Supplementary Material: Placental Transfer and Composition of Perfluoroalkyl Substances (PFASs): A Korean Birth Panel of Parent-Infant Triads

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Supplementary Materials and Methods

Table S1. MS/MS parameters for determination of perfluoroalkyl substances (PFASs) in serum.

Compound	Precursor Ion (m/z)	Product Ions (m/z)	Collision Energy (V)
PFPeA	263.0	218.9	−12
PFHxA	313.0	268.9	−12
		119.0	−30
PFHpA	363.0	318.9	−14
		168.9	−24
PFOA	413.0	368.9	−16
		168.8	−26
PFNA	463.0	418.8	−14
		218.9	−26
PFDA	513.0	468.9	−16
		218.9	−26
PFUnDA	562.9	518.9	−18
		268.8	−26
PFDoDA	613.0	569.0	−18
		168.8	−40
PFTrDA	663.0	619.1	−16
		168.9	−44
PFTeDA	713.1	669.1	−20
		168.9	−44
PFBS	298.9	79.8	−60
		99.0	−42
PFHxS	399.0	79.9	−78
		98.9	−54
PFOS	499.0	80.1	−92
		99.0	−70

Abbreviations: tandem mass spectrometry, MS/MS.

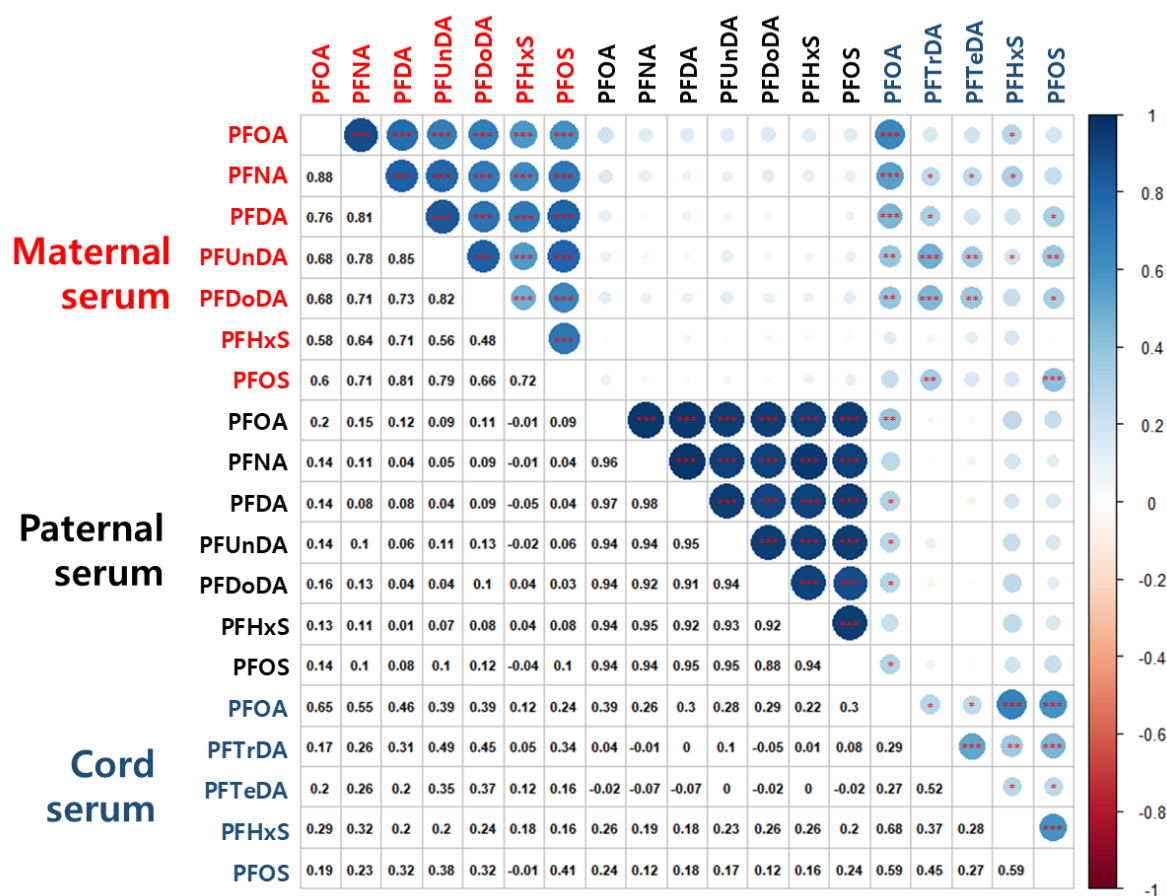**Table S2.** LC-MS/MS conditions for determination of perfluoroalkyl substances (PFASs) in serum.

Parameter		Condition				
HPLC	Column	YMC-Pack ODS-AQ, 2.0 × 150 mm, 3.0 μm				
	Mobile phase	A: 5 mM ammonium acetate and 0.02% formic acid in water B: methanol				
	Gradient	Time (min)	0	5	13	13.1	25
		A (%)	70	0	0	70	70
		B (%)	30	100	100	30	30
	Flow rate	200 μL/min				
	Injection volume	3 μL				
MS/MS	Mode	ESI negative				
	Curtain Gas	25 psi				
	Gas temperature	400 °C				
	Ion spray voltage	−4000 kV				
	Ion source gas 1	40 psi				
	Ion source gas 2	60 psi				
	Collision gas (CAD)	6				

Abbreviations: high-performance lipid chromatography, HPLC; tandem mass spectrometry, MS/MS.

Table S3. Limits of detection (LODs) of perfluoroalkyl substances (PFASs).

Compound	LOD (ng/mL)
PFPeA	0.07
PFHxA	0.06
PFHpA	0.05
PFOA	0.05
PFNA	0.03
PFDA	0.06
PFUnDA	0.05
PFDoDA	0.07
PFTrDA	0.05
PFTeDA	0.03
PFBS	0.08
PFHxS	0.05
PFOS	0.03

Supplementary Results

	PFOA	PFNA	PFDA	PFUnDA	PFDoDA	PFHxS	PFOS	PFOA	PFNA	PFDA	PFUnDA	PFDoDA	PFHxS	PFOS	PFOA	PFTrDA	PFTeDA	PFHxS	PFOS
PFOA																			
PFNA	0.88																		
PFDA	0.76	0.81																	
PFUnDA	0.68	0.78	0.85																
PFDoDA	0.68	0.71	0.73	0.82															
PFHxS	0.58	0.64	0.71	0.56	0.48														
PFOS	0.6	0.71	0.81	0.79	0.66	0.72													
PFOA	0.2	0.15	0.12	0.09	0.11	-0.01	0.09												
PFNA	0.14	0.11	0.04	0.05	0.09	-0.01	0.04	0.96											
PFDA	0.14	0.08	0.08	0.04	0.09	-0.05	0.04	0.97	0.98										
PFUnDA	0.14	0.1	0.06	0.11	0.13	-0.02	0.06	0.94	0.94	0.95									
PFDoDA	0.16	0.13	0.04	0.04	0.1	0.04	0.03	0.94	0.92	0.91	0.94								
PFHxS	0.13	0.11	0.01	0.07	0.08	0.04	0.08	0.94	0.95	0.92	0.93	0.92							
PFOS	0.14	0.1	0.08	0.1	0.12	-0.04	0.1	0.94	0.94	0.95	0.95	0.88	0.94						
PFOA	0.65	0.55	0.46	0.39	0.39	0.12	0.24	0.39	0.26	0.3	0.28	0.29	0.22	0.3					
PFTrDA	0.17	0.26	0.31	0.49	0.45	0.05	0.34	0.04	-0.01	0	0.1	-0.05	0.01	0.08	0.29				
PFTeDA	0.2	0.26	0.2	0.35	0.37	0.12	0.16	-0.02	-0.07	-0.07	0	-0.02	0	-0.02	0.27	0.52			
PFHxS	0.29	0.32	0.2	0.2	0.24	0.18	0.16	0.26	0.19	0.18	0.23	0.26	0.26	0.2	0.68	0.37	0.28		
PFOS	0.19	0.23	0.32	0.38	0.32	-0.01	0.41	0.24	0.12	0.18	0.17	0.12	0.16	0.24	0.59	0.45	0.27	0.59	

Row groups: Maternal serum (PFOA–PFOS), Paternal serum (PFOA–PFOS), Cord serum (PFOA, PFTrDA, PFTeDA, PFHxS, PFOS).

Figure S1. Spearman's correlation among perfluoroalkyl substances (PFASs) in maternal, paternal, and cord serum. The size and the color of the circles represent the correlation coefficients. Asterisks (*, **, and ***) on the circles represent $p < 0.05$, $p < 0.01$, and $p < 0.001$, respectively.