Serum concentrations of eleven polyfluoroalkyl compounds in the U.S. Population: Data from the National Health and Nutrition Examination Survey (NHANES) 1999–2000

Supplementary Information

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The following are available as Supporting Information: Table including analyte name, abbreviated name, CAS numbers, and LOD for the 11 polyfluoroalkyl compounds included in this study (Table S1); table showing the distribution of NHANES 1999–2000 subjects by education and income (Table S2); table including the geometric mean and selected percentiles of PFDeA concentrations in serum (in µg/L) from NHANES 1999–2000 (Table S3); table including the Pearson correlation analysis of PFCs concentrations (Table S4); table including model-estimated geometric mean serum concentrations of PFOS, PFOA, PFHxS, and PFNA (Table S5); table including the least square geometric mean serum concentrations of PFOA and PFOS estimated at

the 25th, 50th, and 75th percentiles of age (Table S6); table including statistical significance differences between model-estimated geometric mean concentrations of PFOS and PFOA for various demographic groups (Table S7); table with the statistical significance differences between model-estimated geometric mean concentrations of PFNA and PFHxS for various demographic groups (Table S8).

Table S1. Analyte name, abbreviation, CAS numbers, and limit of detection (LOD) for the 11 polyfluoroalkyl compounds included in this study.

Analyte	Abbreviation	CAS	LOD (ng/mL) [a]
Perfluorooctane sulfonamide	PFOSA	754-91-6	0.05
2-(N-Methyl-perfluorooctane sulfonamido) acetic acid	Me-PFOSA-AcOH	NA	0.2
2-(N-Ethyl- Perfluorooctane sulfonamido) acetic acid	Et-PFOSA-AcOH	NA	0.2
Perfluorohexane sulfonic acid	PFHxS	355-46-4	0.1
Perfluorooctane sulfonic acid	PFOS	1763-23-1	0.2
Perfluoroheptanoic acid	PFHpA	375-85-9	0.4
Perfluorooctanoic acid	PFOA	335-67-1	0.1
Perfluorononanoic acid	PFNA	375-95-1	0.1
Pefluorodecanoic acid	PFDeA	335-76-2	0.2
Perfluoroundecanoic acid	PFUA	2058-94-8	0.2
Perflurododecanoic acid	PFDoA	307-55-1	0.2

[a] The limit of quantitation (LOQ) is three times the LOD. NA (not available).

Table S2. Distribution of participants by education and income[a]

Education		Income			
		Total	<20K	20K-45K	>45K
<HS	Sample Size	833	415	278	140
	Percentage	34.1	52.2	33.7	18.9
		100	46.6	34.9	19.5
=HS	Sample Size	272	97	108	67
	Percentage	25.4	21.2	29.8	24.9
		100	25.3	40.3	34.4
>HS	Sample Size	378	87	126	165
	Percentage	40.4	26.7	36.6	56.2
		100	20.1	31.1	48.8

[a]Income and education data were available for 1,483 of the 1,562 participants for whom we collected PFC data. Variance Estimation Method: Taylor Series (WR). <HS, less than high school diploma; =HS, high school diploma; >HS, more than high school diploma; <20K, household income < $20,000; 20K-45K, household income between $20,000 and $45,000; >45K, household income > $45,000.

1 Table S3. Geometric mean and selected percentiles of perfluorodecanoic acid (PFDeA) concentrations in serum (in µg/L) for the U.S.

2 population 12 years of age and older: Data from NHANES 1999–2000[a]

	Geometric Mean	Selected Percentiles						N (%)[b]
		10th	25th	50th	75th	90th	95th	
Total	ND	<LOD	<LOD	<LOD	<LOD	0.3 (0.3-0.5)	0.5 (0.4-1.0)	1,562 (25)
Age group (years)								
12-19	ND	<LOD	<LOD	<LOD	<LOD	<LOD	0.4 (0.3-0.4)	543 (15)
20-39	ND	<LOD	<LOD	<LOD	<LOD	<LOD	0.4 (0.3-0.6)	364 (24)
40-59	ND	<LOD	<LOD	<LOD	<LOD	<LOD	0.7 (0.4-1.4)	295 (26)
60+	ND	<LOD	<LOD	<LOD	<LOD	0.6 (0.3-1.4)	1.0 (0.5-1.8)	360 (32)
Sex								
Males	ND	<LOD	<LOD	<LOD	<LOD	0.3 (0.3-0.5)	0.4 (0.3-0.8)	743 (26)
Females	ND	<LOD	<LOD	<LOD	<LOD	0.4 (0.3-0.6)	0.6 (0.3-1.0)	819 (23)
Race/Ethnicity[c]								
MA	ND	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	584 (11)
NHB	ND	<LOD	<LOD	<LOD	<LOD	0.8 (0.5-1.2)	1.0 (0.6-2.3)	309 (39)
NHW	ND	<LOD	<LOD	<LOD	<LOD	0.4 (0.3-0.4)	0.5 (0.4-0.6)	529 (25)

[a] The 95% confidence intervals are shown in parentheses. LOD (limit of detection) is 0.2 ng/mL. [b]N (%), sample size (percentage of

detection). [c]MA (Mexican-Americans), NHB (Non-Hispanic blacks), NHW (Non-Hispanic whites). ND (not determined).

Table S4. Pearson correlation analysis of PFCs concentrations

Analyte		PFOS	PFOA	PFHxS	PFNA	Me-PFOSA -AcOH	Et-PFOSA -AcOH	PFOSA
PFOS	r	1.00	0.64	0.60	0.52	0.35	0.37	0.38
	P		<0.01	<0.01	0.01	0.36	<0.01	<0.01
PFOA	r		1.00	0.51	0.44	0.44	0.29	0.32
	P			<0.01	0.09	0.01	<0.01	<0.01
PFHxS	r			1.00	0.40	0.29	0.17	0.18
	P				0.03	<0.01	0.15	0.01
PFNA	r				1.00	0.26	0.01	0.18
	P					<0.01	<0.01	<0.01
Me-PFOSA-AcOH	r					1.00	0.38	0.37
	P						<0. 01	<0. 01
Et-PFOSA-AcOH	r						1.00	0.45
	P							<0. 01

[a]PFOS, perfluorooctane sulfonic acid; PFOA, perfluorooctanoic acid; PFHxS, perfluorohexane sulfonic acid; PFOSA, perfluorooctane sulfonamide; Et-PFOSA-AcOH, 2-(N-ethyl-perfluorooctane sulfonamido) acetic acid; Me-PFOSA-AcOH, 2-(N-methyl-perfluorooctane sulfonamido) acetic acid; PFNA, perfluorononanoic acid.

1 Table S5. Least square geometric means estimates of PFCs serum concentrations and their

2 corresponding 95% confidence limits (in parentheses)[a]

3	Variable[b]	PFOS[c]		PFOA[d]		PFNA		PFHxS[d]	
4									
5	<HS	28.9	(25.8-32.3)	5.0	(4.5-5.5)				
6	=HS	30.5	(28.1-33.1)	5.4	(4.9-5.9)				
7	>HS	32.9	(29.7-36.5)	5.6	(5.1-6.1)				
8	Female	28.5	(26.3-30.8)	4.9	(4.5-5.4)				
9	Male	33.7	(30.6-37.2)	5.7	(5.3-6.3)				
10	MA	23.0	(20.0-26.5)	4.0	(3.7-4.3)				
11	NHB	34.6	(28.3-42.3)	4.8	(4.3-5.4)				
12	NHW	31.5	(29.1-34.2)	5.6	(5.1-6.2)				
13	NSE			4.9	(4.5-5.4)				
14	PSMK			5.5	(4.9-6.1)				
15	SMK			5.4	(4.9-5.9)				
16	<20K					0.5	(0.4-0.6)		
17	20K-45K					0.5	(0.5-0.6)		
18	>45K					0.6	(0.5-0.7)		
19	Female:<HS					0.5	(0.4-0.6)	2.4	(2.0-2.8)
20	Female:=HS					0.4	(0.4-0.6)	1.7	(1.2-2.4)
21	Female:>HS					0.6	(0.5-0.7)	1.7	(1.5-1.9)
22	Male:<HS					0.5	(0.4-0.6)	2.2	(1.9-2.7)
23	Male:=HS					0.7	(0.6-0.8)	2.7	(2.4-3.0)
24	Male:>HS					0.6	(0.5-0.7)	3.1	(2.7-3.6)
25	Female:MA					0.3	(0.3-0.4)	1.1	(0.9-1.3)
26	Female:NHB					0.7	(0.6-0.9)	1.6	(1.2-2.3)
27	Female:NHW					0.5	(0.4-0.6)	2.1	(1.7-2.5)
28	Male:MA					0.5	(0.4-0.6)	2.3	(1.7-3.1)
29	Male:NHB					1.0	(0.8-1.3)	3.1	(2.5-3.9)
30	Male:NHW					0.6	(0.5-0.7)	2.7	(2.4-3.0)
31	MA:<HS							1.2	(1.0-1.6)
32	MA:=HS							1.8	(1.3-2.6)
33	MA:>HS							1.6	(1.4-2.0)
34	NHB:<HS							2.0	(1.4-2.9)
35	NHB:=HS							2.1	(1.5-2.7)
36	NHB:>HS							2.6	(2.1-3.2)
37	NHW:<HS							2.5	(2.2-3.0)
38	NHW:=HS							2.1	(1.7-2.7)
39	NHW:>HS							2.3	(2.1-2.6)
40									

1   [a]Concentrations in ng/mL. PFCs, polyfluoroalkyl compounds; PFOS, perfluorooctane sulfonic

2   acid; PFOA, perfluorooctanoic acid; PFHxS, perfluorohexane sulfonic acid; PFNA,

3   perfluorononanoic acid. [b]MA, Mexican-Americans; NHB, non-Hispanic blacks; NHW, non-

4   Hispanic whites; <HS, less than high school diploma; =HS, high school diploma; >HS, more than

5   high school diploma; NSE, nondetectable smoke exposure; PSMK, passive smoker; SMK,

6   smoker; <20K, household income < $20,000; 20K-45K, household income between $20,000 and

7   $45,000; >45K, household income > $45,000. [c]Computed at the mean age. [d]Computed at the

8   mean age and BMI.

1   Table S6. Least square geometric mean serum concentrations of PFOA and PFOS and their

2   corresponding 95% confidence limits (in parentheses) estimated at the 25th, 50th, and 75th

3   percentiles of age[a]

	Variable [b]	Age	Analyte	
			PFOS	PFOA
6	Non-Hispanic whites	26	30.3 (28.2-32.6)	5.8 (5.3-6.4)
7	Non-Hispanic whites	39	31.3 (29.0-33.9)	5.6 (5.1-6.1)
8	Non-Hispanic whites	55	32.6 (29.3-36.1)	5.3 (4.7-5.9)
9	Non-Hispanic blacks	26	31.3 (26.1-37.5)	5.0 (4.5-5.6)
10	Non-Hispanic blacks	39	34.0 (27.9-41.5)	4.8 (4.3-5.4)
11	Non-Hispanic blacks	55	37.7 (30.1-47.3)	4.6 (4.0-5.2)
12	Mexican-Americans	26	23.4 (20.6-26.7)	4.2 (3.8-4.5)
13	Mexican-Americans	39	23.1 (20.1-26.5)	4.0 (3.7-4.3)
14	Mexican-Americans	55	22.6 (19.4-26.4)	3.8 (3.4-4.1)
15	Male	26	33.9 (31.0-37.0)	6.5 (6.0-7.0)
16	Male	39	33.7 (30.7-37.0)	5.8 (5.3-6.3)
17	Male	55	33.6 (29.6-38.0)	5.1 (4.5-5.8)
18	Female	26	26.3 (24.6-28.2)	4.8 (4.4-5.3)
19	Female	39	28.1 (26.1-30.3)	4.9 (4.5-5.4)
20	Female	55	30.5 (27.7-33.6)	5.0 (4.5-5.5)

21

22   [a]Concentrations in ng/mL. Percentiles of age : 25th (age=26 years), 50th (age=39 years), and 75th

23   (age=55 years). PFOS, perfluorooctane sulfonic acid; PFOA, perfluorooctanoic acid. [b]The

24   differences among these demographic groups are presented in Table S7.

1   Table S7. Observed statistical significance values for differences between least squares geometric

2   mean concentrations of PFOA and PFOS for various demographic groups

3 Difference	Analyte	
4	PFOS	PFOA
5 $<$HS vs $=$HS	0.43	0.18
6 $<$HS vs $>$HS	0.01	$<$0.01
7 $=$HS vs $>$HS	0.15	0.43
8 M vs F: 25th age[b]	$<$0.01	$<$ 0.01
9 M vs F: 50th age	$<$0.01	$<$ 0.01
10 M vs F: 75th age	0.07	0.64
11 NHB vs MA: 25th age	0.04	
12 NHB vs MA: 50th age	0.01	
13 NHB vs MA: 75th age	$<$0.01	
14 NHW vs MA: 25th age	$<$0.01	
15 NHW vs MA: 50th age	$<$0.01	
16 NHW vs MA: 75th age	$<$0.01	
17 NHW vs NHB: 25th age	0.73	
18 NHW vs NHB: 50th age	0.34	
19 NHW vs NHB: 75th age	0.12	
20 NHB-MA		0.03
21 NHW-MA		$<$0.01
22 NHW-NHB		0.02
23 25th BMI :NSE vs PSMK[c]		0.10
24 25th BMI :NSE vs SMK		0.07
25 25th BMI :PSMK vs SMK		0.38
26 50th BMI :NSE vs PSMK		0.05
27 50th BMI :NSE vs SMK		0.09
28 50th BMI :PSMK vs SMK		0.97
29 75th BMI :NSE vs PSMK		0.04
30 75th BMI :NSE vs SMK		0.50
31 75th BMI :PSMK vs SMK		0.07

32

33   [a]PFOS, perfluorooctane sulfonic acid; PFOA, perfluorooctanoic acid; MA, Mexican-Americans;
34   NHB, non-Hispanic blacks; NHW, non-Hispanic whites; $<$HS, less than high school diploma;
35    $=$HS, high school diploma; $>$HS, more than high school diploma; NSE, nondetectable smoke
36   exposure; PSMK, passive smoker; SMK, smoker. [b]Percentiles of age : 25th (age=26 years), 50th
37   (age=39 years), and 75th (age=55 years). Estimated concentrations are presented in Table S6.
38   [c]Percentiles of BMI: 25th (BMI=23.2), 50th (BMI=26.8), and 75th (BMI=31.5).
39

Table S8. Observed statistical significance values for differences between least squares geometric
mean concentrations of PFNA and PFHxS for various demographic groups.[a]

DIFFERENCE	Analyte	
	PFNA	PFHxS
<20K vs 20K-45K	0.11	
<20K vs >45K	0.03	
20K-45K vs >45K	0.08	
<HS vs =HS:Female	0.37	
<HS vs =HS:Male	0.01	
<HS vs >HS:Female	0.01	
<HS vs >HS:Male	0.07	
=HS vs >HS:Female	0.04	
=HS vs >HS:Male	0.12	
Male vs Female:MA:<HS	0.01	
Male vs Female:MA:=HS	< 0.01	
Male vs Female:MA;>HS	0.06	
Male vs Female:NHB:<HS	0.13	
Male vs Female:NHB:=HS	< 0.01	
Male vs Female:NHB;>HS	0.12	
Male vs Female:NHW:<HS	0.47	
Male vs Female:NHW:=HS	< 0.01	
Male vs Female:NHW;>HS	1.00	
NHB vs MA:Female:25th age [b]	< 0.01	
NHB vs MA: Female:50th age	< 0.01	
NHB vs MA: Female:75th age	< 0.01	
NHB vs MA:Male:25th age	< 0.01	
NHB vs MA:Male:50th age	< 0.01	
NHB vs MA:Male:75th age	< 0.01	
NHW vs MA:Female:25th age	< 0.01	

#	DIFFERENCE	Analyte	
		PFNA	PFHxS
3	NHW vs MA: Female:50th age	< 0.01	
4	NHW vs MA: Female:75th age	< 0.01	
5	NHW vs MA:Male:25th age	0.10	
6	NHW vs MA: Male:50th age	0.10	
7	NHW vs MA: Male:75th age	0.11	
8			
9	NHW vs NHB: Female:25th age	0.23	
10	NHW vs NHB: Female:50th age	0.01	
11	NHW vs NHB: Female:75th age	< 0.01	
12	NHW vs NHB: Male:25th age	0.01	
13	NHW vs NHB: Male:50th age	< 0.01	
14	NHW vs NHB: Male:75th age	< 0.01	
15			
16	<HS vs=HS:Female:MA		0.21
17	<HS vs=HS:Female:NHB		0.13
18	<HS vs=HS:Female:NHW		0.04
19	<HS vs=HS:Male:MA		< 0.01
20	<HS vs=HS:Male:NHB		0.23
21	<HS vs=HS:Male:NHW		0.19
22			
23	<HS vs>HS:Female:MA		0.90
24	<HS vs>HS:Female:NHB		0.69
25	<HS vs>HS:Female::NHW		< 0.01
26	<HS vs>HS:Male:MA		< 0.01
27	<HS vs>HS:Male:NHB		< 0.01
28	<HS vs>HS:Male:NHW		0.10
29			
30	=HS vs>HS:Female:MA		0.35
31	=HS vs>HS:Female:NHB		0.29
32	=HS vs>HS:Female:NHW		0.90
33	=HS vs>HS:Male:MA		0.55
34	=HS vs>HS:Male:NHB		0.16
35	=HS vs>HS:Male:NHW		0.77
36	Male vs Female:MA:<HS:25thAge [c]		0.01
37	Male vs Female:MA:<HS:50thAge		0.13
38	Male vs Female:MA:<HS:75thAge		0.86
39	Male vs Female:MA:=HS:25thAge		< 0.01
40	Male vs Female:MA:=HS:50thAge		< 0.01

	DIFFERENCE	Analyte	
		PFNA	PFHxS
	Male vs Female:MA:=HS:75thAge		< 0.01
	Male vs Female:MA:>HS:25thAge		< 0.01
	Male vs Female:MA:>HS:50thAge		< 0.01
	Male vs Female:MA:>HS:75thAge		< 0.01
	Male vs Female:NHB:<HS:25thAge		0.02
	Male vs Female:NHB:<HS:50thAge		0.17
	Male vs Female:NHB:<HS:75thAge		0.94
	Male vs Female:NHB:=HS:25thAge		< 0.01
	Male vs Female:NHB:=HS:50thAge		< 0.01
	Male vs Female:NHB:=HS:75thAge		0.03
	Male vs Female:NHB:>HS:25thAge		< 0.01
	Male vs Female:NHB:>HS:50thAge		< 0.01
	Male vs Female:NHB:>HS:75thAge		0.01
	Male vs Female:NHW:<HS:25thAge		0.56
	Male vs Female:NHW:<HS:50thAge		0.59
	Male vs Female:NHW:<HS:75thAge		0.13
	Male vs Female:NHW:=HS:25thAge		< 0.01
	Male vs Female:NHW:=HS:50thAge		0.02
	Male vs Female:NHW:=HS:75thAge		0.15
	Male vs Female:NHW:>HS:25thAge		< 0.01
	Male vs Female:NHW:>HS:50thAge		< 0.01
	Male vs Female:NHW:>HS:75thAge		0.01
	NHB vs MA:Female:<HS		0.08
	NHB vs MA:Female:=HS		0.94
	NHB vs MA:Female:>HS		0.03
	NHB vs MA:Male:<HS		0.04
	NHB vs MA:Male:=HS		0.85
	NHB vs MA:Male:>HS		0.03
	NHW vs MA:Female:<HS		< 0.01
	NHW vs MA:Female:=HS		0.17
	NHW vs MA:Female:>HS		< 0.01
	NHW vs MA:Male:<HS		< 0.01
	NHW vs MA:Male:=HS		0.98
	NHW vs MA:Male:>HS		0.39

	DIFFERENCE	Analyte	
		PFNA	PFHxS
3	NHW vs NHB:Female:<HS		0.13
4	NHW vs NHB:Female:=HS		0.25
5	NHW vs NHB:Female:>HS		0.64
6	NHW vs NHB:Male:<HS		0.69
7	NHW vs NHB:Male:=HS		0.76
8	NHW vs NHB:Male:>HS		0.20

[a]PFNA, perfluorononanoic acid; PFHxS, perfluorohexane sulfonic acid; MA, Mexican-Americans; NHB, non-Hispanic blacks; NHW, non-Hispanic whites; <HS, less than high school diploma; =HS, high school diploma; >HS, more than high school diploma; <20K, household income < $20,000; 20K-45K, household income between $20,000 and $45,000; >45K, household income > $45,000. [b]Percentiles of age: 25th (age=26 years), 50th (age=39 years), and 75th (age=55 years).