Supplementary Materials

for

Per- and Polyfluoroalkyl Substances (PFAS) in Urban Stormwater Runoff: Insights from a Roadside Rain Garden

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Table S1. Targeted PFAS species used in this study.

Compound	Abbreviation
Perfluorobutanoic acid	PFBA
Perfluoro-3-methoxypropanoic acid	PFMPA
Perfluoropentanoic acid	PFPeA
Perfluoro-4-methoxybutanoic acid	PFMBA
4:2 Fluorotelomer sulfonic acid	4:2FTS
Nonafluoro-3,6-dioxaheptanoic acid	NFDHA
Perfluorohexanoic acid	PFHxA
Perfluorobutane sulfonic acid	PFBS
Hexafluoropropylene oxide dimer acid	HFPO-DA
Perfluoro (2-ethoxyethane) sulfonic acid	PFEESA
Perfluoroheptanoic acid	PFHpA
Perfluoropentane sulfonic acid	PFPeS
6:2 Fluorotelomer sulfonic acid	6:2FTS
Perfluorohexane sulfonic acid	PFHxS
Perfluorononanoic acid	PFNA
Perfluoroheptane sulfonic acid	PFHpS
8:2 Fluorotelomer sulfonic acid	8:2FTS
Perfluorodecanoic acid	PFDA
N-Ethyl perfluorooctanesulfonamidoacetic acid	NEtFOSAA
Perfluoroundecanoic acid	PFUnA
9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic acid	9Cl-PF3ONS
Perfluorododecanoic acid	PFDoA
11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid	11Cl-PF3OUdS
3-Perfluoropropyl propanoic acid	3:3FTCA
2H,2H,3H,3H-Perfluorooctanoic acid	5:3FTCA
3-Perfluoroheptyl propanoic acid	7:3FTCA
Dodecafluoro-3H-4,8-dioxanoate	ADONA
N-Ethyl perfluorooctane sulfonamide	NEtFOSA
N-ethyl perfluorooctanesulfonamidoethanol	NEtFOSE
N-Methyl perfluorooctane sulfonamide	NMeFOSA
N-Methyl perfluorooctanesulfonamidoacetic acid	NMeFOSAA
N-methyl perfluorooctanesulfonamidoethanol	NMeFOSE
Perfluorodecane sulfonic acid	PFDS
Perfluorododecanesulfonic acid	PFDoS
Perfluorononane sulfonic acid	PFNS
Perfluorooctanoic acid	PFOA
Perfluorooctanesulfonic acid	PFOS
Perfluorooctane sulfonamide	PFOSA
Perfluorotetradecanoic acid	PFTeDA
Perfluorotridecanoic acid	PFTrDA

Table S2. Isotopically labeled PFAS species in extracted internal standard (EIS) used in this study.

Compound	Abbreviation
Perfluorobutanoic acid	$^{13}C_4$ PFBA
Perfluorohexanoic acid	$^{13}C_2$ PFHxA
Sodium perfluorohexane sulfonate	$^{18}O_2$ PFHxS
Perfluorononanoic acid	$^{13}C_5$ PFNA
Perfluorodecanoic acid	$^{13}C_2$ PFDA
Perfluoroundecanoic acid	$^{13}C_2$ PFUnA
Perfluorododecanoic acid	$^{13}C_2$ PFDoA
Perfluorooctanoic acid	$^{13}C_4$ PFOA
Sodium perfluorooctane sulfonate	$^{13}C_4$ PFOS

Table S3. Isotopically labeled PFAS species in non-extracted internal standard (NIS) used in this study.

Compound	Abbreviation
Perfluorobutanoic acid	$^{13}C_3$ PFBA
Perfluoropentanoic acid	$^{13}C_5$ PFPeA
4:2 Fluorotelomer sulfonic acid	$^{13}C_2$ 4:2FTS
Perfluorohexanoic acid	$^{13}C_6$ PFHxA
Perfluorobutane sulfonic acid	$^{13}C_4$ PFBS
Hexafluoropropylene oxide dimer acid	$^{13}C_3$ HFPO-DA
Perfluoroheptanoic acid	$^{13}C_7$ PFHpA
6:2 Fluorotelomer sulfonic acid	$^{13}C_2$ 6:2FTS
Perfluorohexane sulfonic acid	$^{13}C_6$ PFHxS
Perfluorononanoic acid	$^{13}C_9$ PFNA
8:2 Fluorotelomer sulfonic acid	$^{13}C_2$ 8:2FTS
Perfluorodecanoic acid	$^{13}C_9$ PFDA
N-Ethyl perfluorooctanesulfonamidoacetic acid	D_5 N-EtFOSAA
Perfluoroundecanoic acid	$^{13}C_9$ PFUnA
Perfluorododecanoic acid	$^{13}C_{12}$ PFDoA
N-Methyl perfluorooctanesulfonamidoacetic acid	D_3 NMeFOSAA
Perfluorooctane sulfonamide	$^{13}C_8$ PFOSA
Perfluorotetradecanoic acid	$^{13}C_2$ PFTeDA
Perfluorooctanoic acid	$^{13}C_8$ PFOA
Perfluorooctanesulfonic acid	$^{13}C_8$ PFOS

Table S4. Storm events analyzed during this study.

Storm Event No.	Date	Depth (mm)	Duration (h)
1	25 August 23	76.3	14
2	11 September 23	41.2	10
3	14 October 23	88.3	16
4	28 December 23	28.4	21
5	07 June 21	42.6	9
6	10 July 24	62.1	11

Time	Flow Rate	20 mM ammonium acetate	Acetonitrile
0	250	10	90
2	250	10	90
15	250	90	10
18	250	90	10

20	250	10	90
25	250	10	90

Table S5. Mobile phase gradient method employed for elution.

Table S6. Mass Spectrometry tuning parameters for the target PFAS species.

Compound	Abbreviation	Precursor (m/z)	Product (m/z)	Collision Energy (V)	Cone Voltage (V)
Perfluorobutanoic acid	PFBA	213	169	10	15
Perfluoro-3-methoxypropanoic acid	PFMPA	229	85	10	15
Perfluoropentanoic acid	PFPeA	263	219	10	15
Perfluoro-4-methoxybutanoic acid	PFMBA	279	85	10	25
4:2 Fluorotelomer sulfonic acid	4:2FTS	327	307	20	40
Nonafluoro-3,6-dioxaheptanoic acid	NFDHA	295	201	6	20
Perfluorohexanoic acid	PFHxA	313	269	10	15
Perfluorobutane sulfonic acid	PFBS	299	80	35	45
Hexafluoropropylene oxide dimer acid	HFPO-DA	285	169	10	30
Perfluoro (2-ethoxyethane) sulfonic acid	PFEESA	315	135	20	30
Perfluoroheptanoic acid	PFHpA	363	319	10	15
Perfluoropentane sulfonic acid	PFPeS	349	80	40	50
6:2 Fluorotelomer sulfonic acid	6:2FTS	427	407	20	40
Perfluorohexane sulfonic acid	PFHxS	399	80	40	50
Perfluorononanoic acid	PFNA	463	419	10	15
Perfluoroheptane sulfonic acid	PFHpS	449	80	40	50
8:2 Fluorotelomer sulfonic acid	8:2FTS	527	507	25	40

Perfluorodecanoic acid	PFDA	513	469	10	15
N-Ethyl perfluorooctanesulfonamidoacetic acid	NEtFOSAA	584	419	20	25
Perfluoroundecanoic acid	PFUnA	563	519	25	30
9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic acid	9Cl-PF3ONS	531	351	25	30
Perfluorododecanoic acid	PFDoA	613	569	10	20
11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid	11Cl-PF3OUdS	631	451	30	40
3-Perfluoropropyl propanoic acid	3:3FTCA	241	177	15	30
2H,2H,3H,3H-Perfluorooctanoic acid	5:3FTCA	341	237	20	30
3-Perfluoroheptyl propanoic acid	7:3FTCA	441	317	15	30
Dodecafluoro-3H-4,8-dioxanoate	ADONA	377	251	12	20
N-Ethyl perfluorooctane sulfonamide	NEtFOSA	526	169	30	40
N-ethyl perfluorooctanesulfonamidoethanol	NEtFOSE	630	59*	5	40
N-Methyl perfluorooctane sulfonamide	NMeFOSA	512	169	30	40
N-Methyl perfluorooctanesulfonamidoacetic acid	NMeFOSAA	570	419	18	25
N-methyl perfluorooctanesulfonamidoethanol	NMeFOSE	616	59*	5	40
Perfluorodecane sulfonic acid	PFDS	599	80	50	50
Perfluorododecanesulfonic acid	PFDoS	699	80	50	50
Perfluorononane sulfonic acid	PFNS	549	80	45	50
Perfluorooctanoic acid	PFOA	413	369	10	20
Perfluorooctanesulfonic acid	PFOS	499	80	50	80
Perfluorooctane sulfonamide	PFOSA	498	78	30	35
Perfluorotetradecanoic acid	PFTeDA	713	669	10	20
Perfluorotridecanoic acid	PFTrDA	663	619	10	20

Note: The m/z of the Precursor and the Product species are sourced from USEPA 1633.[8]

*The Product species corresponds to the confirmation ions.

Table S7. Mass Spectrometry tuning parameters for the isotopically labeled PFAS species in the non-extracted internal standard (NIS).

Compound	Abbreviation	Precursor (m/z)	Product (m/z)	Collision Energy (V)	Cone Voltage (V)
Perfluorobutanoic acid	$^{13}C_3$ PFBA	216	172	10	15
Perfluoropentanoic acid	$^{13}C_5$ PFPeA	268	223	10	15
4:2 Fluorotelomer sulfonic acid	$^{13}C_2$ 4:2FTS	329	309	20	40
Perfluorohexanoic acid	$^{13}C_6$ PFHxA	319	274	10	15
Perfluorobutane sulfonic acid	$^{13}C_4$ PFBS	303	80	35	45
Hexafluoropropylene oxide dimer acid	$^{13}C_3$ HFPO-DA	287	169	10	30
Perfluoroheptanoic acid	$^{13}C_7$ PFHpA	370	325	10	15
6:2 Fluorotelomer sulfonic acid	$^{13}C_2$ 6:2FTS	429	409	20	25
Perfluorohexane sulfonic acid	$^{13}C_6$ PFHxS	405	80	40	50
PFNA (Perfluorononanoic acid)	$^{13}C_9$ PFNA	472	427	10	15
8:2 Fluorotelomer sulfonic acid	$^{13}C_2$ 8:2FTS	529	509	25	40
Perfluorodecanoic acid	$^{13}C_9$ PFDA	522	477	10	15
N-Ethyl perfluorooctanesulfonamidoacetic acid	D_5 N-EtFOSAA	589	419	20	25
Perfluoroundecanoic acid	$^{13}C_9$ PFUnA	572	527	25	30
Perfluorododecanoic acid	$^{13}C_{12}$ PFDoA	625	580	10	20
N-Methyl perfluorooctanesulfonamidoacetic acid	D_3 NMeFOSAA	573	419	18	25
Perfluorooctane sulfonamide	$^{13}C_8$ PFOSA	506	78	30	35
Perfluorotetradecanoic acid	$^{13}C_2$ PFTeDA	715	670	10	20
Perfluorooctanoic acid	$^{13}C_8$ PFOA	421	376	10	20
Perfluorooctanesulfonic acid	$^{13}C_8$ PFOS	507	80	50	80

Table S8. Mass Spectrometry tuning parameters for the isotopically labeled PFAS species in the extracted internal standard (EIS).

Compound	Abbreviation	Precursor (m/z)	Product (m/z)	Collision Energy (V)	Cone Voltage (V)
Perfluorobutanoic acid	$^{13}C_4$ PFBA	217	173	10	15
Perfluorohexanoic acid	$^{13}C_2$ PFHxA	315	270	10	15
Sodium perfluorohexane sulfonate	$^{18}O_2$ PFHxS	403	84	40	50
Perfluorononanoic acid	$^{13}C_5$ PFNA	468	424	10	15
Perfluorodecanoic acid	$^{13}C_2$ PFDA	515	471	10	15
Perfluoroundecanoic acid	$^{13}C_2$ PFUnA	565	521	25	30
Perfluorododecanoic acid	$^{13}C_2$ PFDoA	615	571	10	20
Perfluorooctanoic acid	$^{13}C_4$ PFOA	417	373	10	20
Sodium perfluorooctane sulfonate	$^{13}C_4$ PFOS	503	84	50	80

Table S9: Average concentrations (ng/L) of the detected PFASs in the stormwater samples.

Compound	Sampling time					
Perfluoroalkyl carboxylic acids (PFCAs)	**Aug-23**	**Sep-23**	**Oct-23**	**Dec-23**	**Jun-24**	**Jul-24**
PFNA	36±5.6	33±7	28±5.6	32±2.3	34±2.8	35±7
PFDA	18±2.8	20±2.8	14±2.8	13±4.2	20±2.3	23±4.2
PFUnA	12±4.2	12±2.3	7±1.1	11±4.4	13±2.1	15±1.4
PFDoA	12±2.1	15±1.4	10±2.8	11±2.1	12±2.3	14±2.8
PFTeDA	8±2.8	7±1.1	8±2.3	7±1.4	8±1.4	10±2.3
PFTrDA	7±1.4	6±1.1	5±0.2	11±1.1	7±0.2	9±2.8
PFOA	288±11.3	308±11.3	300±14.1	244±5.6	296±8.4	263±7
PFBA	78±5.6	73±4.2	68±4.2	64±2.8	75±2.8	78±4.2
PFPeA	53±4.2	53±4.4	48±4.4	62±2.3	51±2.8	55±4.4
PFMBA	10±2.8	10±2.3	6±1.1	15±1.4	11±1.4	14±2.3
PFHxA	141±7	132±10	127±10	115±7.0	132±5.6	134±8.4
PFHpA	20±2.8	20±2.3	18±2.3	18±2.8	20±2.8	22±2.3
PFMPA	20±5.6	25±7	18±2.8	21±4.2	25±4.2	26±5.6
Perfluorosulfonic Acids (PFSAs)						
PFHpS	12±2.8	11±1.4	6±0.2	17±4.2	13±1.4	15±1.4
PFOS	95±4.2	105±14.1	102±9.3	104±5.6	98±8.4	111±8.4
PFNS	18±3.5	16±2.1	12±2.8	16±1.4	18±1.4	20±2.3
PFDS	12±2.1	13±3.5	8±0.2	11±1.1	12±1.1	14±2.8
PFDoS	13±2.8	10±1.4	6±1.4	13±4.2	14±2.8	16±1.4
PFBS	308±25.4	291±15.5	286±8.4	239±12.7	291±9.9	303±11.3
PFPeS	20±2.1	18±2.3	13±1.4	16±2.8	20±2.8	27±4.2
PFHxS	44±5.6	41±7	39±4.2	37±4.4	42±2.3	46±5.6
Fluorotelomer Carboxylic Acids (FTCAs)						
3:3FTCA	17±2.8	19±4.2	14±2.3	14±1.4	17±4.2	19±1.4

5:3FTCA	16±5.6	17±2.8	12±1.4	16±5.6	18±2.3	20±2.8
7:3FTCA	14±2.8	12±4.2	8±2.8	12±2.8	15±1.4	16±2.3
Fluorotelomer Sulfonates (FTSs)						
4:2FTS	17±2.8	20±5.6	16±2.3	17±2.3	19±2.8	21±2.8
8:2FTS	25±4.2	23±5.6	18±3.5	34±2.3	25±4.2	28±3.8
6:2FTS	67±5.6	69±5	64±2.3	59±5.6	70±2.8	74±5.6
Perfluoroalkyl Sulfones (PASFs)						
NEtFOSAA	9±1.4	10±2.3	6±1.4	13±2.1	10±2.3	12±2.9
NEtFOSA	7±2.8	6±1.1	6±1.1	10±2.2	11±1.4	10±1.8
NEtFOSE	10±3.5	9±2.8	7±1.4	12±2.1	11±3.5	13±1.9
NMeFOSA	18±4.9	19±6.3	14±4.9	15±2.2	18±2.8	20±2.7
NMeFOSAA	12±3.5	8±1.4	6±0.2	10±1.4	8±1.4	10±1.5
NMeFOSE	20±5.6	22±2.1	18±3.5	22±2.8	20±2.3	22±2.1
PFOSA	16±2.8	15±1.4	10±2.3	16±2.3	18±2.8	20±1.6
NFDHA	50±2.8	49±5.6	43±4.4	43±4.2	48±4.2	53±4.3
Perfluoroether Carboxylic Acids (PFECAs)						
HFPO-DA	11±4.2	11±1.4	7±1.4	14±1.4	11±1.4	15±1.1
ADONA	15±4.9	17±3.5	12±1.1	14±2.8	16±2.8	18±1.9
Perfluoroether Sulfonic Acids (PFESAs)						
PFEESA	32±2.8	33±4.2	28±2.3	29±4.2	34±5.6	37±2.9
9Cl-PF3ONS	18±2.8	19±4.4	14±3.5	19±2.7	21±2.8	24±3.1
11Cl-PF3OUdS	13±1.2	11±3.2	7±0.2	16±1.4	14±2.3	15±1.3



Figure S1. Leachate lysimeter. (Image credit: Authors).

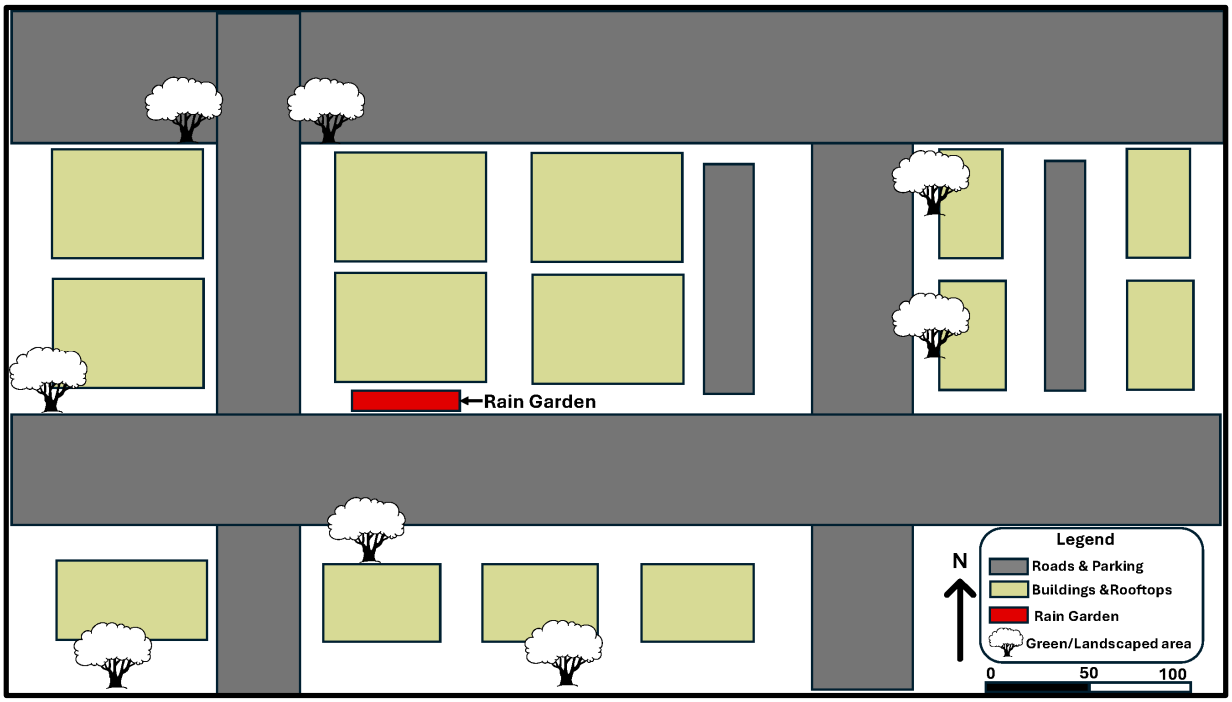


Figure S2. Author-prepared schematic of land use within the Secaucus rain-garden drainage area showing roads/parking (gray), buildings/rooftops (light yellow), and green/landscaped areas (tree symbol). The red area indicates the rain garden location.