Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

A Field-Validated Equilibrium Passive Sampler for the Monitoring of Per- and Polyfluoroalkyl Substances (PFAS) in Sediment Pore Water and Surface Water

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SUPPORTING INFORMATION

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Section S1. The derivation of equations (1) and (2) in the main document

The migration of PFAS analytes from the solution in the jar to the receiving solution of the passive sampler is driven by the concentration gradient. As such, the increase of the concentration *Cs(t)* in the receiving solution over time can be described according to the following equation:

$$\frac{V_s dC_{s(t)}}{dt} = -k_{PFAS} \times A \times (C_{s(t)} - C_{j(t)})$$

where V_s represent the volume of the receiving solution, $C_s(t)$ is the concentration of the analyte (PFAS) in the receiving solution at time *t*, k_{PFAS} is the nass transfer coefficient, and A is the area of the sampling window. Meanwhile, the concentration *Cj(t)* of the analyte in the jar decreases over time. The change in $C_{j(t)}$ as a function of time can be described via the following equation:

$$\frac{V_j dC_{j(t)}}{dt} = -k_{PFAS} \times A \times (C_{j(t)} - C_{s(t)})$$

Solving the two non-linear differential equations above results in equation (1) which was presented in the main text.

Similarly, equation (2) in the main text, which describes the change in the PRC concentration in the receiving solution, can be derived by solving the following equations:

$$\frac{V_s dC_{PRC(t)}}{dt} = -k_{PRC} \times A \times (C_{PRC(t)} - C_{j,\,PRC(t)})$$

$$\frac{V_j dC_{j,\,PRC(t)}}{dt} = -k_{PRC} \times A \times (C_{j,PRC(t)} - C_{\,PRC(t)})$$

Section S2. Measuring diffusion coefficient *D* of PFPeS and PFDA using ^{19}F Diffusion Ordered Spectroscopy (DOSY)

For the measurement of *D*, a single-compound solution of either PFPeS and PFDA was prepared in deuterated water (D_2O) at a concentration 12.0 mg/mL (PFPeS) and 10.0 mg/mL (PFDA). After preparation, samples were place in 5 mm NMR tubes. NMR spectra of PFAS compounds were acquired on an Oxford O500 NMR spectrometer with a OneReynolds probe tuned to fluorine at 470.3 MHz. The OneReynolds probe can generate a maximum field gradient of 60 G/cm. The calibrated fluorine pulse width at 90 degrees was 11.2 µs and the T1 relaxation times for all compounds were measured with the longest T1 being 2.274s. A total relaxation delay of 12.5 seconds was used for all measurements to ensure complete relaxation of all nuclei between pulses. 1D ^{19}F NMR spectra were acquired for all compounds to validate their concentration was acceptable and to confirm purity of at least 95%. NMR parameters for the acquisition of the 1D spectra included a spectral width of 70 – 135 ppm, an acquisition time of 4s, a relaxation delay (d1) of 8.5s, number of transients (scans) between 4 or 64 (concentration dependent) and number of steady states being 4.

Diffusion ordered spectroscopy (DOSY) was completed for all compounds using two modified Oneshot pulse sequences,[7] where the final 45-degree pulse was removed to allow for addition signal-to-noise recovery. The DOSY experiment was performed at a spectral window of -75 - -80 ppm to measure the alkyl CF_3 fluroines, and again between -116 and -128 ppm to measure the remainder of the perfluorinated chain. The magnetic gradient ranged from 5.22 G/cm to 48.8 G/cm. The diffusion delay was set to 200 ms and the gradient was applied for 2 ms with a spectral width identical to the 1D spectra. The calibrated 90-degree pulse width of 11.2 µs was used with an acquisition time of 4.5 s, a relaxation delay of 8.25 s and the told number of scans of 4 or 64 depending on analyte concentration.

The most prominent resonance ^{19}F resonance from all PFAS (terminal CF_3 group) at -80.96 ppm was used to estimate *D* from the DOSY as it provides the highest confidence in diffusion measurement owing to it relatively higher intensity and limited susceptibility to phase twisting during the measurement.

Table S1. Diffusion coefficients of PFAS compounds, $C_8H_{17}SO_3^-$, and Br^-

Compound	Diffusion coefficients (cm^2/s) @ 25°C	Reference
PFBA	2.50×10^{-5}	1
PFPeA	1.20×10^{-5}	1
PFHxA	7.80×10^{-6}	1
PFHpA	7.30×10^{-5}	2
PFOA	4.90×10^{-6}	3
PFNA	4.60×10^{-6}	2
PFDA	2.74×10^{-6}	Measured in this study by ^{19}F NMR
PFBS	1.10×10^{-5}	1
PFPeS	5.32×10^{-6}	Measured in this study by ^{19}F NMR
PFHxS	4.50×10^{-6}	1
PFHpS	6.40×10^{-6}	1
PFOS	5.40×10^{-6}	1
6:2 FTS	4.16×10^{-5}	4
M_3PFPeA	1.20×10^{-5}	Assumed to be similar to PFPeA
M_2PFOA	4.90×10^{-6}	Assumed to be similar to PFOA
M_8PFOA	4.90×10^{-6}	Assumed to be similar to PFOA
M_4PFOS	5.40×10^{-6}	Assumed to be similar to PFOS
$C_8H_{17}SO_3^-$	4.30×10^{-6}	5
Br^-	2.01×10^{-5}	6

Table S2. The concentration of PFAS in a lake-water sample collected at Location A in November 2020.

Compounds	(ng/L)
PFBA	21
PFPeA	98
PFHxA	56
PFHpA	24
PFOA	9
PFNA	2
PFDA	ND
PFUdA	ND
PFDoA	ND
PFTrDA	ND
PFTeDA	ND
PFBS	7
PFPeS	6
PFHxS	63
PFHpS	<0.4
PFOS	32
PFNS	ND
PFDS	ND
4:2 FTS	ND
6:2 FTS	5
8:2 FTS	ND
FOSA	ND
MeFOSAA	ND
EtFOSAA	ND

Table S3. The number and type of passive sampler deployed at Lake Niapenco.

October 2021

Location	Sampled medium	Membrane type	PRCs	# of samplers
A	Pore water	Polycarbonate	Br^-, M_3PFPeA, M_2PFOA, M_4PFOS	32
A	Surface water			16
B	Pore water			16
B	Surface water			16
C	Pore water			16
C	Surface water			16
D	Pore water			16
D	Surface water			16

June 2022

Location	Sampled medium	Membrane type	PRCs	# of samplers
A	Pore water	Polycarbonate	M_8PFOA, $C_8H_{17}SO_3^-$	32
A	Surface water	Polycarbonate		4
B	Pore water	Polycarbonate		4
B	Surface water	Polycarbonate		4

Table S4. The concentration of detected PFAS in sediment in October – November 2021.

Analyte	Location A (t = 0 day) Result (ng/kg)	Location B (t = 0 day) Result (ng/kg)	Location C (t = 0 day) Result (ng/kg)	Location D (t = 0 day) Result (ng/kg)	Location A (t = 46 day) Result (ng/kg)	Location B (t = 46 day) Result (ng/kg)	Location C (t = 46 day) Result (ng/kg)	Location D (t = 46 day) Result (ng/kg)	Method detection limit (MDL) (ng/kg)
4:2 Fluorotelomer sulfonic acid (4:2 FTS)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
6:2 Fluorotelomer sulfonic acid (6:2 FTS)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
8:2 Fluorotelomer sulfonic acid (8:2 FTS)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
Perfluorobutanesulfonic acid (PFBS)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
Perfluorobutanoic acid (PFBA)	120	110	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
Perfluorodecanoic acid (PFDA)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
Perfluorododecanoic acid (PFDoA)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
Perfluoroheptanesulfonic Acid (PFHpS)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
Perfluoroheptanoic acid (PFHpA)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
Perfluorohexanesulfonic acid (PFHxS)	290	300	160	170	280	150	78	62	50
Perfluorohexanoic acid (PFHxA)	96	100	58	56	110	<MDL	<MDL	<MDL	50
Perfluorononanoic acid (PFNA)	80	90	<MDL	<MDL	92	<MDL	<MDL	<MDL	50
Perfluorooctanesulfonic acid (PFOS)	3700	4900	2400	2000	4300	3200	1300	840	100
Perfluorooctanoic acid (PFOA)	120	110	<MDL	<MDL	110	<MDL	<MDL	<MDL	100
Perfluoropentanesulfonic acid (PFPeS)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100
Perfluoropentanoic acid (PFPeA)	130	140	73	81	120	<MDL	<MDL	<MDL	100
Perfluoroundecanoic acid (PFUnA)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	100

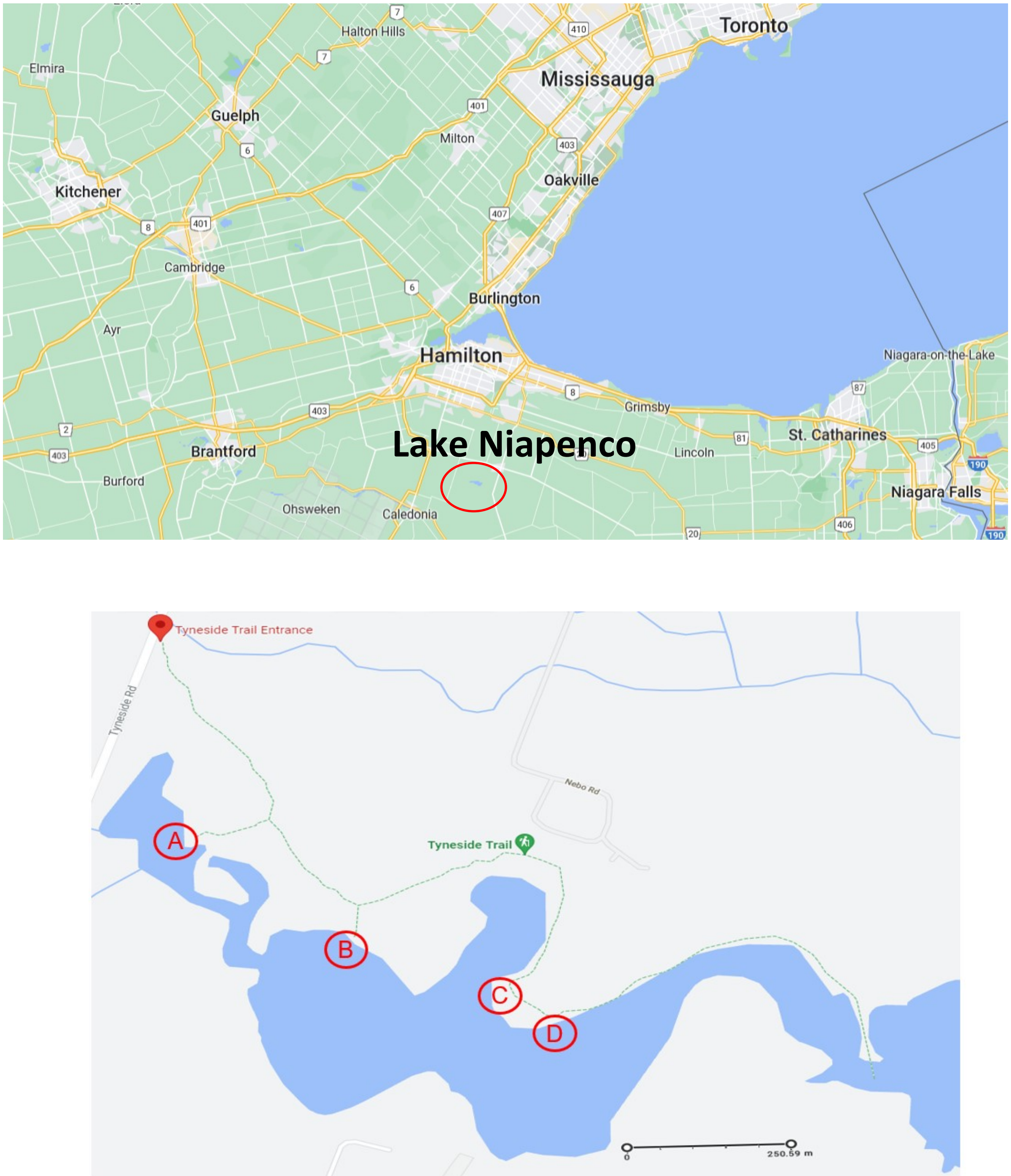

Figure S1. Lake Niapenco and the 4 Locations where the samplers were deployed. Maps were taken from Google Map. The number and type of sampler deployed at each location are presented in Table S3.

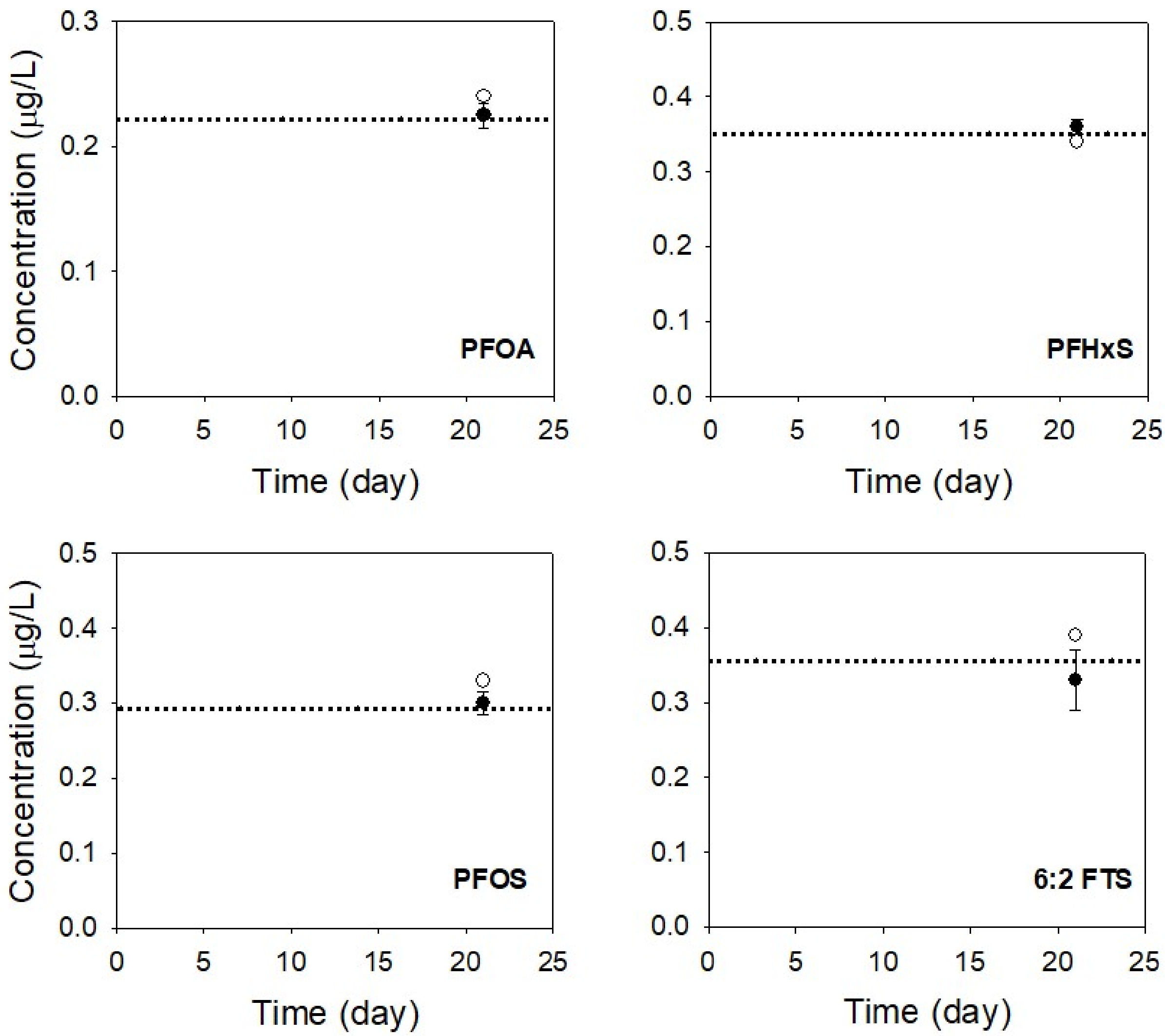

Figure S2. The concentration of PFAS in the receiving solution (black circles) and in the bulk solution (white circles) after 21 days. In this experiment, the initial concentrations of PFAS in the solution in the jar were 0.25 – 0.4 µg/L. The dotted black lines represent the theoretical equilibrium concentration, which was calculated based on mass balance.

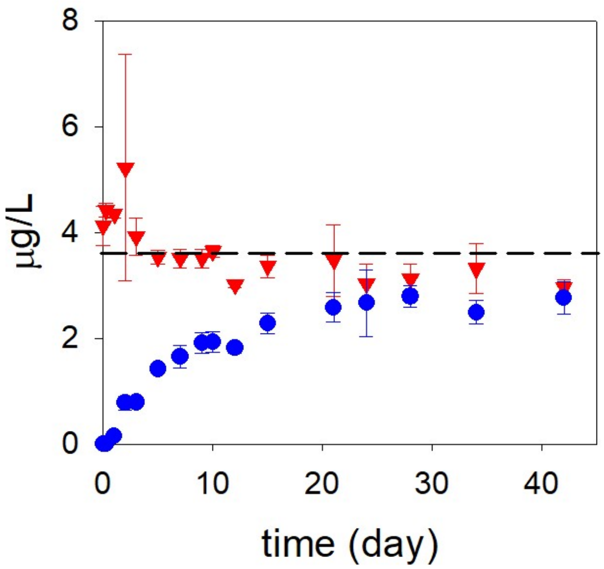

Figure S3. The concentration-time profile of PFOS in a microcosm experiment with a cellulose acetated-based sampler. Red triangles: the concentration in the solution in the jar. Blue and circles: the concentration in the receiving solution. Dashed black line: the equilibrium concentration, which was calculated based on mass balance.

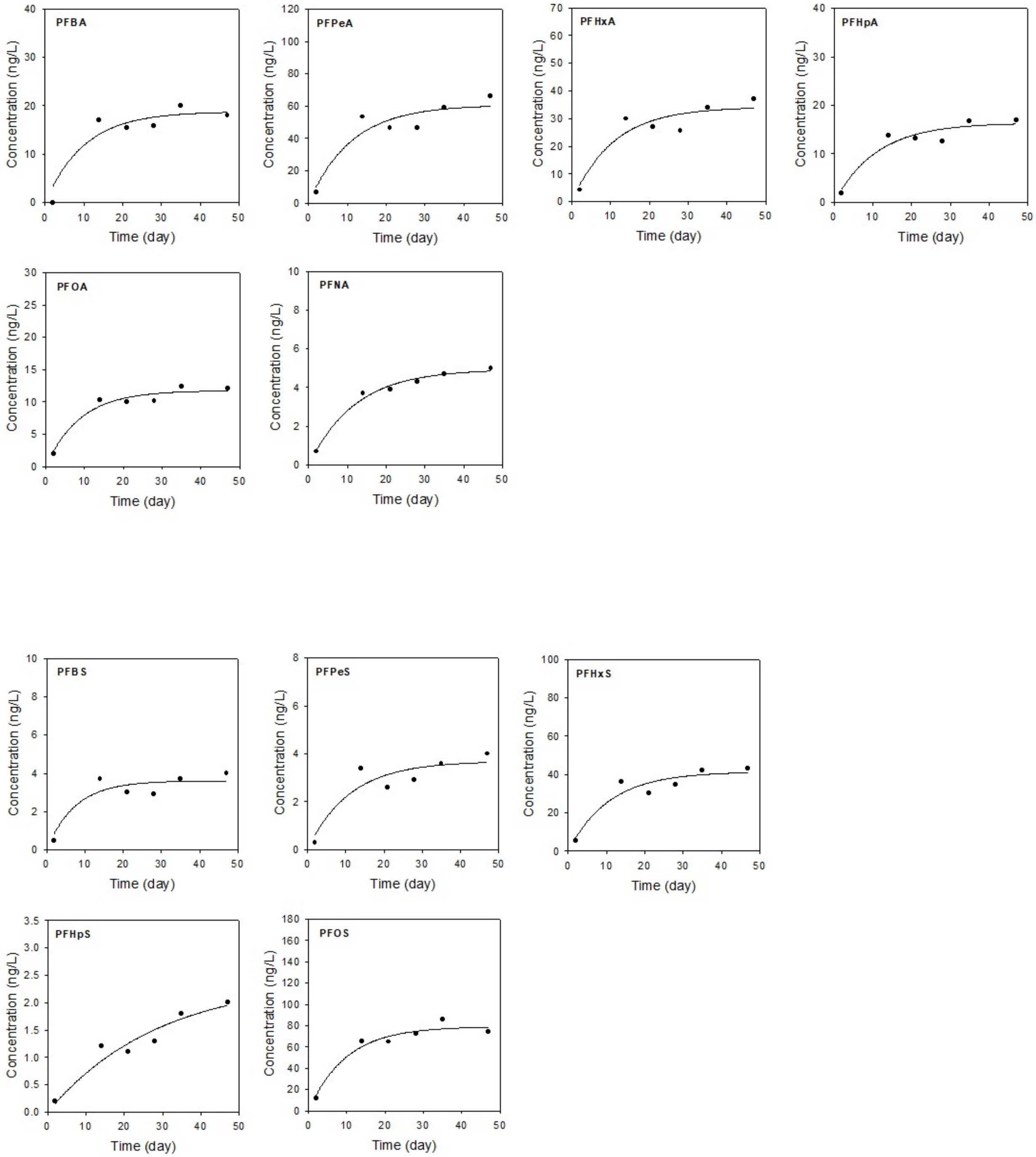

Figure S4. The concentration-time profiles of PFAS in the receiving solution of the samplers deployed in the sediment at Location A in October 2021. The fitting parameters are presented in Table S5 on the following page.

Table S5. Fitting parameters for the fitting of the data presented in Fig. S4.

Compound	R^2	Ceq (ng/L)	k (cm/s)
PFBA	0.90	19 ± 2	$(3.3 \pm 1.5)\times10^{-5}$
PFPeA	0.88	61 ± 7	$(3.0 \pm 1.3)\times10^{-5}$
PFHxA	0.88	34 ± 4	$(3.1 \pm 1.3)\times10^{-5}$
PFHpA	0.91	16 ± 2	$(3.3 \pm 1.1)\times10^{-5}$
PFOA	0.95	12 ± 1	$(3.8 \pm 1.0)\times10^{-5}$
PFNA	0.99	5.0 ± 0	$(2.8 \pm 0.4)\times10^{-5}$
PFBS	0.85	4 ± 0	$(4.5 \pm 2.4)\times10^{-5}$
PFPeS	0.85	4 ± 0	$(3.0 \pm 1.5)\times10^{-5}$
PFHxS	0.91	41 ± 4	$(3.1 \pm 1.1)\times10^{-5}$
PFHpS	0.92	2 ± 1	$(1.2 \pm 0.5)\times10^{-5}$
PFOS	0.95	79 ± 5	$(3.4 \pm 0.9)\times10^{-5}$

Table S6. The concentration of PFAS in the samplers retrieved at day 47 (Location A, October 2021)

Compound	C in the sampler receiving phase (ng/L)	Br-based Ceq (ng/L)	M_3PFPeA-based Ceq (ng/L)	M_2PFOA-based Ceq (ng/L)	M_4PFOS-based Ceq (ng/L)
PFBA	18 ± 6	24 ± 9	20 ± 4	18 ± 6	18 ± 6
PFPeA	66 ± 23	131 ± 46	95 ± 5	71 ± 18	68 ± 22
PFHxA	37 ± 13	102 ± 36	69 ± 10	45 ± 7	41 ± 10
PFHpA	17 ± 5	48 ± 15	32 ± 6	20 ± 2	18 ± 4
PFOA	12 ± 5	48 ± 19	30 ± 9	17 ± 3	15 ± 3
PFNA	5 ± 2	20 ± 7	13 ± 4	7 ± 1	6 ± 1
PFBS	4 ± 2	9 ± 4	7 ± 1	5 ± 1	4 ± 1
PFPeS	4 ± 2	9 ± 5	6 ± 1	4 ± 2	4 ± 2
PFHxS	43 ± 20	185 ± 88	111 ± 19	62 ± 8	55 ± 14
PFHpS	2 ± 1	5 ± 2	3 ± 0	2 ± 0	2 ± 1
PFOS	74 ± 31	274 ± 116	177 ± 73	103 ± 32	90 ± 27

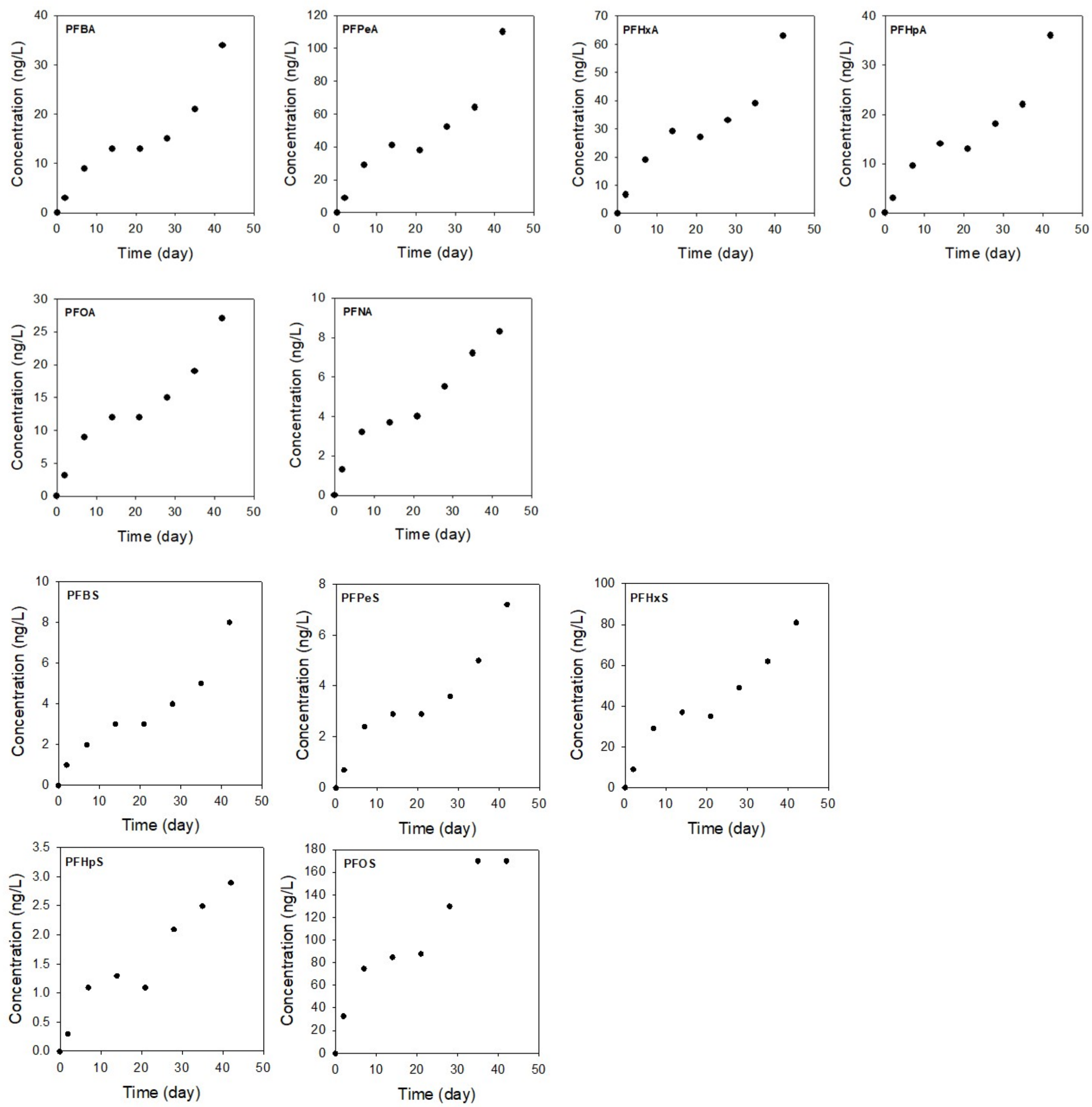

Figure S5. The concentration-time profiles of PFAS in the receiving solution of the samplers deployed in the sediment at Location A in June 2022.

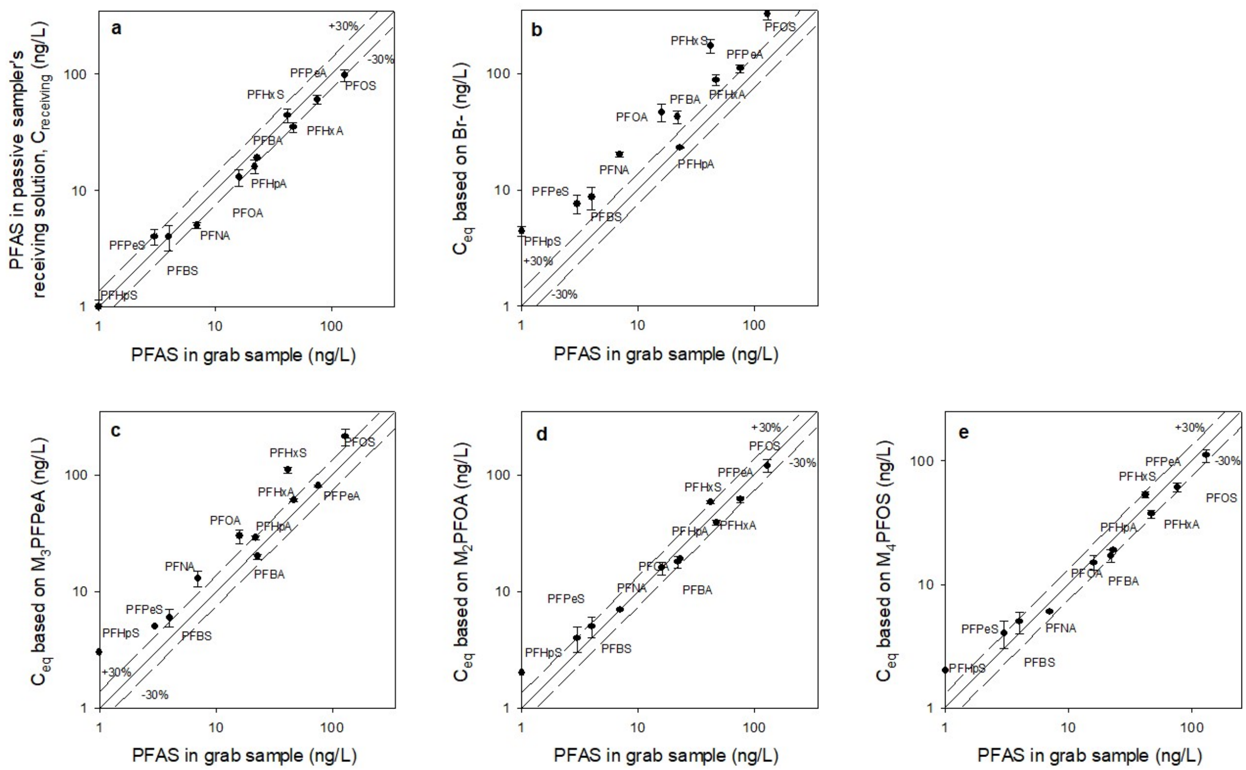

Figure S6. The concentration (C_{grab}) of PFAS in mechanically extracted sediment pore water obtained adjacent to each passive sampler (*x* axis), compared to: **(a)** the concentration of PFAS measured in the receiving solution ($C_{receiving}$) of the sampler that was retrieved at day 47, and **(b, c, d, e)** the equilibrium concentration (C_{eq}), calculated based on $C_{receiving}$ and four different PRCs. The solid lines are the 1:1 lines, whereas the dashed lines represent the ±30% relative percent difference. Samplers were deployed in the sediment at **Location B** in October 2021. Most Br^-- and M_3PFPeA-based C_{eq} values were ≥ 30% compared to the C_{grab} values, while M_2PFOA- and M_4PFOS-based C_{eq} values were within ± 30% of the C_{grab} values.

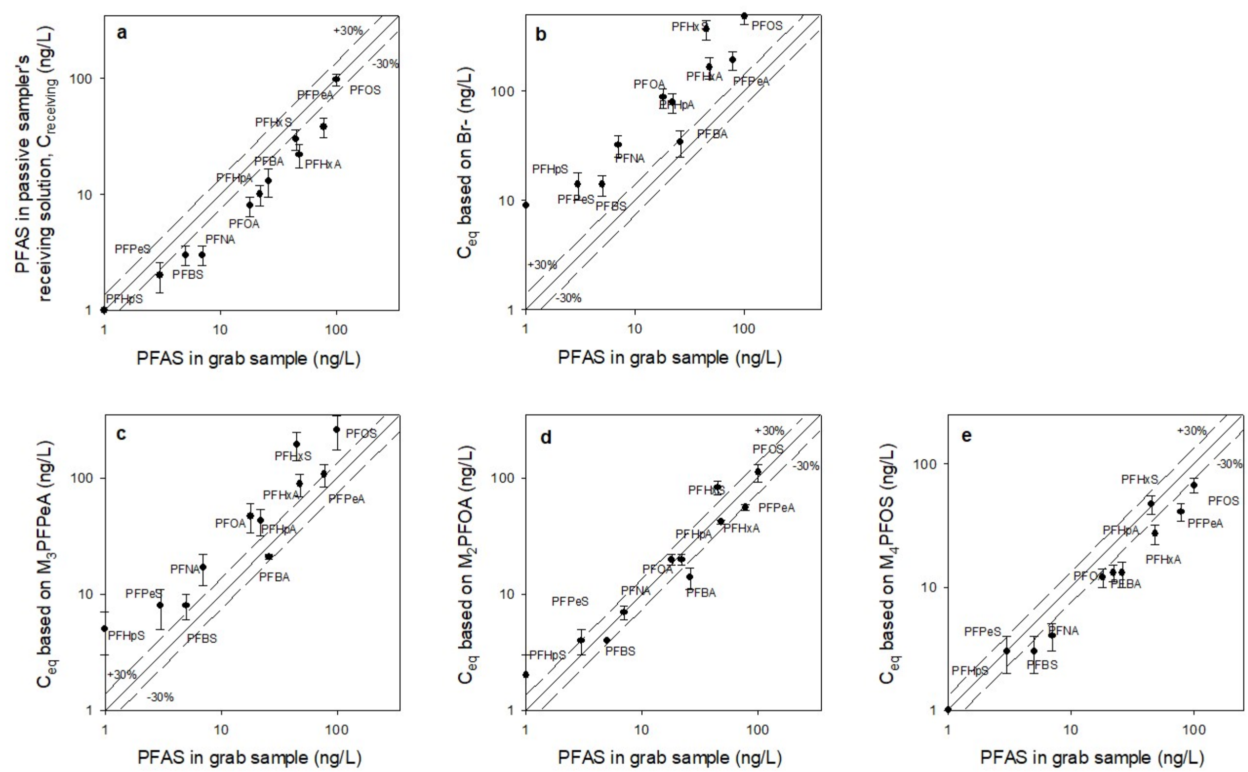

Figure S7. The concentration (C_{grab}) of PFAS in mechanically extracted sediment pore water obtained adjacent to each passive sampler (x axis), compared to: **(a)** the concentration of PFAS measured in the receiving solution ($C_{receiving}$) of the sampler that was retrieved at day 47, and **(b, c, d, e)** the equilibrium concentration (C_{eq}), calculated based on $C_{receiving}$ and four different PRCs. The solid lines are the 1:1 lines, whereas the dashed lines represent the ±30% relative percent difference. Samplers were deployed in the sediment at **Location C** in October 2021. Most Br^-- and M_3PFPeA-based C_{eq} values were ≥ 30% compared to the C_{grab} values, while, with a few exceptions, M_2PFOA- and M_4PFOS-based C_{eq} values were within ± 30% of the C_{grab} values.

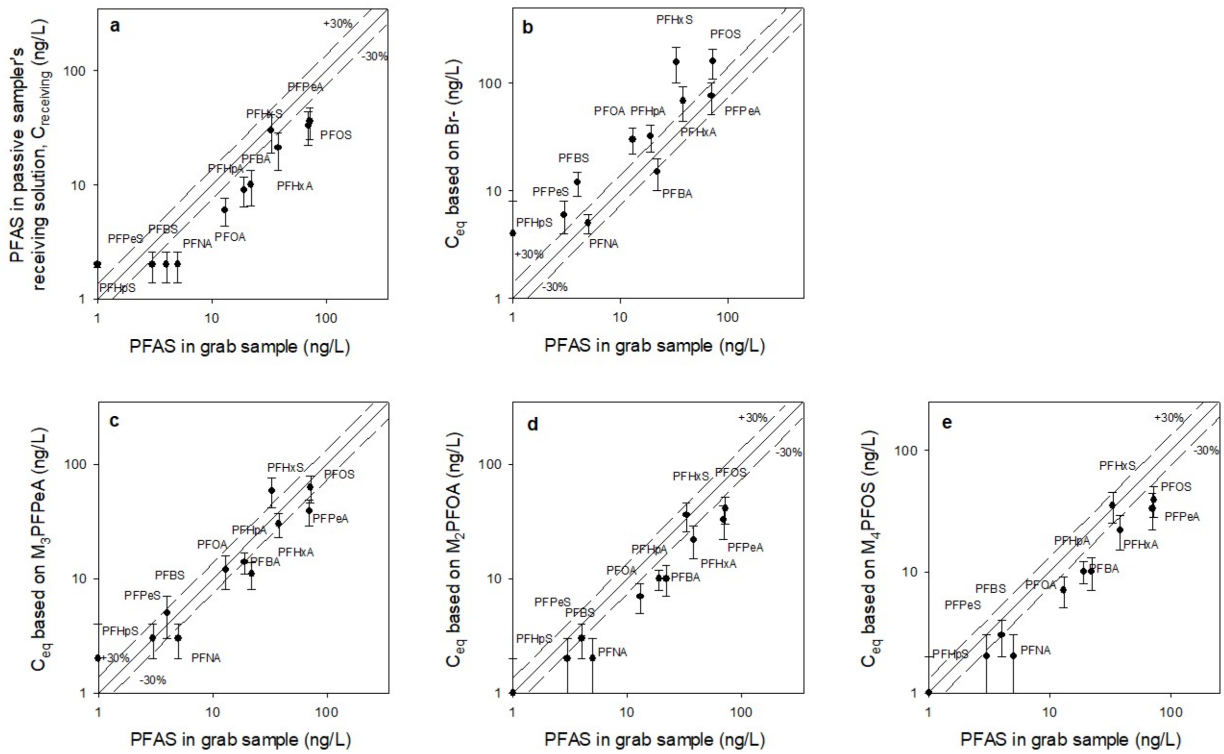

Figure S8. The concentration (C_{grab}) of PFAS in mechanically extracted sediment pore water obtained adjacent to each passive sampler (*x* axis), compared to: **(a)** the concentration of PFAS measured in the receiving solution ($C_{receiving}$) of the sampler that was retrieved at day 47, and **(b, c, d, e)** the equilibrium concentration (C_{eq}), calculated based on $C_{receiving}$ and four different PRCs. The solid lines are the 1:1 lines, whereas the dashed lines represent the ±30% relative percent difference. Samplers were deployed in the sediment at **Location D** in October 2021. Most Br^--based C_{eq} values were ≥ 30% compared to the C_{grab} values, while, with a few exceptions, M_3PFPeA-, M_2PFOA- and M_4PFOS-based C_{eq} values were within ± 30% of the C_{grab} values.

Table S7. Table S7. The concentration of PFAS in the receiving solution ($C_{receiving}$) of the samplers that were retrieved on days 14, 21, 28, 35 and 47. C_{eq} was calculated based on $C_{receiving}$ and the concentration of M_2PFOA remained in the receiving solution. The relative percent difference (RPD) was calculated for C_{eq} and C_{grab}.

	Grab sample collected on day 0	Sampler retrieved on day 14			Sampler retrieved on day 21			Sampler retrieved on day 28			Sampler retrieved on day 35			Sampler retrieved on day 47		
Analyte	(ng/L)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)
PFBA	32	17	17	88	15	17	63	16	17	63	20	20	46	18	18	56
PFPeA	94	53	57	66	46	66	36	46	60	45	59	64	38	66	68	33
PFHxA	57	30	35	61	27	49	15	26	41	32	34	42	30	37	41	34
PFHpA	32	14	17	91	13	25	25	13	21	41	17	21	40	17	19	51
PFOA	20	10	15	34	10	25	24	10	22	10	12	19	5	12	15	27
PFNA	7	4	6	26	4	10	39	4	10	34	5	8	8	5	7	7
PFBS	6	4	4	50	3	4	30	3	4	43	4	4	38	4	4	37
PFPeS	3	3	4	21	3	4	32	3	4	32	4	4	32	4	4	34
PFHxS	49	36	55	10	30	82	50	35	81	50	42	68	33	43	57	15
PFHpS	2	1	2	30	1	2	14	1	2	17	2	2	19	2	2	14
PFOS	110	65	90	23	65	153	33	72	148	29	86	126	13	74	91	19
M2PFOA	-	43	-	-	57	-	-	51	-	-	24	-	-	30	-	-
		[M2PFOA]/[M2PFOA]0 = 0.45			[M2PFOA]/[M2PFOA]0 = 0.6			[M2PFOA]/[M2PFOA]0 = 0.54			[M2PFOA]/[M2PFOA]0 = 0.36			[M2PFOA]/[M2PFOA]0 = 0.21		

Table S8. The concentration of PFAS in the receiving solution ($C_{receiving}$) of the samplers that were retrieved on days 14, 21, 28, 35 and 47. C_{eq} was calculated based on $C_{receiving}$ and the concentration of M_4PFOS remained in the receiving solution. The relative percent difference (RPD) was calculated for C_{eq} and C_{grab}.

	Grab sample collected on day 0	Sampler retrieved on day 14			Sampler retrieved on day 21			Sampler retrieved on day 28			Sampler retrieved on day 35			Sampler retrieved on day 47		
Analyte	(ng/L)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)
PFBA	32	17	17	88	15	16	69	16	16	67	20	20	46	18	18	56
PFPeA	94	53	54	73	46	52	58	46	51	60	59	61	43	66	67	33
PFHxA	57	30	32	77	27	35	48	26	32	55	34	37	41	37	40	36
PFHpA	32	14	15	112	13	17	59	13	16	65	17	19	52	17	19	53
PFOA	20	10	13	56	10	17	19	10	16	22	12	16	23	12	15	30
PFNA	7	4	5	49	4	7	4	4	7	1	5	6	12	5	6	10
PFBS	6	4	4	58	3	3	55	3	3	59	4	4	44	4	4	38
PFPeS	3	3	4	15	3	3	3	3	3	12	4	4	24	4	4	32
PFHxS	49	36	46	6	30	53	7	35	58	17	42	56	14	43	55	11
PFHpS	2	1	1	47	1	2	24	1	2	11	2	2	5	2	2	12
PFOS	110	65	78	41	65	101	9	72	109	1	86	106	4	74	88	22
M4PFOS	-	25	-	-	30	-	-	38	-	-	16	-	-	13	-	-
		[M4PFOS]/[M4PFOS]$_0$ = 0.30			[M4PFOS]/[M4PFOS]$_0$ = 0.36			[M4PFOS]/[M4PFOS]$_0$ = 0.34			[M4PFOS]/[M4PFOS]$_0$ = 0.19			[M4PFOS]/[M4PFOS]$_0$ = 0.16		

Table S9. The concentration of PFAS in the receiving solution ($C_{receiving}$) of the samplers that were retrieved on days 14, 21, 28, 35 and 47. C_{eq} was calculated based on $C_{receiving}$ and the concentration of M_3PFPeA remained in the receiving solution. The relative percent difference (RPD) was calculated for C_{eq} and C_{grab}.

	Grab sample collected on day 0	Sampler retrieved on day 14			Sampler retrieved on day 21			Sampler retrieved on day 28			Sampler retrieved on day 35			Sampler retrieved on day 47		
Analyte	(ng/L)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M3PFPeA	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)	Creceiving (ng/L) in the receiving solution	Ceq (ng/L) predicted based on Creceiving and M4PFOS	Relative percent difference between passive sampler and grab sample (%)
PFBA	32	17	20	62	15	22	38	16	18	56	20	24	29	18	18	56
PFPeA	94	53	88	7	46	103	10	46	72	27	59	101	7	66	68	33
PFHxA	57	30	66	13	27	84	38	26	52	9	34	78	31	37	41	34
PFHpA	32	14	32	1	13	43	30	13	27	17	17	40	23	17	19	51
PFOA	20	10	32	38	10	46	80	10	29	38	12	41	68	12	15	27
PFNA	7	4	12	43	4	19	93	4	13	61	5	16	80	5	7	7
PFBS	6	4	6	7	3	7	17	3	5	24	4	7	11	4	4	37
PFPeS	3	3	6	54	3	7	78	3	5	53	4	7	81	4	4	34
PFHxS	49	36	122	60	30	151	102	35	108	75	42	149	101	43	57	15
PFHpS	2	1	3	35	1	4	68	1	3	42	2	5	82	2	2	14
PFOS	110	65	189	42	65	276	86	72	194	55	86	262	82	74	91	19
M3PFPeA	-	45	-	-	62	-	-	53	-	-	58	-	-	22	-	-
		[M3PFPeA]/[M3PFPeA]0 = 0.47			[M3PFPeA]/[M3PFPeA]0 = 0.65			[M3PFPeA]/[M3PFPeA]0 = 0.55			[M3PFPeA]/[M3PFPeA]0 = 0.60			[M3PFPeA]/[M3PFPeA]0 = 0.23		

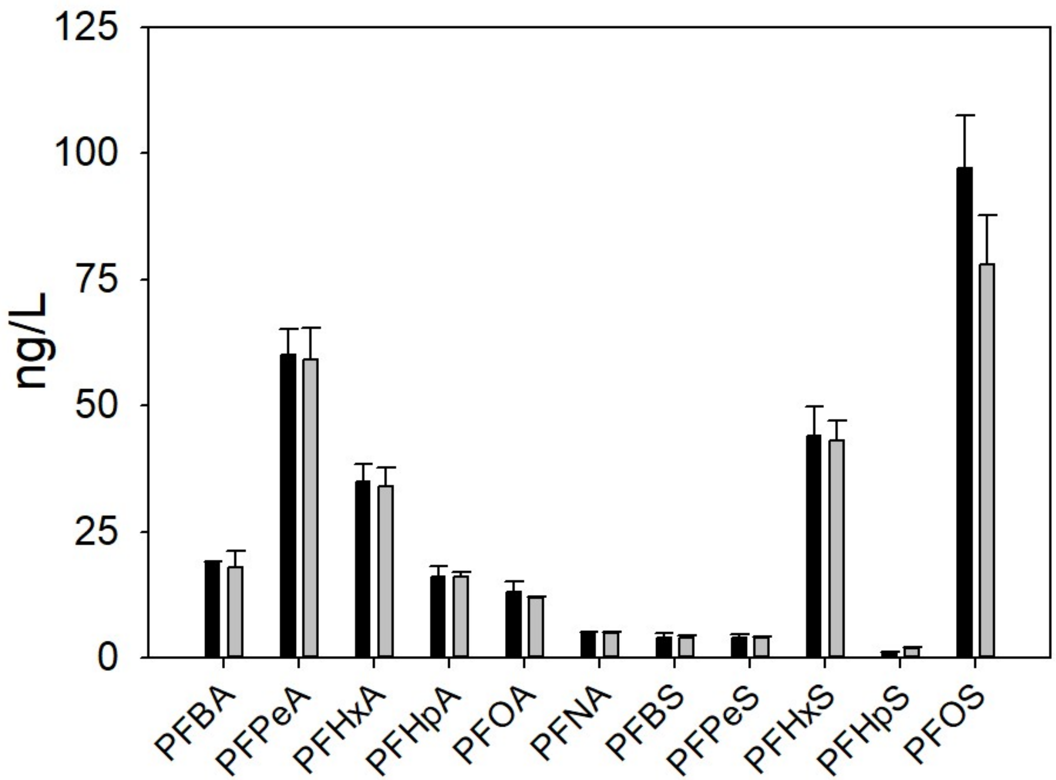

Figure S6. The concentration of PFAS in the pore water sediment at Location B measured by the passive samplers constructed with a polycarbonate (black bars) and a cellulose acetate (grey bars) membranes.

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