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

Supplemental Information for

Distribution and Fate of Per- and Polyfluorinated Alkyl Substances (PFAS) in Wastewater Treatment Facilities

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Table S1. Field collected chemical data for WWTF influent and effluent sampling in March and/or July 2019. Sludge % solids is for individual samples collected in July."

WWTF	Population Served	Sludge % Solids	Location	Flow ($x10^6$L/D)[a]		pH		Conductivity (µS/cm)		DO (mg/L)		REDOX (mV)		Temperature (°C)	
				March	July	March	July	March	July	March	July	March	July	March	July
AL+CD[b]	11000	-	Influent	6.8	-	7.3	-	1092	-	9.7	-	-18.0	-	4.6	-
		-	Effluent	6.8	-	7.6	-	1213	-	6.3	-	-33.1	-	9.4	-
Bard+CD (1)	11000	18	Influent	-	4.9	-	7.7	-	885	-	4.4	-	-34.4	-	20.6
			Effluent	-	4.9	-	7.0	-	780	-	7.2	-	0.3	-	23.0
Bard+CD (2)	7000	26	Influent	1.7	1.3	7.2	7.3	1464	1124	10.2	2.1	-11.2	-22.1	10.4	23.0
			Effluent	1.8	1.4	7.8	7.2	1554	829	6.8	7.9	-44.1	-14.9	10.1	23.7
Bard+CD (3)	16000	0.54	Influent	2.7	2.7	6.7	7.3	1334	839	6.5	4.2	15.2	-22.5	10.4	22.8
			Effluent	2.9	3.1	7.6	6.7	1441	744	7.0	3.7	-36.8	12.7	10.2	24.6
AS+UV (1)	16418	-	Influent	9.8	-	7.2	-	1076	-	10.2	-	-15.4	-	9.2	-
			Effluent	11.9	-	7.5	-	1182	-	5.4	-	-29.7	-	9.6	-
AS+UV (2)	28972	-	Influent	10.8	-	6.7	-	1395	-	7.6	-	13.4	-	10.5	-
			Effluent	15.4	-	7.3	-	1544	-	2.2	-	-18.4	-	10.1	-
OD+CD	1198	17	Influent	0.26	0.19	6.9	7.7	1235	885	4.6	4.4	1.8	-34.4	8.7	20.6
			Effluent	0.26	0.19	8.0	7.1	1176	802	8.2	4.2	-54.9	-10.9	10.7	22.5

[a] Flow data for date of sampling
[b] Abbreviations: AL: Aerated Lagoon, AS: Activated Sludge, Bard: Bardenpho, CD: Chlorination-Dechlorination disinfection, UV: Ultraviolet disinfection

Table S2. Composition of surrogate and recovery standards.

Surrogate (Extracted Internal Standard)	Acceptance Criteria (%) for Recovery
Perfluoro[13C4]Butanoic Acid (MPFBA)	2-156
Perfluoro[13C5]Pentanoic Acid (M5PFPEA)	16-173
Perfluoro[2,3,4-13C3]Butanesulfonic Acid (M3PFBS)	31-159
1H,1H,2H,2H-Perfluoro[1,2-13C2]Hexanesulfonic Acid (M2-4:2FTS)	1-313
Perfluoro[1,2,3,4,6-13C5]Hexanoic Acid (M5PFHxA)	21-145
Perfluoro[1,2,3,4-13C4]Heptanoic Acid (M4PFHpA)	30-139
Perfluoro[1,2,3-13C3]Hexanesulfonic Acid (M3PFHxS)	47-153
Perfluoro[13C8]Octanoic Acid (M8PFOA)	36-149
1H,1H,2H,2H-Perfluoro[1,2-13C2]Octanesulfonic Acid (M2-6:2FTS)	1-244
Perfluoro[13C9]Nonanoic Acid (M9PFNA)	34-146
Perfluoro[13C9]Nonanoic Acid (M9PFNA)	42-146
Perfluoro[1,2,3,4,5,6-13C6]Decanoic Acid (M6PFDA)	38-144
1H,1H,2H,2H-Perfluoro[1,2-13C2]Decanesulfonic Acid (M2-8:2FTS)	7-170
N-Deuteriomethylperfluoro-1-octanesulfonamidoacetic Acid (d3-NMeFOSAA)	1-181
Perfluoro[1,2,3,4,5,6,7-13C7]Undecanoic Acid (M7-PFUDA)	40-144
Perfluoro[13C8]Octanesulfonamide (M8FOSA)	1-87
N-Deuterioethylperfluoro-1-octanesulfonamidoacetic Acid (d5-NEtFOSAA)	23-146
Perfluoro[1,2-13C2]Dodecanoic Acid (MPFDOA)	24-161
Perfluoro[1,2-13C2]Tetradecanoic Acid (M2PFTEDA)	33-143

Isotope Dilution Labeled Recovery Standard

Perfluoro-n-[1,2-13C2]octanoic acid (M2PFOA)

Perfluoro-n-[1,2- 13C2] decanoic acid (M2PFDA)

Sodium perfluoro-[13C8] octane sulfonic acid (M3PFBA)

Sodium perfluoro-[13C8] octane sulfonic acid (M4PFOS)

Tables S3 – S9 Provided in Supplemental File 2 (.xlsx file)

Table S10. Minimum and maximum contribution percentage and data used for calculation. [+]Ref Brown and Arellano, 1980 and Short, 1992

	Minimum	Maximum
Total GBE Volume (L) [+]	1.66E+11	
GBE ΣPFAS (ng/L)	6	17
GBE ΣPFAS (g)	996	2822
GBE Flushing Time (d) [+]	18	36
ΣPFAS WWTF load (g/d)	2.9	3.1
Percentage of GBE PFAS load derived from WWTF	2%	11%

[+]W. S. Brown and E. Arellano, *Estuaries*, 1980, **3**, 248.
[+]F. T. Short, *The ecology of the Great Bay Estuary, New Hampshire and Maine: An Estuarine Profile and Bibliography*, Piscatiqua Region Estuaries Partnership Reports & Publications, 1992.

Table S11. Ratio of the concentration of PFAAs after oxidation by the TOP assay relative to the original PFAA concentration ($C_{TOP}/C_{regular}$) for the OD+CD facility in March

Analyte	Ratio
Perfluorobutanoic Acid (PFBA)	377
Perfluoropentanoic Acid (PFPeA)	207
Perfluorohexanoic Acid (PFHxA)	38.3
Perfluoroheptanoic Acid (PFHpA)	12.2
Perfluorooctanoic Acid (PFOA)	6.3
Perfluorononanoic Acid (PFNA)	0.4
Perfluorodecanoic Acid (PFDA)	0.1
Perfluoroundecanoic Acid (PFUnA)	0.1
Perfluorobutanesulfonic Acid (PFBS)	5.0
Perfluoropentanesulfonic Acid (PFPeS)	1.3
Perfluorohexanesulfonic Acid (PFHxS)	0.1
Perfluorooctanesulfonic Acid (PFOS)	1.5

Table S12 provided in supplemental file 2 (.xlsx file).

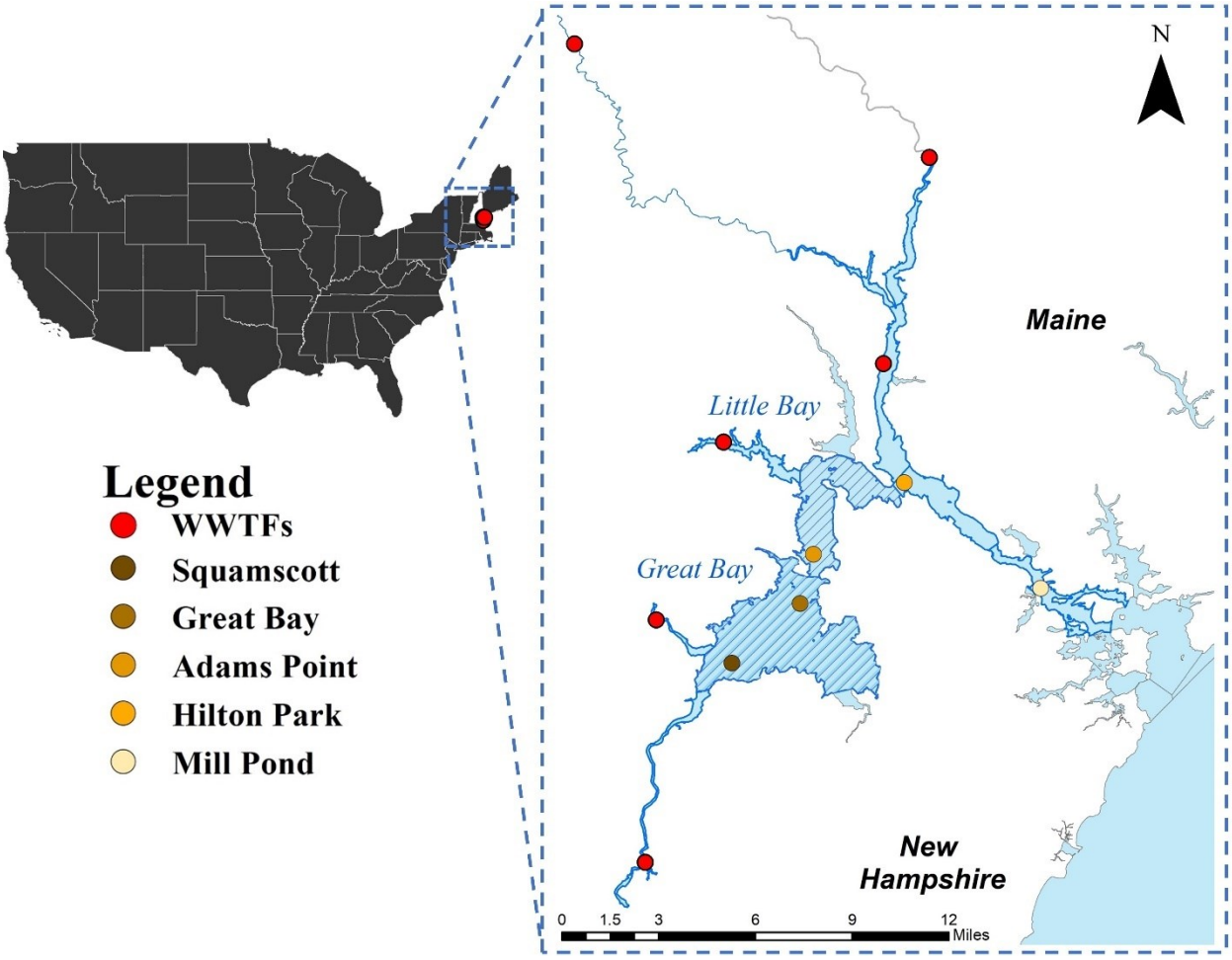

Figure S1. Map of WWTF and Great Bay Estuary sampling sites.

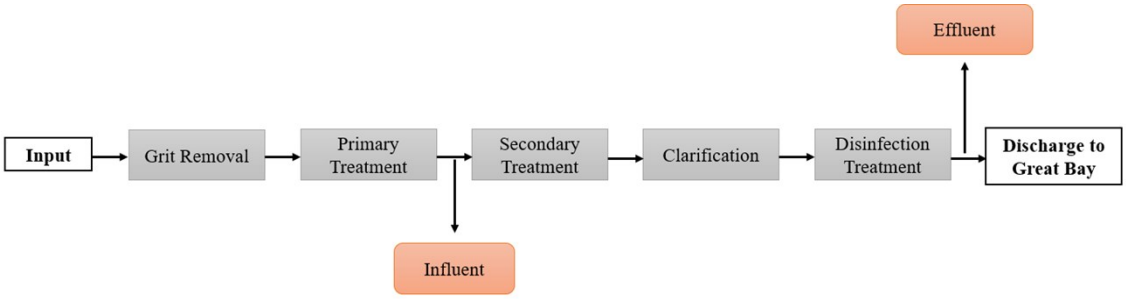

Figure S2. PFAS sampling locations during March sampling campaign.

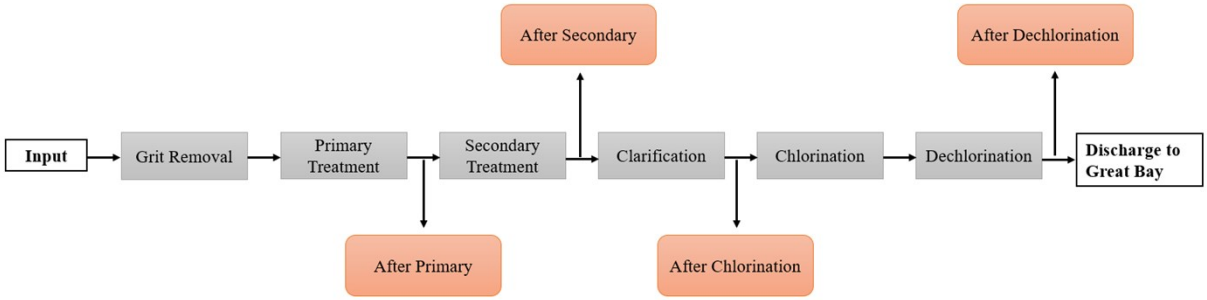

Figure S3. PFAS sampling locations during July sampling campaign.

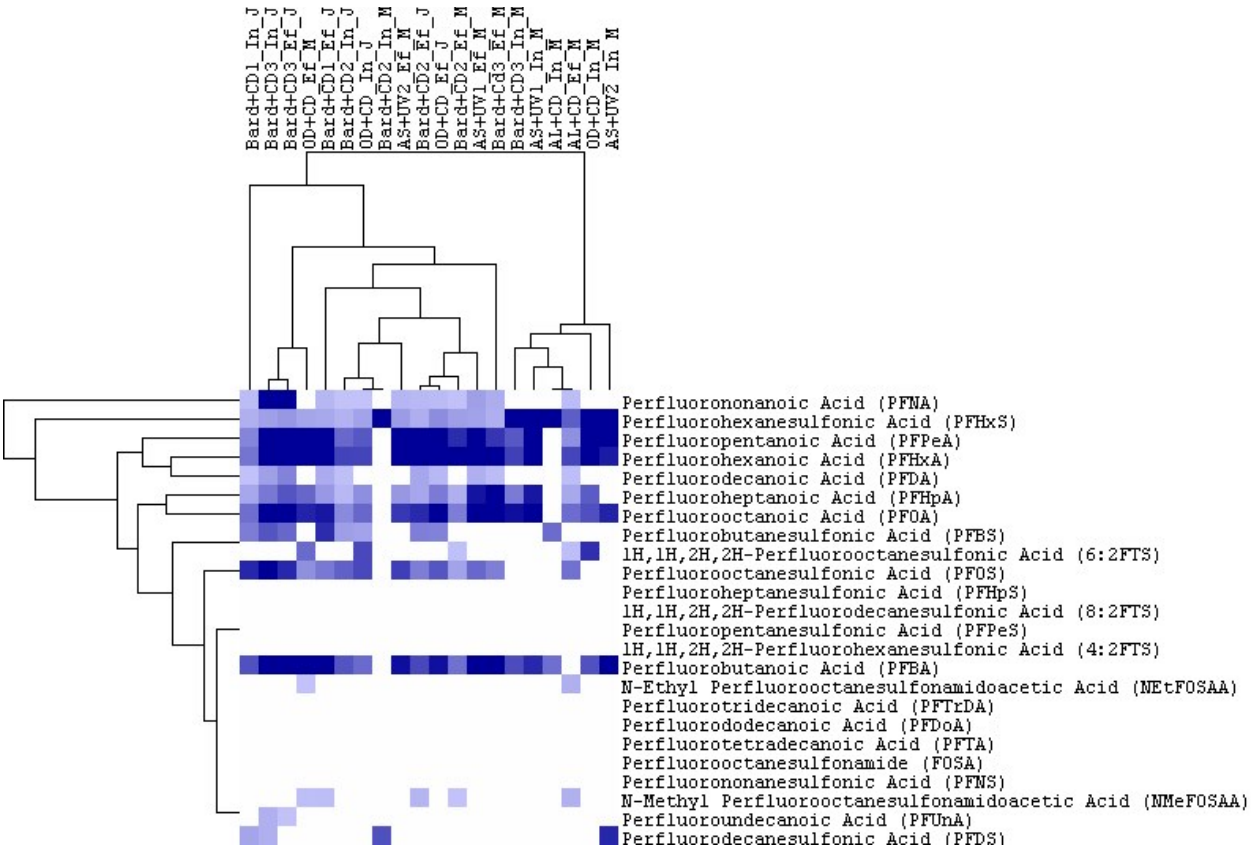

Figure S4. Hierarchical clustering of WWTF influent and effluent samples and PFAS constituent based on average linkage. Sample labeling abbreviations: In-Influent, Ef-Effluent, M-March, J-July.

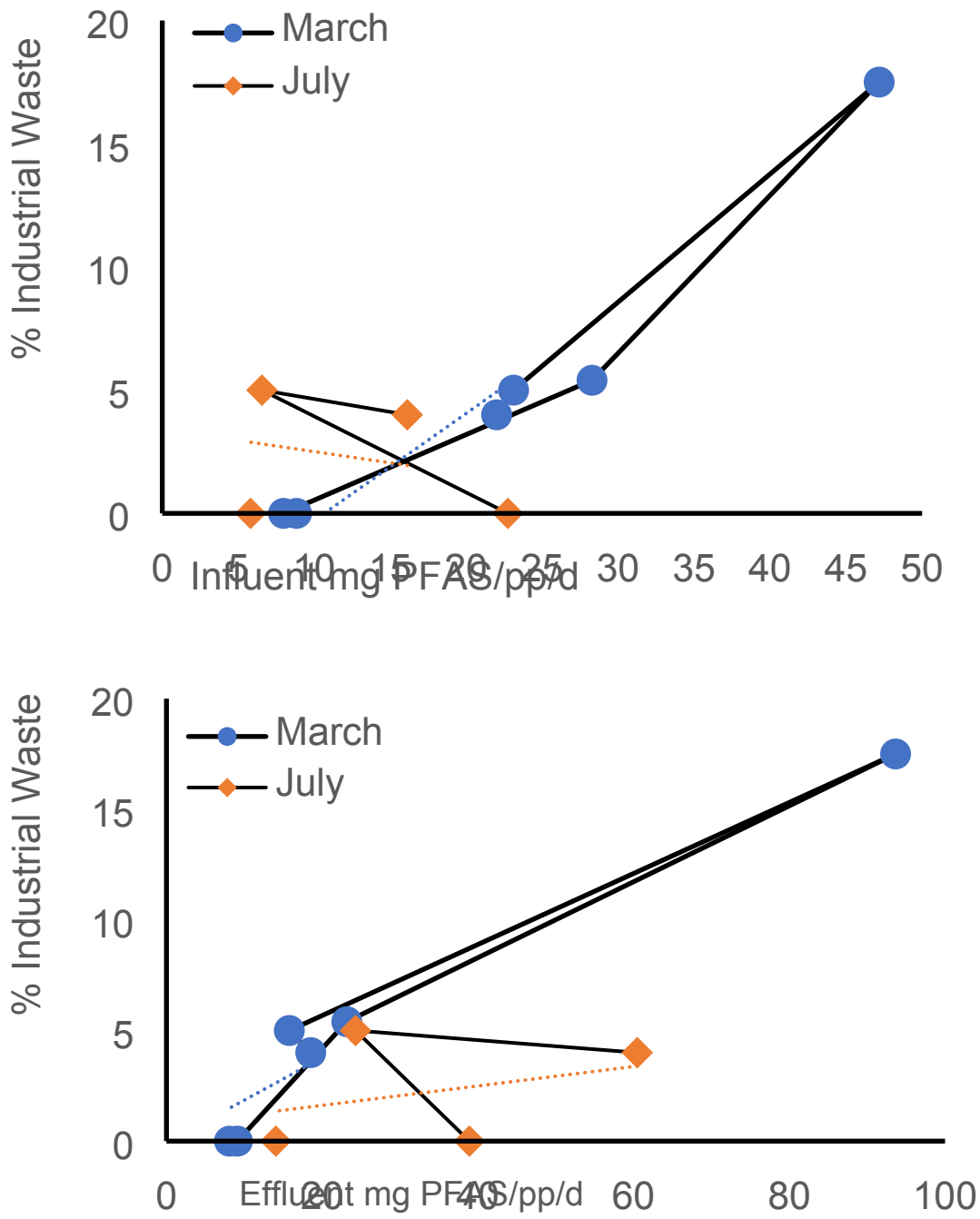

Figure S5. Relationship of population normalized PFAS mass flows in influent (top) and effluent (bottom) to the percentage of known industrial inputs.

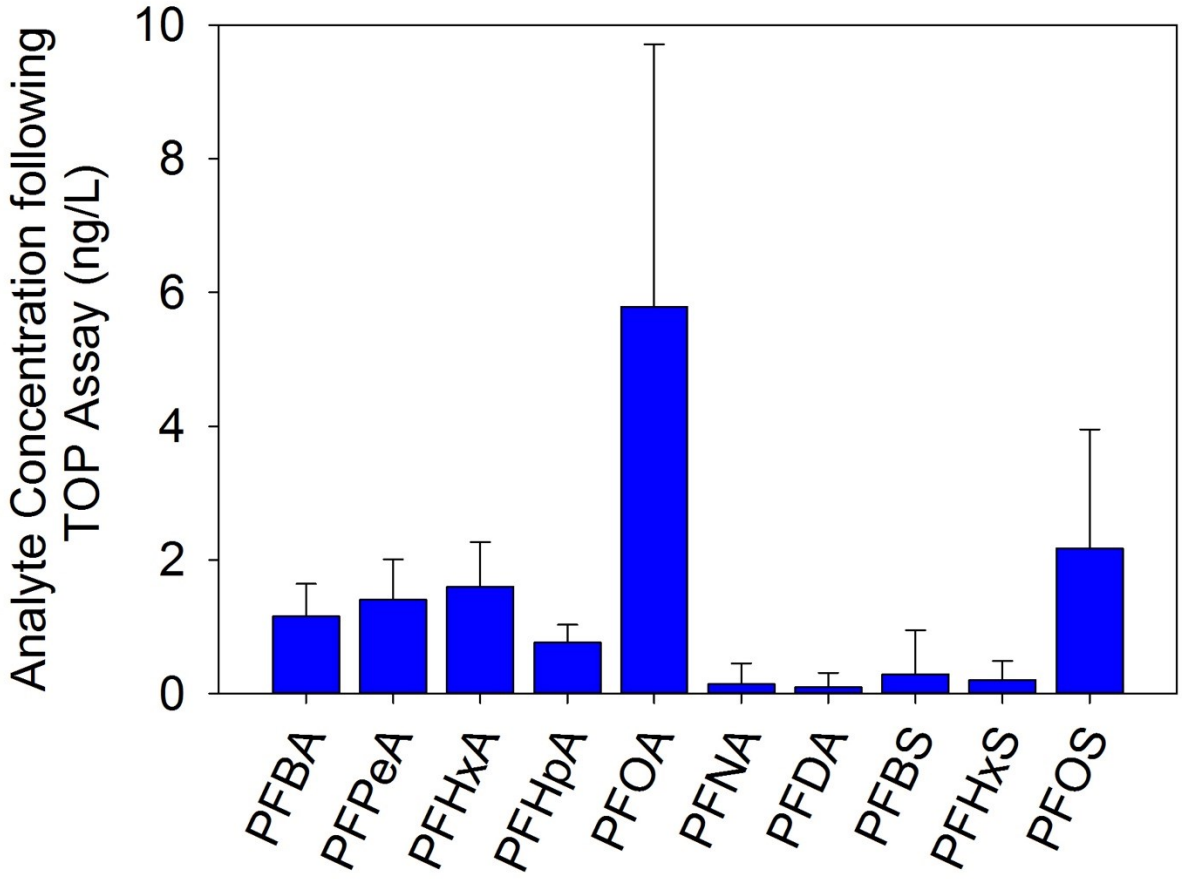

Figure S6. Mean concentration (n=5) of individual PFAAs detected in surface waters following TOP assay, error bars represent standard deviation.