# SUPPLEMENTAL MATERIAL

## Isomer Profiles of Perfluorochemicals in Matched Maternal, Cord and House Dust Samples: Manufacturing Sources and Transplacental Transfer

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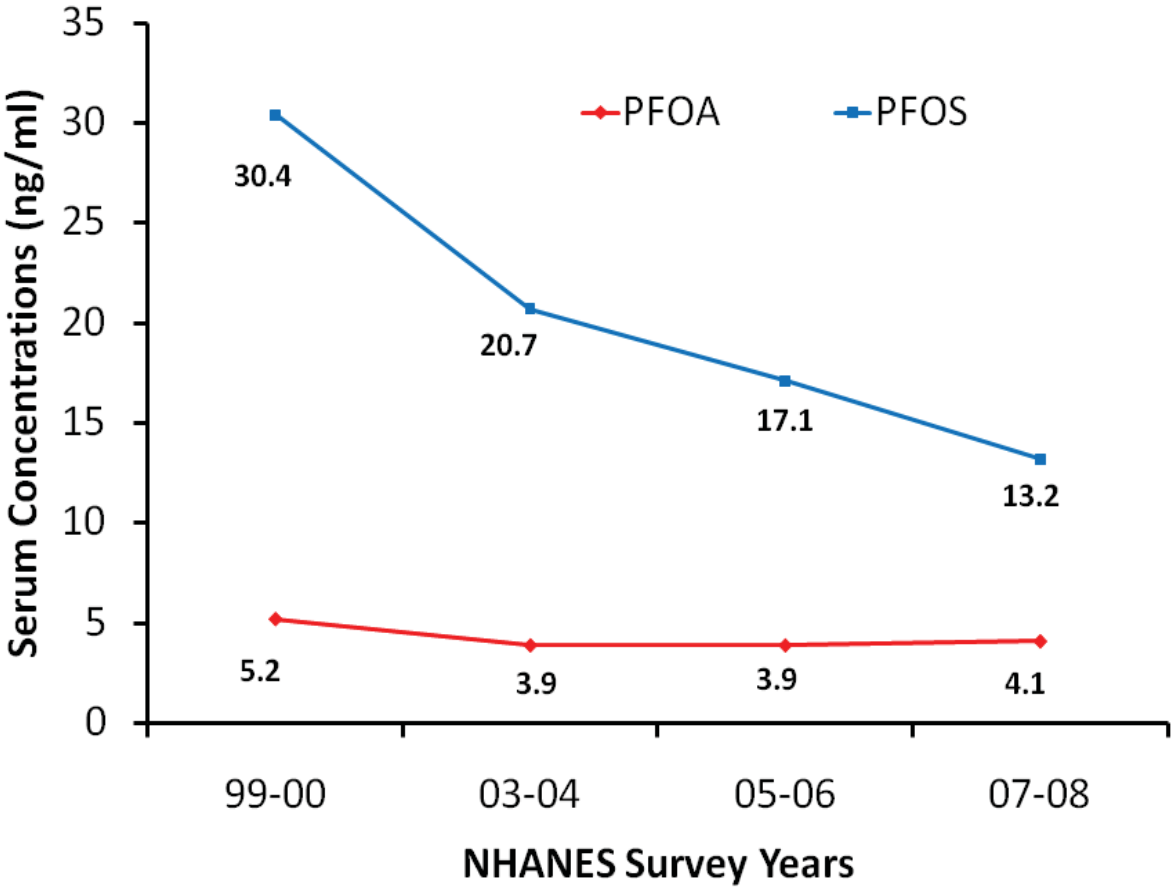
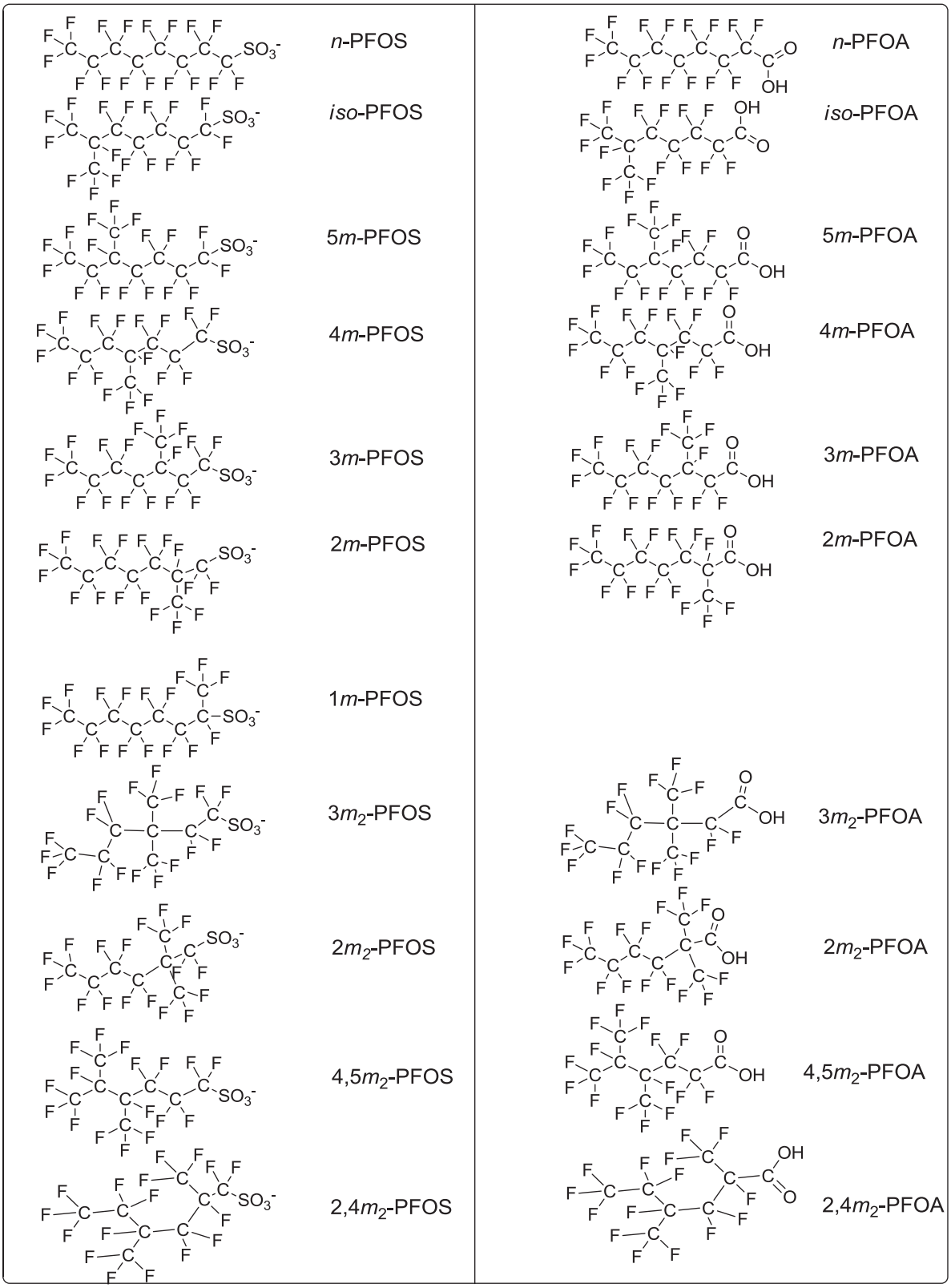
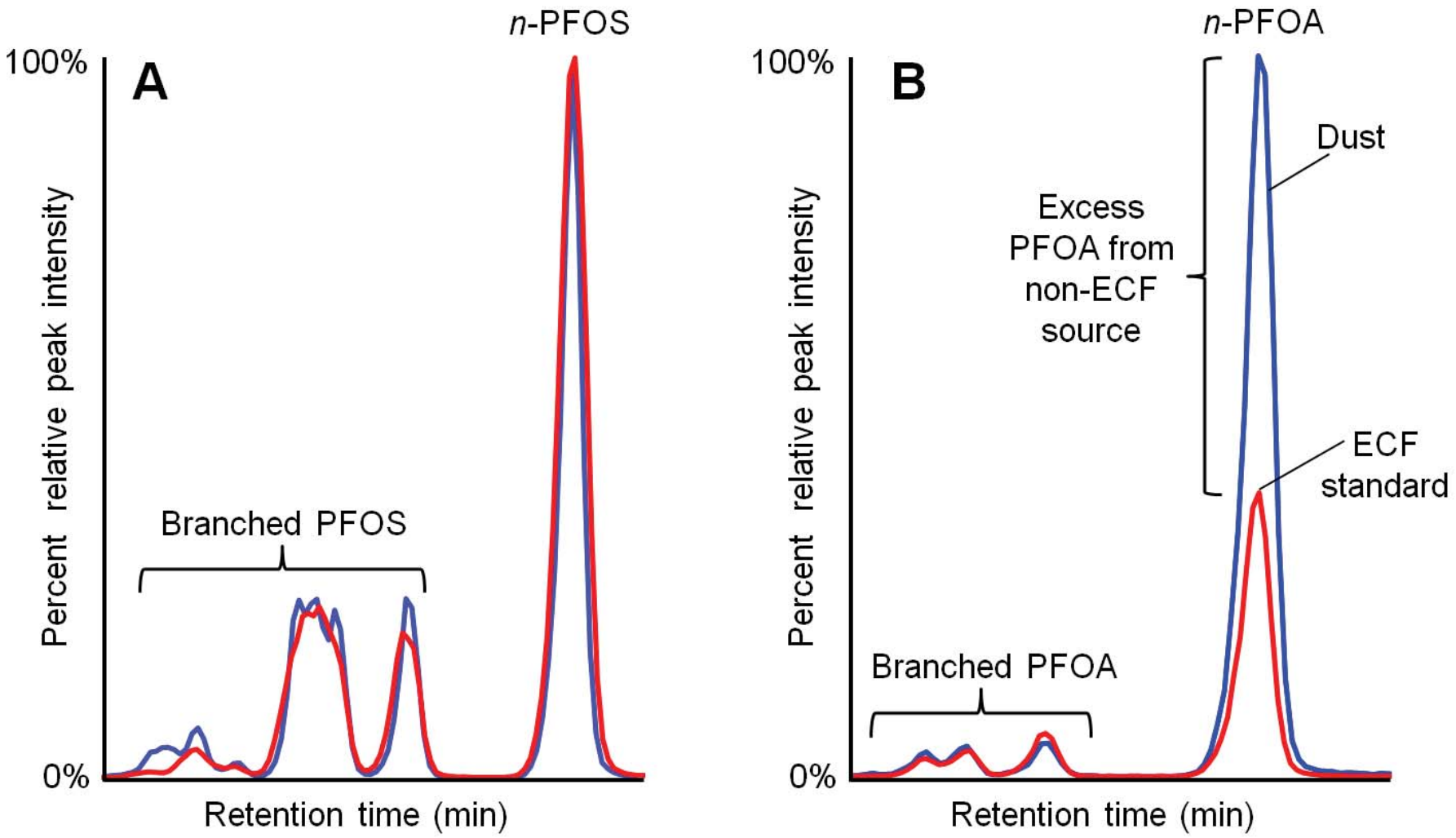



**Supplemental Material, Figure 1.** Trend in the geometric mean concentrations of PFOA and PFOS in the blood of Americans for the 10 year period from 1999 to 2008. PFOS has consistently declined, whereas PFOA has not declined since 2003/2004 and may be increasing. Data for the first 3 NHANES surveys are published data by the CDC, while the geometric means for 2007-2008 were calculated (after weight adjustment) using SAS data files available on the website of the National Center for Health Statistics of the CDC.




**Supplemental Material, Figure 2.** Structures of PFOS and PFOA linear and branched isomers. Note that 1*m*-PFOA does not exist. For geminal diperfluoromethyl-PFOS and geminal diperfluoromethyl-PFOA isomers, only the 3$m_2$ and 2$m_2$ are shown, although other such structures exist. Similarly for non-geminal diperfluoromethyl PFOS and PFOA only the 4,5 $m_2$ and 2,4 $m_2$ are shown, but other structures exist. In the isomer specific analysis, all the diperfluoromethyl PFOS isomers are grouped together and labeled as Σ$m_2$-PFOS. Other nomenclature systems have been proposed (Rayne et al. 2008).




**Supplemental Material Figure 3**. Isomer profiles in a house dust sample for (A) PFOS (*m/z* 499/80) and (B) PFOA (*m/z* 413/369). Red traces represent the isomer profile in a 3M ECF standard, while the blue trace represents the isomer profile in a dust sample. Each profile was normalized to the response of the branched isomers, such that the relative amount of linear isomer in each case is easily compared.

**Supplemental Material, Table 1**. Spike and recovery of native PFCs in serum and dust. Experiments were done in triplicate in each case and figures presented here represent arithmetic means.

| PFCs | Calf serum spiked at 0.5 ng/ml | | Calf serum spiked at 10 ng/ml | | Dust spiked at 60 ng/g | |
|---|---|---|---|---|---|---|
| | Mean % Recovery ±S.D | Range | Mean % Recovery ±S.D | Range | Mean % Recovery ± S.D | Range |
| PFBS | 93.2 ± 16.9 | 79.4-128 | - | - | 71.7 ± 8.1 | 64.0 - 83.0 |
| PFHxS | 79.0 ± 13.0 | 61.8-94.8 | 91.8 ± 12.5 | 75 – 112 | 90.2 ± 12 | 72.1 - 105 |
| PFHpS | 95.5 ± 15.1 | 76.8-123 | - | - | 92.3 ± 27 | 46.8 - 116 |
| PFOS | 82.7 ± 16.8 | 52.0-99.3 | 93.1 ± 11.9 | 82 – 117 | 107 ± 14 | 89.9 - 121 |
| PFDS | 109 ± 8.7 | 93.3-120 | 64.0 ± 8.2 | 52 – 74 | 32.2 ± 15 | 14.7 - 48.9 |
| PFBA | - | - | - | - | 74.3 ± 8.9 | 60.1 - 84.7 |
| PFPeA | - | - | - | - | 83.7 ± 11 | 65.7 - 95.0 |
| PFHxA | 94.2 ± 9.3 | 78.3-108 | - | - | 128 ± 9 | 119 - 141 |
| PFHpA | 78.1 ± 10.7 | 66.2-97.4 | - | - | 97.9 ± 21 | 72.6 - 130 |
| PFOA | 82.5 ± 9.4 | 67.1-99.1 | 95.3 ± 15.5 | 68 – 129 | 83.0 ± 5.3 | 74.6 - 88.5 |
| PFNA | 94.4 ± 5.4 | 84.7-102 | 94.8 ± 8.3 | 74 – 101 | 93.1 ± 20 | 72.0 - 117 |
| PFDA | 81.9 ± 7.6 | 71.6-93.8 | 96.9 ± 4.6 | 91 – 106 | 102 ± 9 | 92.1 - 112 |
| PFUnA | 92.8 ± 7.6 | 81.6-106 | 93.8 ± 10.4 | 78 – 116 | 107 ± 11 | 95.1 - 118 |
| PFDoA | 102 ± 4.9 | 97.3-113 | 93.3 ± 5.8 | 83 – 101 | 95.6 ± 6.3 | 91.3 - 106 |
| PFTrA | 122 ± 6.9 | 115.0-133 | 54.0 ± 11.0 | 33 - 70 | 79.2 ± 17 | 59.9 - 106 |
| PFTA | 105 ± 7.4 | 97.2-117 | - | - | 42.1 ± 24 | 10.2 - 76.3 |
| FOSA-M | 108 ± 7.6 | 92.3-116 | - | - | 42.7 ± 4.9 | 38.2 - 50.9 |

**Supplemental Material, Table 2.** Summary statistics of total PFC concentrations (ng/g, non isomer specific) in house dust samples (n=18 unless otherwise noted). To compute the descriptive statistics, values less than limit of detection (LOD) have been replaced by LOD/2.

| | Min | Max | Median | Mean | Geometric Mean | % above LOD |
|---|---|---|---|---|---|---|
| *Perfluoroalkyl sulfonates* | | | | | | |
| PFBS | <0.5 | 48 | <0.5 | 6.1 | 0.7 | 28 |
| PFHxS | 2.9 | 1300 | 14 | 140 | 21 | 100 |
| PFHpS | <0.5 | 46 | <0.5 | 4.1 | 0.6 | 22 |
| PFOS | <0.5 | 1300 | 37 | 180 | 39 | 94 |
| PFDS | <0.5 | 5.1 | 2.1 | 2.2 | 1.8 | 94 |
| *Perfluoroalkyl carboxylates* | | | | | | |
| PFBA | <0.5 | 42 | 2.6 | 9.2 | 3.6 | 94 |
| PFPeA | <0.5 | 93 | 5.2 | 17 | 4.9 | 83 |
| PFHxA | 2.3 | 390 | 35 | 77 | 33 | 100 |
| PFHpA | 1.4 | 320 | 21 | 55 | 19 | 100 |
| PFOA | 4.3 | 820 | 38 | 120 | 50 | 100 |
| PFNA | 1.4 | 220 | 15 | 44 | 18 | 100 |
| PFDA | 1.7 | 250 | 15 | 44 | 16 | 100 |
| PFUA | <0.5 | 240 | 6.1 | 31 | 8.0 | 94 |
| PFDoA | 1.4 | 160 | 10 | 36 | 13 | 100 |
| PFTrA | <0.5 | 67 | 2.4 | 9.9 | 2.3 | 78 |
| PFTA | <0.5 | 24 | 3.3 | 6.5 | 3.3 | 94 |
| *Perfluoroalkyl sulfonamides* | | | | | | |
| PFOSA | <0.5 | <0.5 | <0.5 | <0.5 | 0.3 | 0 |
| NMeFOSA (n=16) | 1.2 | 13.8 | 2.3 | 3.0 | 2.5 | 100 |
| NEtFOSA (n=16) | <0.06 | 2.8 | 0.15 | 0.55 | 0.14 | 50 |
| NMeFOSAA | <0.5 | 440 | 1.2 | 36 | 2.3 | 50 |
| NEtFOSAA | 3.2 | 240 | 27 | 58 | 32 | 100 |
| NMeFOSE (n=16) | 15 | 910 | 49 | 152 | 65 | 100 |
| NEtFOSE (n=16) | <0.02 | 190 | 10 | 14 | 5.3 | 88 |

**Supplementary Material, Table 3**. Descriptive statistics of the percentage of individual isomers of PFOS and PFOA in house dust samples (N=18), and mean (n=3 injections) of the 3M ECF standard.

| | **PFOS** | | | | | | | **PFOA** | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Linear | *iso* | 5*m* | 4*m* | 3*m* | 1*m* | $\sum m_2$ | Linear | *iso* | 5*m* | 4*m* | 3*m* | $\sum m_2$ | *tb* |
| Mean | 69.4 | 17.6 | 4.55 | 0.61 | 5.08 | 0.81 | 2.13 | 82.0 | 5.54 | 4.77 | 3.12 | 3.21 | 0.80 | 0.56 |
| SD[a] | 4.81 | 3.60 | 1.01 | 0.16 | 1.78 | 0.77 | 0.68 | 11.2 | 3.28 | 3.57 | 3.01 | 1.77 | 0.59 | 0.4 |
| Median | 70.7 | 16.2 | 4.33 | 0.58 | 5.1 | 0.58 | 2.00 | 84.2 | 4.99 | 4.21 | 2.69 | 3.37 | 0.68 | 0.55 |
| Min | 53.4 | 14.8 | 3.20 | 0.42 | <LOD[b] | <LOD | 1.34 | 59.0 | 0.46 | <LOD | <LOD | 0.19 | 0.05 | 0.03 |
| Max | 73.5 | 27.6 | 7.73 | 1.14 | 9.65 | 2.26 | 4.31 | 98.6 | 12.2 | 11.6 | 8.15 | 6.17 | 2.38 | 1.62 |
| Mean ECF Std | 70.2 | 18.1 | 4.83 | 0.58 | 4.18 | 0.46 | 1.69 | 73.4 | 9.05 | 7.35 | 5.80 | 2.98 | 0.74 | 0.67 |

[a] The low relative standard deviations (SDs) associated with the mean percentage of PFOS isomers in the 18 dust samples suggest a similar ECF source, contrasted to the high SD for linear PFOA, suggesting a mixture of ECF and telomer sources.
[b] LOD-Limit of detection.