SUPPLEMENTAL INFORMATION

Identification of an analytical method interference for perfluorobutanoic acid (PFBA) in biological samples

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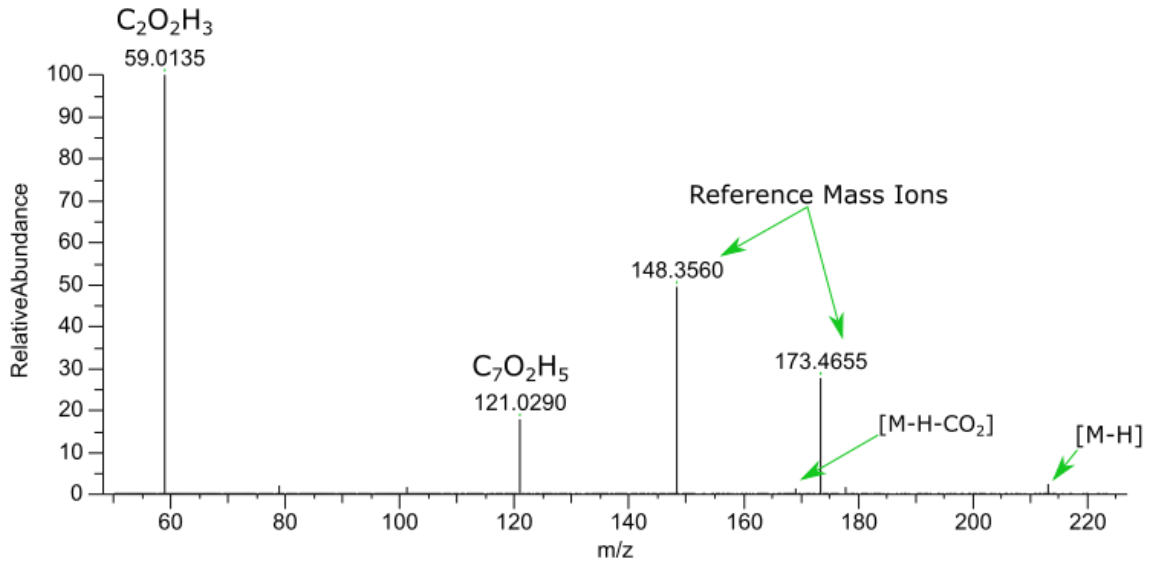
Supplemental Figure S1. Averaged fragmentation spectrum 213.1496 → [52.0000-223.0000] collected at 4Hz with a narrow isolation window (~1.3Da). Averaged spectrum is the result of 105 spectra at collision energy 10, 20, and 40 eV.

Supplemental Table S1. ESI source parameters for MS1 data collection using Agilent 6546 quadrupole time of flight mass spectrometer with electrospray ionization in negative mode.

Materials and Methods

Initial, targeted HPLC-MS/MS analysis of placental samples was completed as detailed in Bangma et al. 2020.[12] In brief, samples originally were analyzed using an Agilent 1100 High Performance Liquid Chromatography system (HPLC; Santa Clara, CA) coupled to an Applied Biosystems API 4000 triple quadrupole mass spectrometer (Applied Biosystems, Foster City, CA) with electrospray ionization in negative mode. Samples (5 µL) were injected onto a Kinetex 2.6 µ PFP analytical column, (50 mm x 3 mm). The full chromatographic run involved a ramping LC solvent gradient with methanol and de-ionized water both containing 2.5mmol/L ammonium acetate and lasted 70 minutes per sample. System chromatographic pressure maintained around 200 bar (system max pressure 400 bar). For the initial analysis, the reporting limit (RL) was calculated in two ways using an established NIST protocol: (1) using the lowest detectable calibrant divided by the mass of extracted sample or (2) taking the average amount of compound detected in the blanks divided by the mass of extracted sample. From the two methods of calculating the RL, the RL that was the highest for that PFAS and sample was designated as the respective RL for PFAS in that sample and as a result, PFBA RLs ranged between 0.268 and 0.502 ng/g.



Supplemental Figure S1. Averaged fragmentation spectrum 213.1496 → [52.0000-223.0000] collected at 4Hz with a narrow isolation window (~1.3Da). Averaged spectrum is the result of 105 spectra at collision energy 10, 20, and 40 eV.

Supplemental Table S1. ESI source parameters for MS1 data collection using Agilent 6546 quadrupole time of flight mass spectrometer with electrospray ionization in negative mode.

Parameter (unit)		
Mass range (m/z)	100-1000	
Gas temp (°C)	175	225
Drying gas (l/min)	11	3.0
Nebulizer (psi)	35	15
Sheath gas temp (°C)	275	125
Sheath gas flow (l/min)	11	3.0
VCap (V)	35000	
Capillary (µA)	0.056	
Nozzle voltage (Expt) (V)	1000	
Chamber (µA)	0.25	
Fragmentor (V)	105	
Skimmer (V)	45	
Oct 1 RF Vpp (V)	750	