

Supplemental Information

The Human Fecal Microbiome Contributes to the Biotransformation of the PFAS Surfactant 8:2 Monosubstituted Polyfluoroalkyl Phosphate Ester

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Table S1. LC-MS/MS analyte mass transitions, cone and collision energies

Compound	Precursor ion (m/z)	Product ion (m/z)	Cone energy (V)	Collision energy (V)
PFPeA	263.0	219.0	24	8
PFHxA	313.2	269.0	26	6
PFHpA	363.0	319.0	30	10
7:2 sFTOH	393.0	219.0	20	14
PFOA	413.0	369.0	30	10
7:2 Ketone	413.0	393.0	30	10
7:3 u acid	439.0	395.0	30	20
7:3 FTCA	441.0	337.0	15	10
8:2 FTUCA	457.0	393.2	10	18
PFNA	463.0	219.2	30	15
8:2 FTA	477.0	393.0	14	15
8:2 monoPAP	543.1	97.2	16	20
8:2 monoPAP_Qual	543.1	523.0	16	20

Table S2. Absolute recovery data for PFCA metabolites. Recovery values were obtained in triplicate after 1 hour incubation at 37°C in 100 mM phosphate buffer with the NADPH regeneration system.

	Average peak area of samples spiked before incubation	Peak area of samples spiked after incubation	Absolute Recovery (%)	Standard Error
PFPeA	1329	1055	126	21.1
PFHpA	8924	7220	124	5.9
PFHxA	5195	3549	146	13.6
PFOA	2825	2367	119	7.6
PFNA	64	49	130	16.8

Table S3. Metabolites reported as percent dose from incubation with NADPH and 6 µM 8:2 monoPAP.

	Liver S9	Intestine S9	Fecal suspension
1 min			
8:2 FTOH	2.94%	3.83%	23.05%
Oxidation Products	1.34%	0.22%	0.02%
Total	4.29%	4.06%	23.07%
5 min			
8:2 FTOH	2.15%	4.38%	26.02%
Oxidation Products	3.53%	0.24%	0.13%
Total	5.68%	4.62%	26.15%
10 min			
8:2 FTOH	3.39%	15.22%	27.49%
Oxidation Products	3.78%	0.22%	0.19%
Total	7.16%	15.45%	27.68%
30 min			
8:2 FTOH	6.01%	25.48%	29.89%
Oxidation Products	4.26%	0.20%	0.20%
Total	10.27%	25.67%	30.08%
60 min			
8:2 FTOH	11.14%	26.28%	27.67%
Oxidation Products	7.03%	0.21%	0.21%
Total	18.17%	26.50%	27.88%
120 min			
8:2 FTOH	12.01%	30.65%	25.93%
Oxidation Products	7.20%	0.19%	0.21%
Total	19.21%	30.84%	26.14%