Supplemental Information for

Interlaboratory Comparison of Extractable Organofluorine Measurements in Groundwater and Eel (*Anguilla rostrata*): Recommendations for Methods Standardization

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Supplementary Introduction

Table S1. Comparison of bulk PFAS methods

Analytical method	Description	Comments
Extractable organofluorine (EOF)	Measures the concentration of fluorine extracted from a sample *Applications*: aqueous, solid & biological matrices, consumer products	*Strengths*: • Applicable to most matrices • Sensitivity (sub-ppb detection limits) *Limitations:* • Extraction procedure must remove inorganic fluorine to prevent interference • High levels of chloride and alkaline earth elements can affect combustion process
Adsorbable organofluorine (AOF)	Measures the concentration of fluorine adsorbed from a sample *Applications*: aqueous matrices	*Strengths*: • Activated carbon absorbent is nonselective allowing for broader collection of organofluorine chemicals • Less analytical steps, reducing time and potential introduction of contamination *Limitations:* • Adsorption procedure must remove inorganic fluorine to prevent interference • Limited applicability outside of aqueous matrices
^{19}F nuclear magnetic resonance (NMR)	Measures the concentration of organofluorine extracted from a sample *Applications*: aqueous, solid & biological matrices, consumer products	*Strengths*: • Distinguishes between organic & inorganic fluorine • Applicable to most matrices • Nondestructive with simple sample prep and minimal matrix interference *Limitations:* • Low sensitivity – extensive pre-concentration or prolonged acquisition time required
Particle induced gamma emission (PIGE)	Measures the concentration of fluorine on a solid surface *Applications*: solid samples (i.e. consumer products)	*Strengths*: • Nondestructive and high throughput *Limitations:* • Does not distinguish between organic & inorganic • Sensitivity (ppm detection limits)
X-ray photoelectron spectroscopy (XPS)	Measures the atomic organofluorine percentage on a solid surface *Applications*: solid samples (i.e. consumer products)	*Strengths*: • Detection of true surface (<0.01 μm) fluorine present • Distinguishes between organic & inorganic fluorine • Common instrument in research labs *Limitations:* • Requires assumptions to convert measurement to concentration • Sensitivity (High detection limits)
Total oxidizable precursor (TOP) assay	Measures the concentration of PFAA produced due to oxidative conversion of precursor compounds *Applications*: aqueous, solid & biological matrices, consumer products	*Strengths*: • Low detection limits (ppt levels) • Utilizes common instrumentation (LC-MS/MS) *Limitations:* • Only measures compounds that oxidize into PFAA • Matrix interferences and recovery issues for non-aqueous matrices

Supplementary Materials and Methods

Interlaboratory coordination.

Table S2. Participant labs and materials received by each lab for sample extraction and analysis

Lab	Sector	CIC instrument	Materials Received
Bureau Veritas (Canada)	Commercial lab	Thermo	- Groundwater (500 mL) - Eel Homogenate (25 g) - Field Blank (200 mL) - Fluoride Spike Solution (Eel: 10 mg F L^{-1}; Groundwater: 100 mg F L^{-1}) - PFAS Spike Solution (0.62 mM F)
Eurofins Environment Testing (Australia)	Commercial lab	Metrohm	
Federal Institute for Materials Research and Testing (Germany)	Government lab	Thermo	
Harvard University (USA)	Academic lab	Metrohm	
North Carolina State University (USA)	Academic lab	Thermo	
Norwegian Institute for Water Research (Norway)	Non-profit research lab	Metrohm	
Örebro University (Sweden)	Academic lab	Metrohm	

Example recruitment email sent to invite participant laboratories:

"Dr. XXX,

My name is Bridger and I am a PhD student in Dr. Elsie Sunderland's lab at Harvard University. Our group is trying to organize a lab inter-comparison on the use of CIC to characterize organofluorine in groundwater and biota. We are reaching out to you because XXX from XXX recommended your group.

We are in the early stages of planning and are currently trying to gauge interest from labs that use CIC for fluorine analyses. Would your group be interested in potentially participating in a lab inter-comparison this year?

Sincerely,
Bridger Ruyle"

Methods overview for groundwater and eel sent to participants:

For groundwater:

1. Shake groundwater and field blank stocks vigorously prior to subsampling 50 mL for each replicate. Additionally, sample 50 mL of laboratory deionized water (DI H_2O) for each extraction blank.
    a. For spiked samples, add appropriate PFAS or IF spikes to subsample
    b. For targeted analysis samples, add IS to subsample
2. Shake subsamples vigorously and let equilibrate overnight
3. Attach SPE cartridges to manifold and condition them with sequential additions of 4 mL of 0.1% NH_4OH in MeOH, 4 mL of MeOH, and 4 mL of DI H_2O

4. Shake subsample vigorously prior to loading all volume (50 mL) onto cartridge
5. After the sample has been extracted, rinse cartridge with 10 mL of 0.01% NH_4OH in DI H_2O to remove inorganic fluoride followed by a 4 mL DI H_2O rinse
6. Under vacuum, dry cartridge
7. Add labeled vials to manifold eluents to collect elution. Elute cartridge with sequential additions of 4 mL MeOH followed by 4 mL 0.1% NH_4OH in MeOH. Vortex sample
8. Blow down elution under gentle stream of nitrogen to dryness
9. Reconstitute sample in 1 mL of MeOH. Vortex sample and then heat reconstituted sample for 40 minutes at 40°C. Vortex sample again
10. For EOF samples only:
    a. Subsample 0.75 mL for duplicate injections on the CIC to measure EOF
    b. Make up the remaining 0.25 mL according to your lab's SOP for PFAS analysis on the LC-MS/MS including the addition of IS
11. For Targeted analysis samples only:
    a. Prepare the sample according to your lab's SOP for PFAS analysis on the LC-MS/MS

For eel:

1. Weigh out 1 g of wet weight homogenized fish tissue (frozen or partly thawed) into 15 mL polypropylene (PP) tubes and record exact mass of wet tissue.
2. If spiking with sodium fluoride (NaF, 100 ul of 10 mg/L), native PFAS standards (100 ul of 0.62 mM F), or internal standards (IS, your labs procedures), add spike and vortex samples, and let equilibrate for 30 mins.
3. For lab blanks, add 1 ml of DI H_2O to sample tube.
4. Add 4 mL acetonitrile (ACN) to samples, vortex and sonicate for 30 mins in a water bath.
5. Centrifuge samples for 10 mins at 4000 rpm. Decant supernatant to a new 15 mL PP tube.
6. Repeat the process a second time by adding another 4 mL of ACN to the initial homogenate, vortexing, sonicating, centrifuging, and transferring to the second PP tube, for a combined total of ~8 mL of ACN supernatant. Put extract in freezer (-20°C) for at least 4 hrs (or overnight) to allow lipids to precipitate out.
7. Remove samples from the freezer. If lipid precipitate is present centrifuge (under refrigeration if possible) for 2 mins at 4000 rpm and immediately decant to new 15 mL PP tube.
8. Evaporate extracts under nitrogen to just dryness and reconstitute in 1 ml LCMS-grade MeOH and vortex the reconstituted sample.
9. Weigh out 50 mg of loose dispersive ENVI-carb into a 1.7 mL microcentrifuge tube and add 100 µL glacial acetic acid. Decant the 1 mL extract into the microtube containing ENVI-carb. Vortex immediately for 10 seconds and centrifuge for 20 mins at 13000 rpm. *Note: If your lab has availability to ENVI-carb cartridges and those are preferred, your lab can use those cartridges instead.
10. From the centrifuged extract in ENVI-carb, pipette the desired amount of supernatant into additional vials for CIC and LC-MS/MS analysis, according to your lab's final extract prep procedures. (E.g.: 0.6 ml supernatant to CIC vial for EOF analysis, 0.3 ml to LC vial for LC-MS analysis, 0.1 mL leftover in ENVI-carb tube).
11. Spike the LC-MS/MS extract with IS (except the ones spiked at the beginning for targeted PFAS only) and dilute according to your own procedures prior to analysis.

Table S3. Composition of organofluorine PFAS spike[a]

PFAS	Concentration in fluorine equivalents [μg F L^{-1}]
PFBA	500
PFPeA	520
PFHxA	534
PFHpA	544
PFOA	552
PFNA	558
PFDA	563
PFUnDA	567
PFDoDA	570
PFTrDA	573
PFTeDA	576
FOSA	518
N-MeFOSAA	453
N-EtFOSAA	442
PFBS	405
PFPeS	450
ΣPFHxS[b]	452
PFHpS	482
ΣPFOS[b]	479
PFNS	505
PFDS	514
4:2 FTSA	391
6:2 FTSA	440
8:2 FTSA	471
Total	12059

[a]Spike is a 2.5x dilution in methanol of Wellington's PFAC-24PAR technical mixture
[b]Σ denotes the sum of linear and branched isomers

Groundwater extraction – specific lab protocols.

Lab 1:

Groundwater subsamples (50 mL) were extracted by solid phase extraction using Phenomenex PFAS WAX/GCB (6 mL, 200 mg/50 mg). The extraction included triplicates of un-spiked groundwater, groundwater spiked with sodium fluoride (2000 μg F L^{-1}), field blanks

consisting of deionized water pumped through the sampling equipment in the field prior to groundwater sample collection, and extraction blanks in deionized water. Spiked samples were left to equilibrate for 12 hr prior to extraction. The extraction was performed by preconditioning the cartridges with 4 mL 0.3% NH_4OH/MeOH + 4 mL MeOH + 5 mL Milli-Q water, loading the samples onto the cartridges, and rinsing the cartridges with 10 mL 0.03% NH_4OH in Milli-Q water + 4 mL Milli-Q water. Cartridges were then dried under vacuum for 30 minutes and eluted with 4 mL MeOH + 4 mL 0.3% NH_4OH/MeOH. Sample extracts were blown to dryness under nitrogen using an N-EVAP system at room temperature. Extracts were reconstituted in 1.5 mL methanol, vortexed for 1 min, and analyzed for EOF.

Lab 2:

Groundwater subsamples (50 mL) were extracted by solid phase extraction using Oasis WAX (6 mL, 150 mg, 30 μm). The extraction included triplicates of un-spiked groundwater, groundwater spiked with 50 uL of the supplied GW fluoride spike (1000 μg L^{-1}), groundwater spiked with 60 uL of the supplied PFAS spike (14.6 μg L^{-1}), field blanks consisting of deionized water pumped through the sampling equipment in the field prior to groundwater sample collection, and extraction blanks in deionized water. Samples were additionally spiked with internal standards prior to extraction totaling 0.02 ug L^{-1} which was roughly 0.2% of the measured EOF concentrations. Spiked samples were left to equilibrate for overnight at room temperature (>12 hrs) prior to extraction. The extraction was performed by preconditioning the cartridge with 4 mL 0.1% NH_4OH/MeOH + 4 mL MeOH + 4 mL Milli-Q water, loading the samples onto the cartridges (by gravity, ca. 1 drop per sec), and rinsing the cartridges with 10 mL 0.01% NH_4OH in Milli-Q water + 4 mL Milli-Q water. Cartridges were then dried under

maximum vacuum for approximately 5 minutes. 4 mL of methanol was added to each retained water sample bottle and used to vigorously rinse the inner walls of the bottle. The methanol rinsate was transferred to the corresponding SPE cartridges with a disposable transfer pipet and eluted by gravity into the SPE eluent collection tubes. Just before the methanol level in the SPE cartridges reached the sorbent bed 4 mL of 0.1% NH_4OH/MeOH was added to each SPE cartridge to continue the elution. Sample extracts were blown to dryness at 45 °C ± 10 °C under nitrogen using Thermo Scientific™ Reacti-Vap™ Evaporator. Extracts were reconstituted in 1 mL methanol, vortexed, heated at 40°C for 40 mins and then vortexed again, and split for EOF (0.82 mL) and LC-MS/MS (0.18 mL) analysis. For LC-MS/MS analysis, the split extract was mixed with 20 µL of injection internal standard solution containing 13C6-PFHxA and 13C9-PFDA, (Cambridge Isotope Laboratories) at 100 ng/mL each) and analyzed for mass balance comparison to EOF results.

Lab 3:

Groundwater subsamples (50 mL) were extracted by solid phase extraction using weak anion exchange cartridges (Phenomenex PWAX, 6cc, 150 mg). The extraction included triplicates of un-spiked groundwater, groundwater spiked with 100 µL of 1000 mg/L sodium fluoride (nominal concentration 2000 µg L^{-1} in sample), groundwater spiked with 100 µL of Wellington PFAC-24PAR PFAS mixture (provided; nominal concentration 24 µg L^{-1} in sample), field blanks consisting of deionized water pumped through the sampling equipment in the field prior to groundwater sample collection, and extraction blanks consisting of ultrapure water. Spiked samples were left to equilibrate for a minimum of 30 minutes prior to extraction.

Extraction was performed by preconditioning the cartridge with 5 mL 0.1% NH_4OH/MeOH, followed by 5 mL MeOH and 5 mL Milli-Q water. Samples were loaded under gravity, then rinsed with 10 mL 0.01% NH_4OH in Milli-Q water followed by 5 mL Milli-Q water. Cartridges were then dried under vacuum for a minimum of 30 minutes, or until friable. Cartridges were eluted with 4 mL MeOH followed by 4 mL 0.1% NH_4OH/MeOH. Extracts were reduced to near dryness (~20 µL) under a gentle stream of nitrogen using a Biotage TurboVap Evaporator Concentrator unit (10 psi, 40 °C). Extracts were reconstituted in 400 µL methanol:water (1:1) by vortexing for 30 sec. Extracts were split for EOF and LC-MS/MS analysis. For LC-MS/MS analysis 100 µL extract was fortified with 50 µL of a 10 µg/L PFAS Isotope Working internal standard mixture. For samples with PFAS concentration that exceeded the calibration range, extracts were diluted up to 50-fold with 20% methanol and re-analyzed.

Lab 4:

Groundwater subsamples (50 mL) were extracted by solid phase extraction using Oasis WAX (6 mL, 150 mg, 30 µm). The extraction included triplicates of un-spiked groundwater, groundwater spiked with sodium fluoride (2000 µg F L^{-1}), groundwater spiked with Wellington PFAC-24PAR PFAS mixture (24 µg F L^{-1}), field blanks consisting of deionized water pumped through the sampling equipment in the field prior to groundwater sample collection, and extraction blanks in deionized water. Spiked samples were left to equilibrate for 12 hr prior to extraction. The extraction was performed by preconditioning the cartridges with 4 mL 0.1% NH_4OH/MeOH + 4 mL MeOH + 4 mL Milli-Q water, loading the samples onto the cartridges, and rinsing the cartridges with 10 mL 0.01% NH_4OH in Milli-Q water + 4 mL Milli-Q water. Cartridges were then dried under vacuum for 30 minutes and eluted with 4 mL MeOH + 4 mL

0.1% NH_4OH/MeOH. Sample extracts were blown to dryness under nitrogen using an N-EVAP system. Extracts were reconstituted in 1 mL methanol, vortexed, heated at 40°C for 40 minutes, and split for EOF (0.75 mL) and LC-MS/MS (0.25 mL) analysis. For LC-MS/MS analysis, the split extract was mixed with 0.75 mL Milli-Q water, 0.46 mL MeOH, and 0.04 mL Wellington MPFAC-24ES isotopically-labeled PFAS mixture (0.03 ng μL^{-1}) and analyzed for mass balance comparison to EOF results.

Lab 5:

Groundwater subsamples (50 mL) were extracted by solid phase extraction using Oasis WAX (3 mL, 60 mg, 60 μm). The extraction included triplicates of un-spiked groundwater, groundwater spiked with sodium fluoride (2000 μg F L^{-1}), groundwater spiked with a PFAS mixture (24 μg F L^{-1}), field blanks consisting of deionized water pumped through the sampling equipment in the field prior to groundwater sample collection, and extraction blanks in deionized water. Spiked samples were left to equilibrate for 12 hr prior to extraction. The extraction was performed using an automated SPE system designed for PFAS analysis (Thermo Scientific, Dionex™ AutoTrace™ 280 PFAS) by preconditioning the cartridges with 2 mL 0.1% NH_4OH/MeOH + 2 mL MeOH + 2 mL Milli-Q water, loading the samples onto the cartridges, and rinsing the cartridges with 10 mL 0.01% NH_4OH in Milli-Q water + 4 mL Milli-Q water. Cartridges were then dried under vacuum for 30 minutes and eluted with 2 mL MeOH + 2 mL 0.1% NH_4OH/MeOH. Sample extracts were blown to dryness under nitrogen using a TurboVap LV evaporator (Biotage, Sweden). Extracts were reconstituted in 1 mL methanol, vortexed, heated at 40°C for 40 mins, and split for EOF (0.8 mL) and LC-MS/MS (0.2 mL) analysis. For LC-MS/MS analysis, the split extract was mixed with 1.77 mL Milli-Q water, 0.01 mL 1000 mM

ammonium acetate solution, and 0.02 mL Wellington MPFAC-24ES isotopically-labeled PFAS mixture (0.05 ng μL^{-1}) and analyzed for mass balance comparison to EOF results.

Lab 6:

Groundwater subsamples (50mL) were extracted by solid phase extraction using Oasis WAX (6 mL, 150 mg, 30 μm). The extraction included triplicates of un-spiked groundwater, groundwater spiked with sodium fluoride (2000 μg F L^{-1}) and field blanks consisting of deionized water pumped through the sampling equipment in the field prior to groundwater sample collection, and extraction blanks in deionized water. Spiked samples were left to equilibrate for 12 hr prior to extraction. The extraction was performed by preconditioning the cartridges with 4 mL 0.1% NH_4OH/MeOH + 4 mL MeOH + 4 mL Milli-Q water, loading the samples onto the cartridges, and rinsing the cartridges with 10 mL 0.01% NH_4OH in Milli-Q water + 4 mL Milli-Q water. Cartridges were then dried under vacuum for 15 minutes and eluted with 4 mL MeOH + 4 mL 0.1% NH_4OH/MeOH. Sample extracts were blown to dryness under nitrogen. Extracts were then reconstituted in 1 mL methanol and vortexed prior to EOF analysis.

Lab 7:

Groundwater subsamples (50 mL) were extracted by solid phase extraction using Oasis WAX (6 mL, 150 mg, 30 μm). The extraction included triplicates of un-spiked groundwater, groundwater spiked with sodium fluoride (2000 μg F L^{-1}), groundwater spiked with a PFAS mixture (24 μg F L^{-1}), field blanks consisting of deionized water pumped through the sampling equipment in the field prior to groundwater sample collection, and extraction blanks in laboratory-produced ultrapure water (18.2 MΩ). Spiked samples were vortex mixed and left to

equilibrate for 12 hr prior to extraction. The extraction was performed by preconditioning the cartridges with 4 mL 0.1% NH_4OH/MeOH + 4 mL MeOH + 4 mL ultrapure water, loading the samples onto the cartridges, and rinsing the cartridges with 10 mL 0.01% NH_4OH in ultrapure water + 4 mL ultrapure water. Cartridges were then dried under vacuum for 30 minutes, and centrifuged for 2 min at 3000 rpm, eluted with 4 mL MeOH + 4 mL 0.1% NH_4OH/MeOH. Sample extracts were blown to dryness under nitrogen using PIERCE Reacti-Term Heating module at a constant temperature at 30°C. Extracts were reconstituted in 1 mL methanol, vortexed, heated at 40°C for 40 mins, and split for EOF (0.25 mL) and LC-MS/MS (0.20 mL) analysis. For LC-MS/MS analysis, the split extract was mixed with 0.3 mL water phase (e.g. ultrapure water with 2 mM ammonium acetate and 0.01 mL Wellington isotopically-labeled PFAS mixture[1] (0.2 ng μL^{-1})] and analyzed for mass balance comparison to EOF results.

Eel extraction – specific lab protocols.

Lab 1:

Eel samples were provided as a composite of homogenized wet-weight whole body tissue. Eel subsamples (1 g) were extracted by solid-liquid extraction using acetonitrile. The extraction included triplicates of un-spiked eel, eel spiked with 100 µl of the provided fluoride standard, eel spiked with 100 µl of 0.62 mM F PFAS mixture, and extraction blanks in acetonitrile. Spiked samples were left to equilibrate for 1 hr prior to extraction. The extraction was performed by adding acetonitrile (4 mL), vortexing and sonicating for 30 mins, and centrifuging at 4000 rpm for 10 mins. The supernatant was decanted to a new 15 mL polypropylene (PP) tube and the extraction was repeated once, yielding a final extract volume of 8 mL. Extracts were frozen (-20°C) for 4 hours to allow for lipid precipitation, centrifuged at

4000 rpm for 2 mins and decanted to a new PP tube. Extracts were then blown to dryness under nitrogen using a nitrogen evaporation system (Cole-Parmer® SC-200 Sample Concentrator). Extracts were reconstituted in 1.5 mL methanol, vortexed, and then used for CIC analysis.

Lab 2:

Eel samples were provided as a composite of homogenized wet-weight whole body tissue. Eel subsamples (1 ± 0.1 g) were extracted by solid-liquid extraction using acetonitrile. The extraction included triplicates of un-spiked eel, eel spiked with 150 µL of fluoride spike (1500 µg kg^{-1}), eel spiked with 100 µL of PFAS spike (1200 µg kg^{-1}), and extraction blanks in acetonitrile. Samples were additionally spiked with internal standards prior to extraction totaling 0.07 ug kg^{-1} which was roughly 35% of the measured EOF concentrations if fully recovered. Spiked samples were not equilibrated prior to extraction. The extraction was performed by adding acetonitrile (4 mL), vortexing briefly, sonicating for 30 mins, and centrifuging at 4000 rpm for 10 mins. The supernatant was decanted to a new 15 mL polypropylene (PP) tube and the extraction was repeated once, yielding a final extract volume of 8 mL. Extracts were frozen (-20°C) for at least 4 hours to allow for lipid precipitation, centrifuged at 4000 rpm for 2 mins and decanted to a new PP tube. Extracts were then blown to dryness at 45 °C ± 10 °C under nitrogen using Thermo Scientific™ Reacti-Vap™ Evaporator. Extracts were reconstituted in 1 mL methanol, vortexed, and combined with dispersive ENVI-carb (50 mg) and glacial acetic acid (100 µL), vortexed immediately for 10 sec, centrifuged (20 min), and then split for EOF (0.82 mL) and LC-MS/MS (0.18 mL) analysis. For LC-MS/MS analysis, the split extract was mixed with 20 µL of injection internal standard solution containing 13C6-PFHxA and 13C9-PFDA

(Cambridge Isotope Laboratories at 100 ng/mL each) and analyzed for mass balance comparison to EOF results.

Lab 3:

Eel samples were provided as a composite of homogenized wet-weight whole body tissue. Eel subsamples (~1 g) were extracted by solid-liquid extraction using acetonitrile. Samples included triplicates of un-spiked eel, eel spiked with 100 µL of 10 mg/L sodium fluoride (nominal concentration of 1000 µg kg^{-1}), eel spiked with 100 µL of Wellington PFAC-24PAR PFAS mixture (nominal concentration 1200 µg kg^{-1}), and extraction blanks consisting of ultrapure water. Spiked samples were left to equilibrate for a minimum of 30 minutes prior to extraction.

Extraction was performed by adding 4 mL acetonitrile to each sample, vortexing for 60 sec, then centrifuging at 3500 rpm for 5 min. The supernatant was transferred with a pipette to a new 15 mL polypropylene (PP) tube. The extraction was repeated with a second aliquot of acetonitrile (4 mL) and the supernatant combined for a final extract volume of 8 mL. Extracts were frozen (-18°C) for >8 hours to allow for lipid precipitation, centrifuged at 3500 rpm for 2 mins, and the supernatant transferred to a new PP tube. The extract was cleaned up using Bond Elut Carbon cartridges (250mg, 6cc; Agilent Technologies) preconditioned with acetonitrile and ultrapure water. Extracts were reduced to near dryness (~20 µL) under a gentle stream of nitrogen using a Biotage TurboVap Evaporator Concentrator unit (10 psi, 40 °C). Extracts were reconstituted in 400 µL methanol:water (1:1) by vortexing for 30 sec. Extracts were split for EOF and LC-MS/MS analysis. For LC-MS/MS analysis, 100 µL extract was fortified with 50 µL of a 10 µg/L PFAS Isotope Working internal standard mixture. For samples with PFAS

concentration that exceeded the calibration range, extracts were diluted up to 50-fold with 20% methanol and re-analyzed.

Lab 4:

Eel samples were provided as a composite of homogenized wet-weight whole body tissue. Eel subsamples (1 g) were extracted by solid-liquid extraction using acetonitrile. The extraction included triplicates of un-spiked eel, eel spiked with sodium fluoride (1000 μg F kg^{-1}), eel spiked with Wellington PFAC-24PAR PFAS mixture (1200 μg F kg^{-1}), and extraction blanks in acetonitrile. Spiked samples were left to equilibrate for 30 minutes prior to extraction. The extraction was performed by adding acetonitrile (4 mL), and vortexing, sonicating for 30 mins, and centrifuging at 4000 rpm for 10 mins. The supernatant was decanted to a new 15 mL PP tube and the extraction was repeated once yielding a final extract volume of 8 mL. Extracts were frozen (-20°C) for 12 hr to allow for lipid precipitation, centrifuged at 4000 rpm for 2 mins and decanted to a new PP tube. Extracts were then blown to dryness under nitrogen using an N-EVAP system. Extracts were reconstituted in 1 mL methanol, vortexed, and combined with dispersive ENVI-carb (50 mg) and glacial acetic acid (100 μL), vortexed, centrifuged, and then split for EOF (0.6 mL) and LC-MS/MS (0.3 mL) analysis. For LC-MS/MS analysis, the split extract was mixed with 0.75 mL Milli-Q water, 0.41 mL MeOH, and 0.04 mL Wellington MPFAC-24ES isotopically-labeled PFAS mixture (0.03 ng μL^{-1}) and analyzed for mass balance comparison to EOF results.

Lab 5:

Eel samples were provided as a composite of homogenized wet-weight whole body tissue. Eel subsamples (1 g) were extracted by solid-liquid extraction using acetonitrile. The extraction included triplicates of un-spiked eel, eel spiked with sodium fluoride (1000 μg F kg^{-1}), eel spiked with a PFAS mixture (1200 μg F kg^{-1}), and extraction blanks in acetonitrile. Spiked samples were left to equilibrate for 30 minutes prior to extraction. The extraction was performed by adding acetonitrile (4 mL), and vortexing, sonicating for 30 mins, and centrifuging at 4000 rpm for 10 mins. The supernatant was decanted to a new 15 mL PP tube and the extraction was repeated once, yielding a final extract volume of 8 mL. Extracts were frozen (-20°C) for 12 hr to allow for lipid precipitation, centrifuged at 4000 rpm for 2 mins and decanted to a new PP tube. Extracts were then blown to dryness under nitrogen using a TurboVap LV evaporator (Biotage, Sweden). Extracts were reconstituted in 1 mL methanol, vortexed, and passed through 1 mL ENVI-carb (100 mg) cartridges, and then split for EOF (0.6 mL) and LC-MS/MS (0.3 mL) analysis. For LC-MS/MS analysis, the split extract was mixed with 2.665 mL Milli-Q water, 0.015 mL 1000 mM ammonium acetate solution, and 0.02 mL Wellington MPFAC-24ES isotopically-labeled PFAS mixture (0.05 ng μL^{-1}) and analyzed for mass balance comparison to EOF results.

Lab 6:

Eel samples were provided as a composite of homogenized wet-weight whole body tissue. Eel subsamples (1 g) were extracted by solid-liquid extraction using acetonitrile. The extraction included triplicates of un-spiked eel, eel spiked with sodium fluoride (1000 μg F kg^{-1}) and extraction blanks in acetonitrile. Spiked samples were left to equilibrate for 30 minutes prior

to extraction. The extraction was performed by adding acetonitrile (4 mL), and vortexing, sonicating for 30 mins, and centrifuging at 4000 rpm for 10 mins. The supernatant was decanted to a new 15 mL PP tube and the extraction was repeated once, yielding a final extract volume of 8 mL. Extracts were frozen (-20°C) for 12 hr to allow for lipid precipitation, centrifuged at 4000 rpm for 2 mins and decanted to a new PP tube. Extracts were then blown to dryness under nitrogen. Extracts were reconstituted in 1 mL methanol, vortexed, and combined with dispersive ENVI-carb (50 mg) and glacial acetic acid (100 μL), vortexed, and centrifuged prior to EOF determination.

Lab 7:

Eel samples were provided as a composite of homogenized wet-weight whole body tissue. Eel subsamples (1 g) were extracted by solid-liquid extraction using acetonitrile. The extraction included triplicates of un-spiked eel, eel spiked with sodium fluoride (1000 μg F kg^{-1}), eel spiked with a PFAS mixture (1200 μg F kg^{-1}), and extraction blanks in acetonitrile. Spiked samples were vortex mixed and left to equilibrate for 30 minutes prior to extraction. The extraction was performed by adding acetonitrile (4 mL), and vortexing, sonicating for 30 mins, and centrifuging at 4000 rpm for 10 mins. The supernatant was decanted to a new 15 mL PP tube and the extraction was repeated once yielding a final extract volume of 8 mL. Extracts were frozen (-20°C) for 12 hr to allow for lipid precipitation, centrifuged at 4000 rpm for 2 mins and decanted to a new PP tube. Extracts were then blown to dryness under nitrogen using a PIERCE Reacti-Term Heating module at a constant temperature at 30°C. Extracts were reconstituted in 1 mL methanol, vortexed, and purified with by using graphitized carbon SPE columns (100 mg, 1 mL, Supelclean™ ENVI-Carb ™). The ENVI-Carb ™ SPE cartridges were conditioned with 4

mL MeOH before the sample extract was loaded on the cartridge and collected, and then blown to 1 mL under nitrogen. The extracts were then split for EOF (0.25 mL) and LC-MS/MS (0.2 mL) analysis. For LC-MS/MS analysis, the split extract was mixed with 0.3 mL water phase (e.g. ultrapure water with 2 mM ammonium acetate and 0.01 mL Wellington isotopically-labeled PFAS mixture[1] (0.2 ng μL^{-1})] and analyzed for mass balance comparison to EOF results.

EOF determination.

Lab 1:

Extracts were analyzed for EOF using a 1-Enviroscience CIC with AQF-2100H combustion unit combined with an ASC-240s ceramic boat autosampler from Mitsubishi (Mitsubishi Chemical Analytech, Tokyo, Japan), GA-210 Absorber Module, and IC; ICS Integrion, Thermo Fisher Scientific GmbH (Dreieich, Germany). Aliquots of 500 μL were combusted in ceramic boats for 860 seconds at 1050°C. A steady supply of oxygen (300 mL min^{-1}) and argon (150 mL min^{-1}) were supplied to the combustion chamber (water supply level 2). The combusted fluorine was absorbed in ~11 mL deionized water including internal standards and transferred to the IC. The IC was operated with a mobile phase consisting of gradient potassium hydroxide (KOH) and pumped at a flowrate of 0.25 mL min^{-1}. The IC was equipped with AG20 2x50mm guard column guard column and Dionex IonPac AS20 2x250mm column at 30°C. The height of the fluorine peak was measured using a conductivity detector.

Measured fluorine peak areas were corrected by subtracting the average peak area of empty boat blanks analyzed during the run. Concentrations of EOF were determined from the area of the fluorine peak using an eleven-point calibration curve from 1.0 to 20.0 μg F L^{-1} as

aqueous NH_4F solution ($R^2 > 0.997$). Two calibration quality control samples were run throughout the worklist and were within ±10% of the nominal concentration.

The detection limits were instrumental limits of detection (LOD) based on blank combustions of different ceramic boats. The detection limit was calculated according to DIN 32645.[1] Ten repeated measurements of ten different blank samples (empty sample boats) were conducted. Subsequently, the standard deviation (SD) was calculated, divided by the slope of the calibration curve (1-20 μg F L^{-1}) and multiplied by 3, resulting in the instrumental LOD value.

Lab 2:

Extracts were analyzed for EOF using Mitsubishi Chemical Analytech Adsorption Unit Model TXA-04 and a Mitsubishi Chemical Analytech Automatic Combustion Unit Model AQF-2100H system, including Ceramic Boat Autosampler- ASC 240 S, Horizontal Furnace Model HF-210 and Gas Absorbtion Unit GA-211. Aliquots of 100 μL were combusted in ceramic boats for 50 min at 1000°C. A steady supply of oxygen (300 mL min^{-1}) and argon (100 mL min^{-1}) were supplied to the combustion chamber. The combusted fluorine was absorbed in 10 mL deionized water and transferred to the IC Thermo Scientific Dionex Integration HPIC system with Chromeleon software. The IC was operated with a mobile phase consisting of 2 mM to 100 mM KOH 30 min gradient and pumped at a flowrate of 0.25 mL min^{-1}. The IC was equipped with Dionex IonPac AG20 (2 × 50 mm) guard column and Dionex IonPac AS20 (2 × 250 mm) analytical column at 30°C. The height of the fluorine peak was measured using a conductivity detector.

Measured fluorine peak areas were corrected by subtracting the peak area of empty boat blanks that were injected immediately before or after the extract. Concentrations of EOF were

determined from the area of fluorine peak using a 8-point quadratic calibration curve from 0.2 ug to 50 ug as fluoride (Fluoride Primary Standard, 1,000 ppm F-, 500 mL, Fisher (P/N 3173-6) (coefficient of determination $R \geq 0.99$). One calibration quality control sample was run at the beginning and after every 20 samples for each worklist and were within ±20% of mid-level calibration standard. The Limits of Quantification and Detection respectively were 20 and 10 ug/L for groundwater and 1.0 and 0.5 ug/g wet weight tissue. The Limits of Quantification and Detection were calculated according to TNI standard 2009.

Lab 3:

Extracts were analyzed for EOF using Metrohm CIC with combustion unit from Analytik Jena (Jena, Germany), 920 Absorber Module, and 930 Compact IC Flex from Metrohm (Herisau, Switzerland). Aliquots of 200 µL were loaded manually into quartz boats containing a small plug of quartz wool. Boats were combusted for 7.5 minutes (nested) at 1050°C. A steady supply of oxygen (300 mL min^{-1}) and argon (100 mL min^{-1}) were supplied to the combustion chamber. The combusted fluorine was absorbed in 5.345 mL deionized water and transferred to the IC. The IC was operated with a mobile phase consisting of 3.2 mM sodium bicarbonate + 1 mM sodium carbonate and pumped at a flowrate of 0.7 mL min^{-1}. The IC was equipped with Metrosep A Supp 5 Guard/4.0 guard column and Metrosep A Supp 5-150/4 column at 26°C. The height of the fluorine peak was measured using a conductivity detector.

Concentrations of EOF were determined from the height of fluorine peak using a 7-point calibration curve from 0.013 to 1 µg L^{-1} as sodium fluoride ($R^2 > 0.99$). A continuing calibration verification standard was run once every 10 samples, with acceptance criteria ±20% of the nominal concentration. Reporting limits for all matrices were determined by the instrument

detection limit, determined by the lowest calibration standard, equivalent to 20 μg/mL on column.

Lab 4:

Extracts were analyzed for EOF using a Metrohm CIC with combustion unit from Analytik Jena (Jena, Germany), and 920 Absorber Module and 930 Compact IC Flex from Metrohm (Herisau, Switzerland). Aliquots of 100 μL were combusted in ceramic boats for 360 seconds at 1050°C. A steady supply of oxygen (300 mL min^{-1}) and argon (100 mL min^{-1}) were supplied to the combustion chamber. The combusted fluorine was absorbed in 9.7 mL deionized water and transferred to the IC. The IC was operated with a mobile phase consisting of 3.2 mM sodium bicarbonate/1 mM sodium carbonate and pumped at a flowrate of 0.7 mL min^{-1}. The IC was equipped with Metrosep A Supp 5 Guard/4.0 guard column and Metrosep A Supp 5-150/4 column at 30°C. The height of the fluorine peak was measured using a conductivity detector.

Measured fluorine peak areas were corrected by subtracting the peak area of empty boat blanks that were injected immediately before or after the sample extract. Concentrations of EOF were determined from the height of fluorine peak using a 9-point calibration curve from 50 to 10000 μg F L^{-1} as PFOA in methanol ($R^2 > 0.99$). Four calibration quality control samples were run throughout the worklist and were within ±15% of the nominal concentration.

The detection limits were between 1.5 and 2.2 μg F L^{-1} for groundwater and 18.6 μg F g^{-1} for eel. The detection limit represents the method detection limit (MDL) and was calculated as the average plus three times the standard deviation of the extraction blanks multiplied by the dilution factor.

Lab 5:

Extracts were analyzed for EOF using a CIC system with a Thermo Scientific™ Dionex™ Integrion™ HPIC™ system and a Nittoseiko AQF-2100H combustion system. Aliquots of 100 μL were combusted in ceramic boats for 180 seconds at 900 °C (Outlet temp: 1075°C). A steady supply of oxygen (400 mL min^{-1}) and argon (200 mL min^{-1}) were supplied to the combustion chamber. The combusted fluorine was absorbed in 10.295 mL deionized water and transferred to the IC. The IC was operated with a mobile phase consisting of a KOH (Thermo Scientific™) gradient starting at 3 mM for 3 min, increasing to 50 mM over a 9 min period, and held at 50 mM for 3 min before re-equilibrating to 3 mM KOH for 5 min. The flow rate was 0.25 mL min^{-1}. The IC was equipped with Thermo Dionex IonPac AS18 (2 x 250 mm) with AS18 guard column at 35°C. The height of the fluorine peak was measured using a conductivity detector.

Measured fluorine peak areas were corrected by subtracting the peak area of empty boat blanks that were injected immediately before or after the sample extract. Concentrations of EOF were determined from the height of fluorine peak using a 12-point calibration curve from 25 to 3000 μg F L^{-1} as a mixture of 13 PFAS in methanol ($R^2 > 0.99$). Ten calibration quality control samples (at 250 μg F L^{-1}) were run throughout the worklist and were on average within ±30% of the nominal concentration.

The detection limits were 0.5 μg F L^{-1} for groundwater and 0.025 μg F g^{-1} for eel. The detection limit represents the method reporting limit (MRL) and was calculated from the lowest calibration point (25 μg F L^{-1}) of the applied calibration curve.

Lab 6:

Extracts were analyzed for EOF using a Metrohm CIC with combustion unit from Analytik Jena (Jena, Germany), and 920 Absorber Module and 930 Compact IC Flex from Metrohm (Herisau, Switzerland). Aliquots of 100 μL were combusted in quartz boats for 360 seconds at 1050°C. A steady supply of oxygen (300 mL min^{-1}) and argon (100 mL min^{-1}) were supplied to the combustion chamber. The combusted fluorine was absorbed in 9.7 mL deionized water and transferred to the IC. The IC was operated with a mobile phase consisting of 3.2 mM sodium bicarbonate/1 mM sodium carbonate and pumped at a flowrate of 0.7 mL min^{-1}. The IC was equipped with a Metrosep A Supp 5 Guard/4.0 guard column and a Metrosep A Supp 5-150/4 column at 30°C. The area of the fluorine peak was measured using a conductivity detector.

Measured fluorine peak areas were corrected by subtracting the peak area of empty boat blanks that were injected immediately before or after the extract. Concentrations of EOF were determined from the area of fluorine peak using a seven-point calibration curve from 50 to 2000 μg F L^{-1} as PFOA in methanol ($R^2 > 0.99$). Calibration quality control samples were run throughout the worklist and were within ±15% of the nominal concentration.

The detection limits were between 0.7 and 1.0 μg F L^{-1} for groundwater and 0.06 μg F g^{-1} for eel. The detection limit represents the MDL and was calculated as the average plus three times the standard deviation of the extraction blanks multiplied by the dilution factor.

Lab 7:

Extracts were analyzed for EOF using a Metrohm CIC with combustion unit from Analytik Jena (Jena, Germany), and 920 Absorber Module and 930 Compact IC Flex from Metrohm (Herisau, Switzerland). Aliquots of 50 μL were combusted in quartz glass boats

monitored by a flame sensor (combustion time for all samples 6.7 min) at 1050°C. A steady supply of oxygen (300 mL min^{-1}) and argon (100 mL min^{-1}) were supplied to the combustion chamber. The combusted fluorine was absorbed in approximately 4.9 mL ultrapure water (range 4.8 to 5.7 mL) and then 2000 µL of the absorbed solution was transferred onto a trap column before being transferred to the IC. The IC was operated with a mobile phase consisting of 64 mM sodium carbonate and 20 mM sodium bicarbonate and pumped at a flowrate of 0.7 mL min^{-1}. The IC was equipped with Metrosep A Supp 5-150/4 column. The height of the fluorine peak was measured using a conductivity detector.

Measured fluorine peak areas were corrected by subtracting the peak area of empty boat blanks that were injected immediately before or after the sample extract. Concentrations of EOF were determined from the height of fluorine peak using a six-point calibration curve from 50 to 2000 µg F L^{-1} as PFOA in methanol ($R^2 > 0.99$). The 19 calibration quality control samples were run throughout the worklist and were within ±10% of the nominal concentration.

The detection limits were 1000 ng F L^{-1} for groundwater and 50 ng F g^{-1} for eel. The detection limit represents the MRL and was determined as the lowest point of a seven-point calibration.

Table S4. EOF results in groundwater

See accompanying Excel

Table S5. PFAS results in groundwater

See accompanying Excel

Table S6. EOF results in eel

See accompanying Excel

Table S7. PFAS results in eel

See accompanying Excel

Quality Control.

Inorganic fluorine removal:

$$\text{Equation S1:} \quad f_{removal} = 1 - \frac{C_{meas,fluoride\ spike} - C_{meas,unspiked}}{C_{fluoride\ spike}}$$

Where $f_{removal}$ is the fractional removal of the inorganic fluorine spike, $C_{meas,fluoride\ spike}$ is the measured fluorine concentration in the fluoride-spiked extract, $C_{meas,unspiked}$ is the measured fluorine concentration in the unspiked extract, and $C_{fluoride\ spike}$ is the nominal concentration of the fluoride spike (2000 μg F L^{-1} in groundwater and 1200 μg F kg^{-1} in eel).

Organofluorine recovery:

$$\text{Equation S2:} \quad f_{recovery} = \frac{C_{meas,PFAS\ spike} - C_{meas,unspiked}}{C_{PFAS\ spike}}$$

Where $f_{recovery}$ is the fractional recovery of the PFAS spike, $C_{meas,PFAS\ spike}$ is the measured fluorine concentration in the PFAS-spiked extract, $C_{meas,unspiked}$ is the measured fluorine concentration in the unspiked extract, and $C_{PFAS\ spike}$ is the concentration of the PFAS spike (Figure S1).

Evaluation of PFAS extraction losses:

$$\text{Equation S3:} \quad f_{loss} = \frac{C_{EOF} - C_{targeted}}{C_{targeted}}$$

Where f_{loss} is the fractional loss of PFAS due to extraction, C_{EOF} is the concentration of PFAS in the EOF extract (internal standard added after extraction), and $C_{targeted}$ is the concentration of PFAS in the targeted extract (internal standard added before extraction).

Data and statistical analyses.

When adding or subtracting two numbers A and B with standard deviations of σ_A and σ_B to obtain a new value of C, the standard deviation σ_C was calculated as:

$$\text{Equation S4:} \quad \sigma_C = \sqrt{\sigma_A^2 + \sigma_B^2}$$

When multiplying or dividing two numbers A and B with standard deviations of σ_A and σ_B to obtain a new value of C, the standard deviation σ_C was calculated as:

$$\text{Equation S5:} \quad \sigma_C = |C|\sqrt{\left(\frac{\sigma_A}{A}\right)^2 + \left(\frac{\sigma_B}{B}\right)^2}$$

PFAS concentrations in ng L^{-1} (C_{PFAS}) were converted to fluorine equivalents in ng F L^{-1} (C_F) as:

$$\text{Equation S6:} \quad C_F = 19\frac{C_{PFAS}n_F}{MW}$$

where n_F is the number of fluorine's per molecule and MW is the molecular weight. To obtain the concentration of all PFAS in fluorine equivalents, C_F is summed across all targeted analytes.

Interlaboratory averages in EOF concentrations (Figure 2) and the fraction of PFAS-quantified EOF (Figure 5) were calculated from the measured data using Markov chain Monte Carlo (MCMC) analysis:

$$\text{Equation S7:} \quad P(k|X) \propto P(X|k) \times P(k)$$

Where P(k|X) is the posterior probability distribution of the interlaboratory average, P(X|k) is the likelihood equation, and P(k) is the prior. A uniform prior with bounds [0,∞) and normal likelihood function were used.

MCMC analysis was performed using *emcee* version 3.1.1 with eight independently seeded walkers that update their sampling location according to the Gaussian algorithm.[2] The

analyses were run until the MCMC error was $2500^{-0.5}$. We present results for the expected mean and standard deviation throughout the manuscript.

Supplementary Results

Table S8. Intra-laboratory precision

	Groundwater		Eel	
Lab	Average extract COV [%]	Replicate percent difference [%]	Average extract COV [%]	Replicate percent difference [%]
1	35	NA[a] 113 NA[a]	27	150 NA[a] NA[a]
2	2	2 3 3	18	9 24 108
3	16	–[b]	14	–[b]
4	7	3 11 9	3	5 6 5
5	22	122 14 159	6	16 3 17
6	3	2 6 7	18	14 4 7
7	33	18 NA[a] 131	21	10 4 8

[a]One or both replicates were above detection limit
[b]Only one sample injection per extract was performed

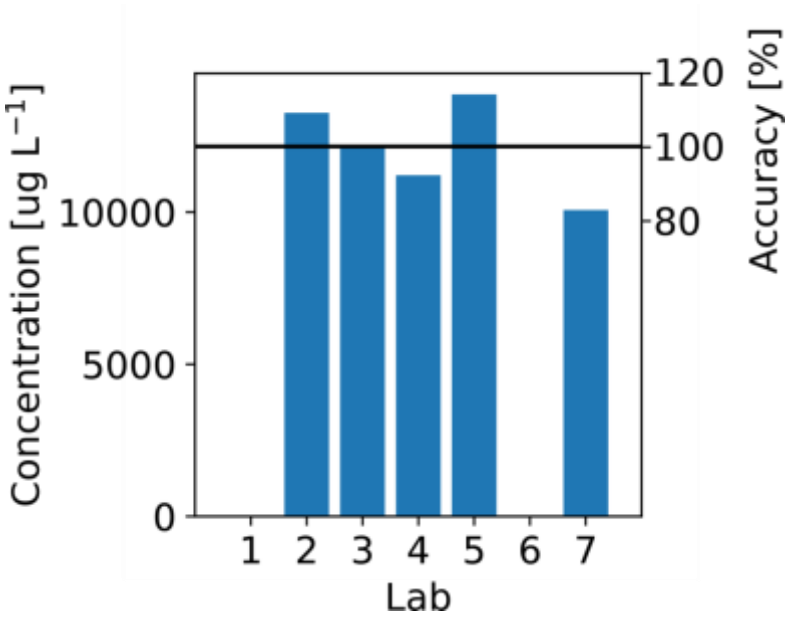

Figure S1. Measured PFAS mixture spike concentration

Table S9. Fluorine recovery of a PFAS mixture in groundwater and eel[a]

Lab	Groundwater fluorine recovery (μ±σ) [%]	Eel fluorine recovery (μ±σ) [%]
1	NR[b]	NR[b]
2	94±8	64±14
3	83±5	67±12
4	77±6	79±4
5	119±20	106±16
6	NR[b]	NR[b]
7	78±60	104±28

[a]Calculated from the average and standard deviation of all injections from a lab
[b]Spike not reported (NR) because it was either not performed or not measured

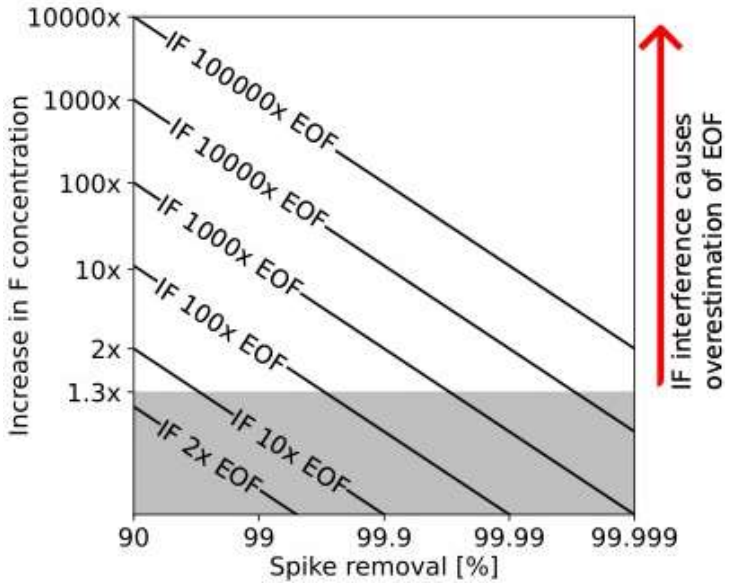

Figure S2. Increase in fluorine (F) concentration due to incomplete removal of the inorganic fluorine (IF) fraction. Lines represent different scenarios where IF exceeds organofluorine (EOF) by a factor of 2 to 100,000. The gray shaded area represents conditions in which the residual IF increases F concentrations by no more than 30%. The white area represents conditions in which the residual IF increases F concentrations by more than 30% resulting in an overestimation of EOF concentrations.

Table S10. Fluoride spike removal per lab

Lab	Groundwater				Eel			
	Spike removal [%]		Interference due to residual IF [%]		Spike removal [%]		Interference due to residual IF [%]	
	Mean	Standard deviation	Mean	Standard deviation	Mean	Standard deviation	Mean	Standard deviation
1	99.86	0.27	47	100	110.29	6.54	0	72
2	99.89	0.16	10	15	88.87	8.98	83	76
3	99.46	0.98	210	380	102.24	2.30	0	15
4	99.95	0.03	14	9	97.91	2.66	13	16
5	99.23	0.48	250	210	92.43	7.38	19	19
6	100.19	0.04	0	6	108.23	4.34	0	22
7	100.05	0.38	0	42	61.32	20.48	45	25

Table S11. EOF composition in groundwater

See accompanying Excel

Table S12. EOF composition in eel

See accompanying Excel

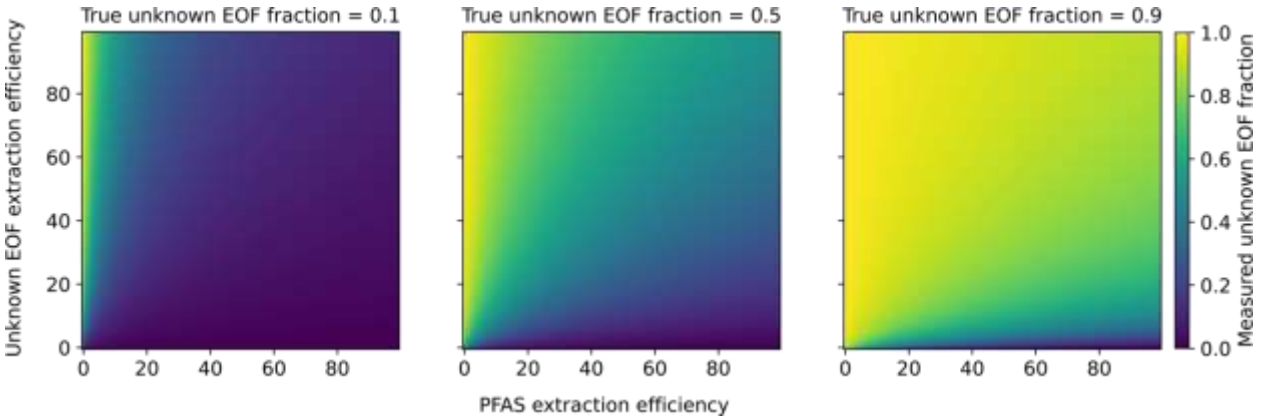

Figure S3. Effect of extraction efficiency on measured unknown EOF fraction for three scenarios.

Table S13. Percent loss of PFAS due to extraction

See accompanying Excel

EOF Data Evaluation Checklist

Extraction and analysis

☐ Are concentrations of PFAS reported along with EOF data?

☐ Are concentrations of inorganic fluorine reported along with EOF data?

☐ Have the precision of replicate extractions and instrumental injections been evaluated?

Notes:

QA/QC

☐ Does the chosen extraction method demonstrate adequate recovery of representative PFAS?

☐ Does the chosen extraction method demonstrate adequate removal of inorganic fluorine?

☐ Are PFAS with internal standard added before and after extraction to compared to quantify extraction efficiency

☐ Are concentrations from extraction and field blanks presented?

Notes:

Quantification and data processing

☐ Has any instrumental background contamination been subtracted from the reported concentration?

☐ Has any extraction/field blank contamination been subtracted from the reported concentration?

☐ Has the chosen detection limit been explained and is it appropriate for the presented data?

☐ Are PFAS concentrations compared to EOF concentrations from the same split extract?

Notes:

References

(1) DIN 32645:2008-11 Chemical Analysis - Decision Limit, Detection Limit and Determination Limit under Repeatability Conditions - Terms, Methods, Evaluation, 2008. https://dx.doi.org/10.31030/1465413.
(2) Foreman-Mackey, D.; Hogg, D. W.; Lang, D.; Goodman, J. Emcee: The MCMC Hammer. *arXiv:1202.3665 [astro-ph, physics:physics, stat]* **2013**. https://doi.org/10.1086/670067.