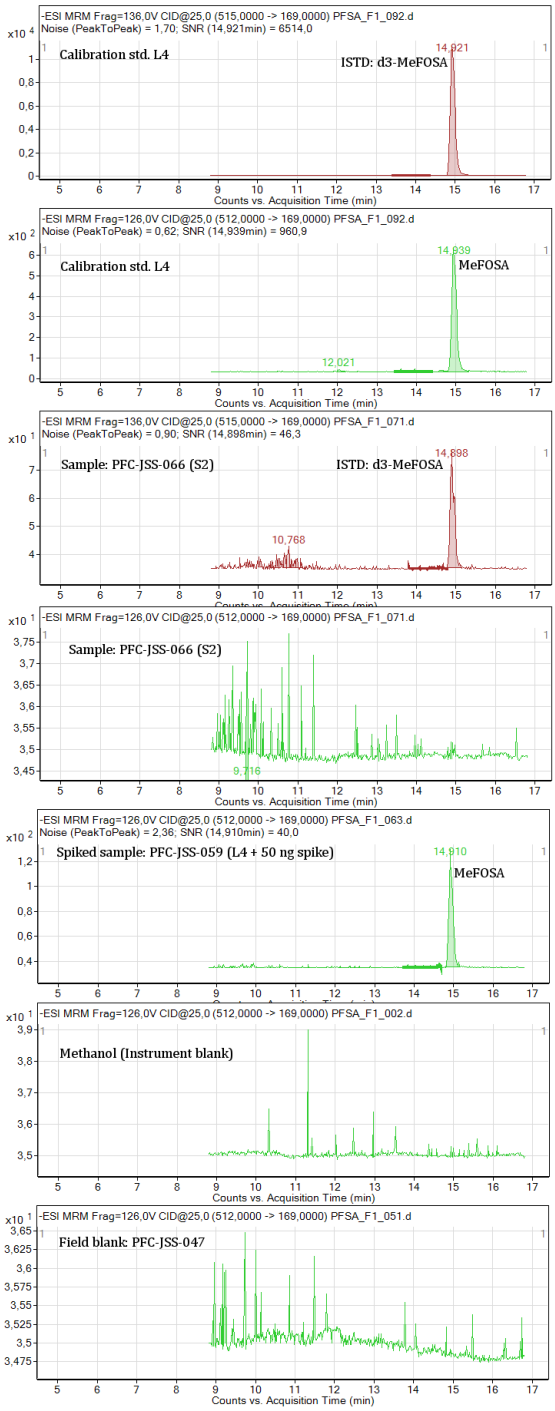


Figure G.15. MRM Chromatograms MeFOSA.

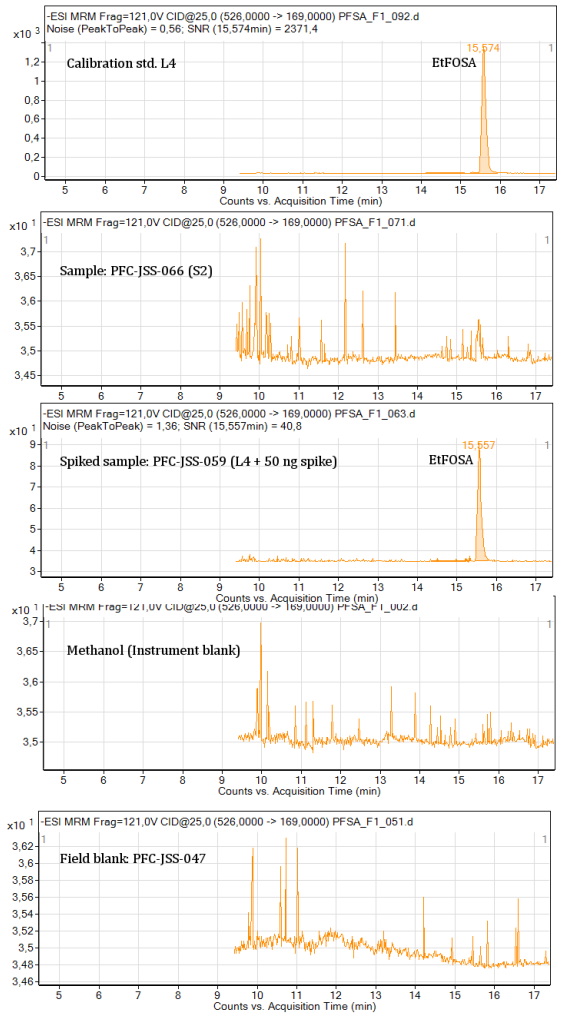


Figure G.16. MRM Chromatograms EtFOSA.

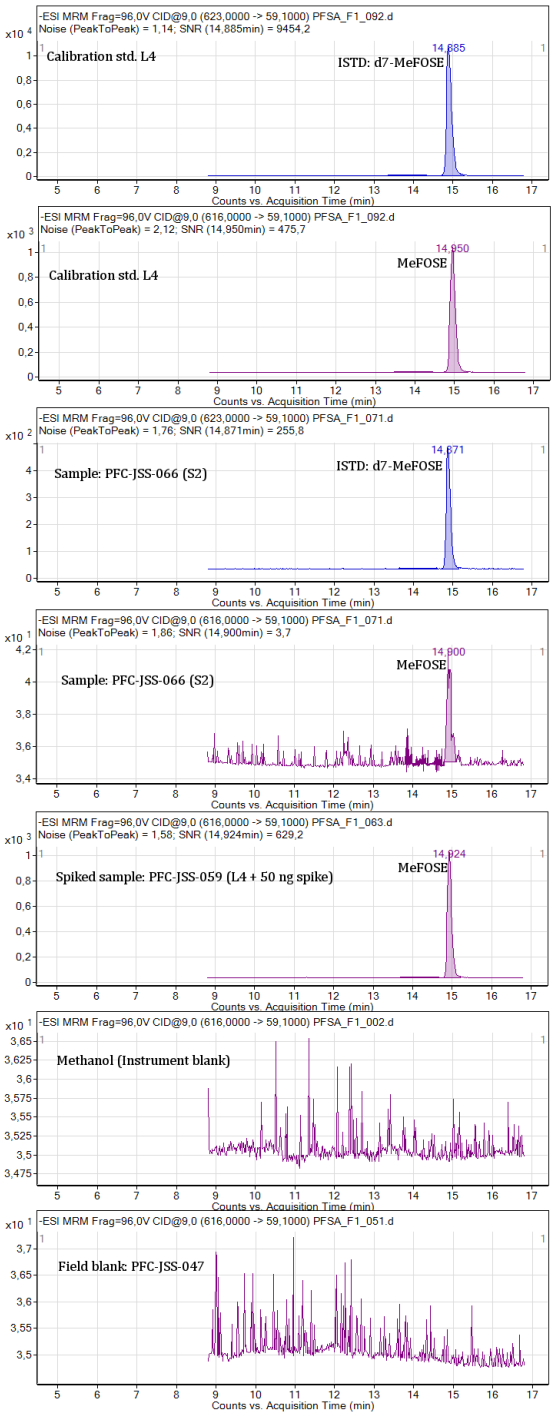


Figure G.17. MRM Chromatograms MeFOSE.

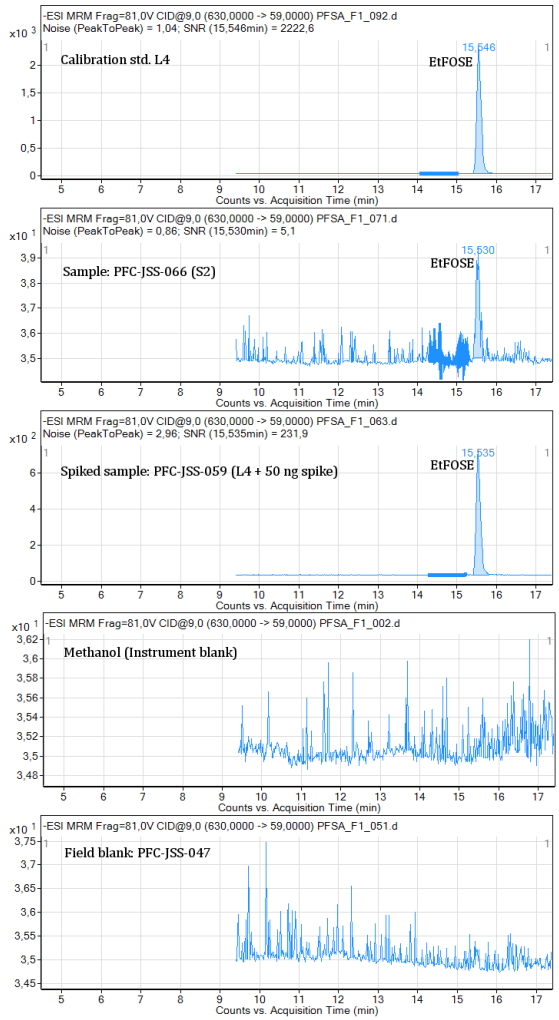


Figure G.18. MRM Chromatograms EtFOSE.

H Statistics

All results above MDL were included. Results below MDL were set to half MDL, except values very close to MDL, which were kept as their original value.

Table H.1. Raw data uses for statistics.

Lok. ID	PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnDA	PFDoDA	PFBS	PFHxS	6:2 FTSA	Br-PFOS	L-PFOS	Sum PFAS
L5-1	0,58	0,071	0,41	0,32	2,66	0,32	0,92	0,070	0,22	0,013	0,022	0,055	0,12	0,14	5,92
L5-2	1,09	0,089	0,34	0,26	1,78	0,24	0,61	0,056	0,16	0,013	0,023	0,027	0,083	0,11	4,88
A1-nov-1	0,25	1,29	2,66	0,57	0,31	0,03	0,004	0,012	0,003	0,035	0,21	0,004	0,088	0,10	5,56
A1-nov-2	0,31	1,55	3,02	0,40	0,36	0,04	0,004	0,017	0,003	0,14	0,43	0,004	0,20	0,24	6,70
A1-nov-3	0,47	2,16	2,65	0,81	0,02	0,01	0,004	0,013	0,003	0,013	0,014	0,004	0,006	0,008	6,18
L1-apr-1	0,99	0,046	0,15	0,17	0,47	0,16	0,11	0,071	0,033	0,013	0,010	0,004	0,038	0,042	2,30
L1-apr-2	0,86	0,024	0,11	0,14	0,39	0,16	0,12	0,092	0,047	0,013	0,005	0,004	0,035	0,033	2,03
L1-apr-3	0,93	0,084	0,14	0,15	0,45	0,16	0,11	0,032	0,029	0,013	0,015	0,019	0,041	0,041	2,20
L2-apr-1	1,15	0,030	0,076	0,14	0,24	0,12	0,050	0,055	0,019	0,013	0,012	0,015	0,029	0,024	1,97
L2-apr-2	1,01	0,065	0,075	0,13	0,25	0,12	0,061	0,043	0,015	0,013	0,007	0,016	0,028	0,027	1,86
L2-apr-3	1,08	0,059	0,079	0,14	0,26	0,14	0,043	0,021	0,007	0,013	0,014	0,021	0,032	0,024	1,94
L3-apr-1	4,63	0,21	0,34	0,50	1,36	0,32	0,041	0,014	0,003	0,013	0,17	0,026	0,11	0,069	7,80
L3-apr-2	5,23	0,21	0,38	0,53	1,28	0,30	0,030	0,021	0,003	0,013	0,16	0,021	0,10	0,060	8,35
L3-apr-3	2,81	0,14	0,21	0,31	0,84	0,21	0,025	0,009	0,003	0,013	0,10	0,022	0,077	0,051	4,81
L4-apr-1	1,37	0,042	0,10	0,42	0,18	0,10	0,044	0,046	0,003	0,013	0,007	0,004	0,028	0,044	2,38
L4-apr-2	1,23	0,059	0,10	0,24	0,18	0,10	0,041	0,033	0,010	0,013	0,010	0,004	0,034	0,025	2,07
A1-jun-1	3,99	3,16	14,76	4,07	5,53	0,85	0,19	0,13	0,009	2,40	14,80	4,25	27,05	41,24	122,44
A1-jun-2	3,92	3,86	16,48	4,48	5,35	0,86	0,17	0,13	0,009	2,41	14,77	4,17	25,97	38,58	121,15
A1-jun-3	4,07	3,07	15,22	4,32	5,62	0,87	0,15	0,076	0,008	2,33	14,79	4,35	24,70	37,18	116,75
L1-jun-1	0,25	0,012	0,12	0,15	0,16	0,14	0,052	0,049	0,017	0,013	0,010	0,025	0,085	0,087	1,16
L1-jun-2	0,25	0,012	0,10	0,13	0,14	0,13	0,048	0,040	0,009	0,013	0,003	0,016	0,095	0,085	1,07
L1-jun-3	0,25	0,012	0,13	0,14	0,13	0,11	0,049	0,036	0,015	0,013	0,006	0,010	0,073	0,079	1,05
L2-jun-1	0,39	0,012	0,06	0,05	0,16	0,11	0,071	0,028	0,021	0,013	0,007	0,050	0,056	0,054	1,09
L2-jun-2	0,44	0,012	0,059	0,05	0,15	0,14	0,061	0,028	0,014	0,013	0,008	0,038	0,060	0,057	1,13
L3-jun-1	0,89	0,025	0,074	0,11	0,20	0,16	0,076	0,030	0,024	0,013	0,016	0,075	0,080	0,11	1,88
L3-jun-2	0,70	0,012	0,047	0,087	0,14	0,14	0,054	0,036	0,016	0,013	0,013	0,033	0,068	0,091	1,44
L3-jun-3	0,68	0,012	0,044	0,068	0,16	0,14	0,048	0,027	0,021	0,013	0,011	0,043	0,071	0,084	1,42
L4-jun-1	0,77	0,049	0,079	0,076	0,30	0,14	0,086	0,037	0,026	0,013	0,016	0,077	0,086	0,14	1,89
L4-jun-2	0,59	0,028	0,058	0,071	0,21	0,11	0,083	0,034	0,025	0,013	0,011	0,040	0,077	0,15	1,50
L4-jun-3	0,40	0,012	0,014	0,017	0,02	0,01	0,008	0,017	0,003	0,013	0,003	0,007	0,035	0,083	0,63
I	1,50	0,24	0,11	0,19	0,29	0,20	0,036	0,020	0,011	0,013	0,022	0,008	0,066	0,057	2,76
O	1,34	0,072	0,15	0,19	0,26	0,15	0,035	0,076	0,030	0,013	0,021	0,004	0,051	0,066	2,46
S1	0,46	0,012	0,070	0,029	0,41	0,94	0,17	0,13	0,017	0,013	0,007	0,048	0,21	0,23	2,75
S2	0,25	0,012	0,014	0,017	0,086	0,66	0,12	0,17	0,035	0,013	0,003	0,017	0,092	0,13	1,62
M1	2,85	0,15	0,25	0,46	0,54	0,61	0,10	0,055	0,003	0,013	0,041	0,004	0,152	0,16	5,39
M2	2,65	0,072	0,59	0,25	0,41	0,20	0,025	0,025	0,003	0,013	0,020	0,004	0,057	0,06	4,38

Table H.2. PCA loadings

	PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnDA	PFDoDA	PFBS	PFHxS	6:2 FTSA	Br-PFOS	L-PFOS
PC-1	0,8844	-0,1639	-0,3461	0,0098	0,0619	0,0094	-0,0053	0,0055	0,0004	-0,0162	-0,0895	-0,0140	-0,1362	-0,2002
PC-2	0,2332	0,4462	0,6205	0,1359	-0,2169	-0,3451	-0,1395	-0,0721	-0,0335	-0,0041	-0,0345	-0,0567	-0,2203	-0,3133
PC-3	0,2115	-0,0548	-0,0450	-0,0371	-0,6123	-0,2512	-0,2467	-0,0504	-0,0610	0,0320	0,1992	0,0475	0,3254	0,5430
PC-4	0,0036	-0,1123	-0,0315	0,0117	0,5568	-0,7684	0,0664	-0,1622	0,0197	0,0121	0,1289	0,0140	0,0877	0,1735
PC-5	0,1226	0,2623	0,1118	-0,9046	0,1527	0,1160	-0,0205	-0,0921	-0,0085	0,0184	0,1498	0,0421	-0,0581	0,1082
PC-6	0,0863	-0,7399	0,5693	-0,0848	0,0825	0,1423	-0,1679	0,0157	-0,0436	0,0411	0,1891	-0,0652	0,0725	-0,0973
PC-7	0,0105	0,2404	-0,1381	0,2147	0,2802	0,2532	-0,5536	-0,3010	-0,2289	-0,0168	0,4182	-0,2706	0,1728	-0,0810

Table H.3. PCA Scores.

Lok. ID	PC-1	PC-2	PC-3	PC-4	PC-5	PC-6	PC-7
L-mar-1	-0,1977	-0,1534	-0,3103	0,1988	0,0085	-0,0130	-0,0035
L-mar-2	-0,0919	-0,0940	-0,2259	0,1535	0,0126	-0,0084	-0,0080
A1-nov-1	-0,4469	0,3211	-0,0573	-0,0261	0,0049	0,0428	-0,0076
A1-nov-2	-0,4447	0,2885	-0,0331	-0,0202	0,0455	0,0363	-0,0018
A1-nov-3	-0,4153	0,3767	-0,0440	-0,0736	-0,0082	-0,0820	0,0025
L1-apr-1	0,0851	-0,0056	-0,0713	0,0373	-0,0013	0,0084	0,0016
L1-apr-2	0,0831	-0,0209	-0,0727	0,0247	-0,0053	0,0073	-0,0123
L1-apr-3	0,0750	-0,0041	-0,0735	0,0398	0,0080	-0,0078	0,0117
L2-apr-1	0,2278	0,0365	0,0164	0,0013	0,0027	0,0063	-0,0054
L2-apr-2	0,1906	0,0335	0,0005	0,0030	0,0044	-0,0112	-0,0016
L2-apr-3	0,1998	0,0323	0,0018	-0,0018	0,0049	-0,0029	0,0137
L3-apr-1	0,2334	0,0472	-0,0009	0,0465	0,0233	0,0104	0,0340
L3-apr-2	0,2621	0,0638	0,0183	0,0377	0,0227	0,0127	0,0261
L3-apr-3	0,2246	0,0439	-0,0029	0,0449	0,0223	0,0074	0,0345
L4-apr-1	0,2147	0,0685	0,0489	-0,0085	-0,1014	-0,0108	0,0067
L4-apr-2	0,2271	0,0707	0,0442	-0,0123	-0,0415	-0,0048	0,0023
A1-jun-1	-0,4011	-0,1534	0,2341	0,0846	0,0067	-0,0055	0,0098
A1-jun-2	-0,4032	-0,1333	0,2216	0,0791	0,0050	0,0000	0,0106
A1-jun-3	-0,3980	-0,1394	0,2203	0,0824	0,0049	0,0020	0,0123
L1-jun-1	-0,1398	-0,0677	-0,0414	-0,0266	-0,0771	0,0134	-0,0010
L1-jun-2	-0,1218	-0,0708	-0,0262	-0,0232	-0,0778	0,0075	0,0027
L1-jun-3	-0,1286	-0,0351	-0,0262	-0,0245	-0,0790	0,0248	-0,0091
L2-jun-1	0,0130	-0,0605	-0,0352	-0,0054	0,0056	-0,0015	-0,0263
L2-jun-2	0,0440	-0,0548	-0,0167	-0,0288	0,0177	0,0062	-0,0169
L3-jun-1	0,1154	-0,0201	0,0292	-0,0135	0,0063	-0,0050	-0,0200
L3-jun-2	0,1258	-0,0272	0,0406	-0,0270	0,0009	-0,0020	-0,0150
L3-jun-3	0,1272	-0,0320	0,0325	-0,0197	0,0144	-0,0006	-0,0126
L4-jun-1	0,0523	-0,0448	-0,0048	0,0268	0,0248	-0,0170	-0,0157
L4-jun-2	0,0368	-0,0579	0,0180	0,0217	0,0130	-0,0202	-0,0260
L4-jun-3	0,2379	0,0246	0,1827	0,0030	0,0380	-0,0188	-0,0457
I	0,1739	0,0575	0,0238	-0,0232	0,0183	-0,0460	0,0265
O	0,1764	0,0477	0,0280	-0,0092	-0,0037	0,0054	-0,0013
S1	-0,1533	-0,2282	-0,1045	-0,1861	0,0395	0,0093	0,0326
S2	-0,1627	-0,2435	-0,0810	-0,2999	0,0246	-0,0057	-0,0066
M1	0,1679	0,0173	0,0216	-0,0485	-0,0076	0,0014	0,0212
M2	0,2112	0,1164	0,0454	-0,0068	0,0234	0,0617	-0,0124

Table H.4. PCA explained variance.

	PC-1	PC-2	PC-3	PC-4	PC-5	PC-6	PC-7
Calibration	58,8420	77,7960	90,1241	97,4577	98,7335	99,3348	99,6938
Validation	45,8429	65,1536	75,8332	94,4233	96,1265	96,5582	98,4980
PFBA	96,6239	98,7884	99,9465	99,9467	99,9870	99,9964	99,9964
PFPeA	26,6816	90,4116	91,0367	92,5987	94,0807	99,6396	99,9900
PFHxA	48,2756	98,2538	98,4251	98,4748	98,5840	99,9186	99,9655
PFHpA	0,3896	24,6981	25,8786	25,9486	98,4459	98,7465	99,8962
PFOA	2,7911	13,8254	71,0318	99,1682	99,5364	99,5871	99,9360
PFNA	0,0701	30,4616	40,9338	99,2391	99,4701	99,6341	99,9439
PFDA	0,1274	28,5412	86,3265	88,8176	88,8589	90,1648	98,6358
PFUnDA	0,4128	23,4261	30,7529	75,8627	78,3944	78,4292	86,0323
PFDoDA	0,0087	22,0660	69,5935	72,5294	72,6256	73,8082	93,2876
PFBS	42,7551	43,6240	78,8413	81,8148	83,0157	85,8429	86,1231
PFHxS	37,2881	39,0689	77,7343	87,3691	89,6323	91,3311	96,2939
6:2 FTSA	5,1086	32,2576	44,6156	45,2564	46,2614	47,4005	59,1044
Br-PFOS	31,9084	58,7920	96,9530	98,6019	98,7277	98,8200	99,1333
L-PFOS	29,0120	51,8993	96,6249	99,3399	99,5237	99,5937	99,6227
PFBA	95,9356	97,8130	99,4647	99,8897	99,9490	99,9614	99,9805
PFPeA	1,5629	76,2792	79,5186	81,8321	81,4060	85,8090	99,7735
PFHxA	28,8756	96,6651	96,9786	96,1617	95,6239	97,3319	99,8400
PFHpA	-17,7262	2,5087	-2,9033	-28,2402	94,8491	94,6205	99,4201
PFOA	-9,9658	-17,1371	12,2466	98,4078	98,7589	98,7262	99,5945
PFNA	-13,4713	-2,7488	-18,0144	98,7704	98,9916	99,0984	99,8090
PFDA	-16,5352	-6,3172	64,8810	78,6956	73,8552	72,7265	94,2434
PFUnDA	-13,2451	-8,2288	-24,4754	60,2422	52,9415	44,4717	52,4989
PFDoDA	-15,8012	-13,4409	49,4484	45,0405	33,3112	25,8344	70,4225
PFBS	19,0883	-32,3005	31,9261	37,7138	30,9121	13,6859	-20,5793
PFHxS	12,1804	-27,5534	41,1808	64,6044	67,0201	63,2668	66,5773
6:2 FTSA	-12,0152	16,0946	25,4854	2,5594	-18,0575	-39,3571	-63,2250
Br-PFOS	2,8584	24,6951	90,5572	95,2854	94,8642	94,3372	93,6303
L-PFOS	0,6739	15,1728	91,4843	98,5619	98,8330	98,7527	98,4939

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