Environ Health Perspect

DOI: 10.1289/EHP7169

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Supplemental Material

A Roadmap to the Structure-Related Metabolism Pathways of Per- and Polyfluoroalkyl Substances in the Early Life Stages of Zebrafish (*Danio rerio*)

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Figure S2. Metabolites of NMe-FOSA and NEt-FOSA. Nontargeted detection of metabolites in zebrafish larvae exposed to 5 μM of NMe-FOSA (top panel) and NEt-FOSA (bottom panel) was accomplished using the R scripts as detailed in method section. The sizes and colors of the dots are proportional to intensities. PFOS (46) and PFOSA (60) were confirmed with authentic standards (confidence level 1). Notes: NMe-FOSA, N-Methylperfluorooctanesulfonamide; NEt-FOSA, N-Ethylperfluorooctanesulfonamide; PFOSA, perfluorooctanesulfonamide; PFOS, perfluorooctanesulfonic acid.

Figure S3. Metabolites of perfluorooctane sulfonamide quaternary ammonium salt (PFOSAmS, 5). Tentative identification of metabolites from PFOSAmS was accomplished by interpreting the high-resolution MS^2 spectra of the three most abundant metabolite.

Figure S4. Representative chromatograms of shorter-chain PFCAs in zebrafish larvae metabolized from perfluoroalkyl carboxamides. (A) The chromatograms of 1H-PFPeA metabolized from amide 38 (top), and 1H-PFBA (bottom) directly exposed to zebrafish larvae. (B) The chromatograms of PFPeA metabolized from amide 19 (top), and PFHxA directly exposed to zebrafish larvae. (C) The chromatograms of PFBA metabolized from amide 38 (top), and PFBA directly exposed to zebrafish larvae. 1H-PFBA (4), PFHxA (20), PFBA (12) and PFPeA were confirmed with authentic standards (confidence level 1). The authentic standard of 1H-PFPeA was not available (confidence level 3). Note: PFBA, perfluorobutanoic acid; PFHxA, perfluorohexanoic acid; PFPeA, perfluoropentanoic Acid.

Figure S5. Time courses of carboxamides and polyfluoroalkyl carboxylic acids metabolites. Parent compound and carboxylic acids metabolites of 19, 31 and 38 were monitored separately across development in zebrafish exposed to 5 μM of each parent carboxamides. The peak areas of polyfluoroalkyl carboxylic acid metabolites were plotted against the left y-axis, while the peak area of carboxamide 38 was plotted against the right y-axis. Perfluorobutanoic acid (PFBA, 12) and perfluoropentanoic acid (PFPeA) were confirmed with authentic standards (confidence level 1). The authentic standard of 1H-PFPeA was not available (confidence level 3). The summary data can be found in Excel Table S8.

Figure S6. Hydrolysis products of 8:2 FTOH. Representative metabolites of 8:2 FTOH were detected in zebrafish larvae exposed to 5μM of 8:2 FTOH after 120h exposure. (A) Chromatograms of representative metabolites; (B) Proposed metabolism pathways. PFOA (74) was confirmed with authentic standards (confidence level 1). The authentic standards of 7:3 FTUCA, 8:2 FTUCA, 8:2 FTOH sulfate, 8:2 FTOH Gluc, 7:3 FTUCA cysteine were not available (confidence level 3). Note: FTOHs, fluorotelomer alcohols; FTUCA, fluorotelomer unsaturated carboxylic acids; PFOA, perfluorooctanoic acid.

Figure S7. Metabolites of two FTOH. Metabolites detected in zebrafish larvae exposed to H-6:1 FTOH (67) and 4:4 FTOH (40) were plotted versus the intensities of metabolites from 8:2 FTOH. Blue dots represent metabolites showing significantly higher fold-changes (FC>20, $p<0.05$, student's t-test) relative to 8:2 FTOH. The authentic standards of 1H-PFHxA, 6:1 FTOH sulfate and 6:1 FTOH glucuronide were not available (confidence level 3). Note: FTOHs, fluorotelomer alcohols; PFHxA, perfluorohexanoic acid.

Figure S8. Taurine metabolites of PFAS 49, 30, and 56 in zebrafish. Taurine conjugates from PFAS were identified by employing high-resolution MS^2 spectra. The authentic standards of metabolites were not available, so they were tentatively identified at confidence level 3.

Figure S9. Metabolite of 6:2 FTMAC. 6:2 FTOH sulfate was detected in zebrafish larvae exposed to 5 μM of compound 2. The chromatograms of 6:2 FTOH sulfate from compound 2 and the control are shown in the top and bottom panels. Note that minor background contamination was detected from the control. The proposed metabolism pathway of compound 2 is shown on the right. 6:2 FTOH (70) was confirmed with authentic standards (confidence level 1). The authentic standards of 6:2 FTOH sulfate was not available (confidence level 3). Note: FTOHs, fluorotelomer alcohols.

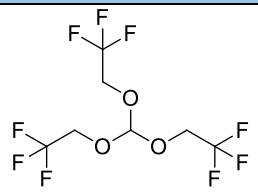
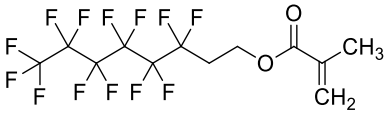
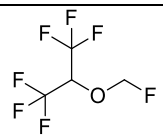
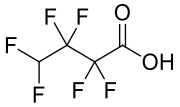
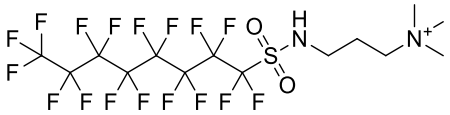
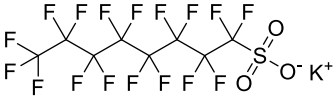
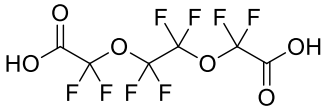
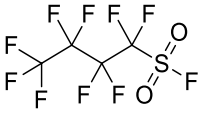
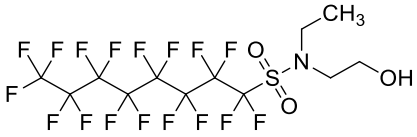
Figure S10. Hydrolysis of polyfluoroalkyl carboxamide 19 by hCES1. Reaction mixtures contained various concentrations 19 and 100 μg/L human recombinant human liver carboxylesterase 1 (*h*CES1) was incubated with 100 μL phosphate buffer at 37 °C for 1 hour, N=3. (A) The percentages of parent PFAS hydrolyzed by *h*CES1. (B) The concentrations of corresponding hydrolysis product perfluoropentanoic acid (PFPeA) detected. One-way ANOVA with Dunnett test was employed for the statistical test. Asterisk indicates *$0.01<p<0.05$, **$0.01<p<0.001$ and ***$p<0.0001$. Bars represent mean ± SD (n=3). Notes: The summary data can be found in Excel Tables S9 and S10.

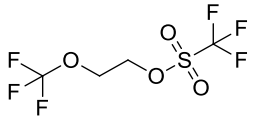
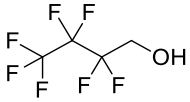
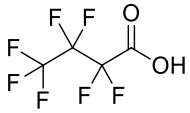
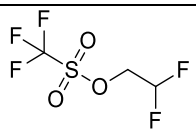
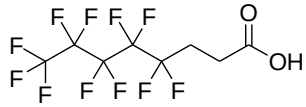
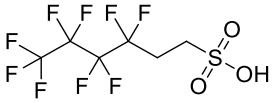
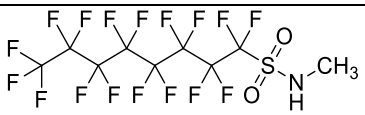
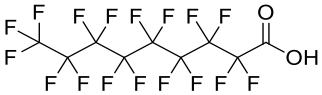
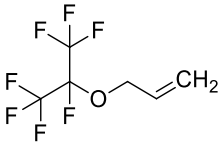
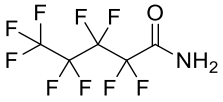
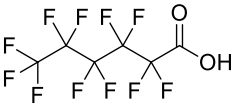
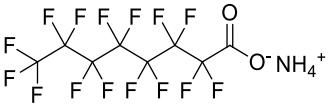
Figure S11. Structures of hydrolysis products detected in human recombinant human liver carboxylesterase 1 (*h*CES1) hydrolysis assay. Perfluorobutanoic acid (PFBA, 12) and perfluoropentanoic acid (PFPeA) were confirmed with authentic standards, the confidence level was assigned to level 1. The authentic standards of 1H-PFPeA and 4:3 fluorotelomer carboxylic acid (FTCA) were not available, so they were confirmed with high resolution MS^1 and MS^2 spectra at confidence level 3.

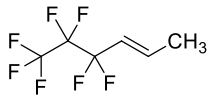
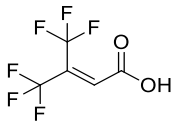
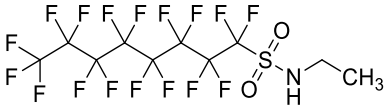
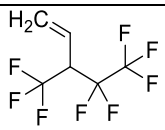
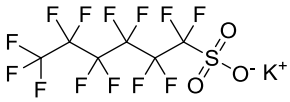
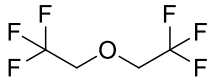
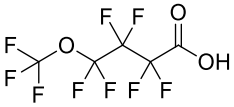
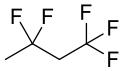
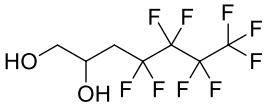
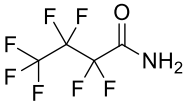
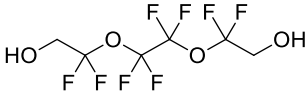
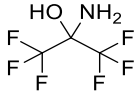
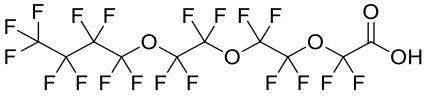
References

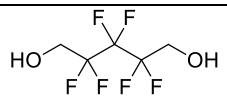
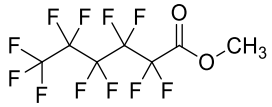
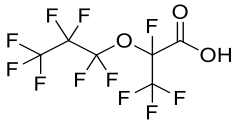
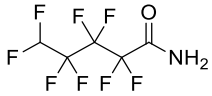
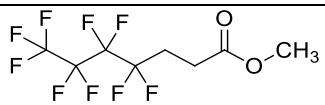
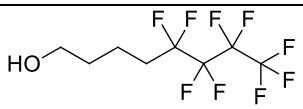
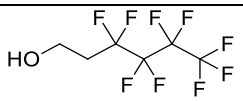
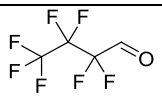
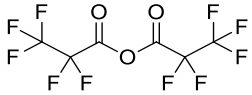
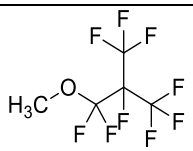
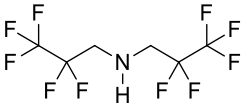
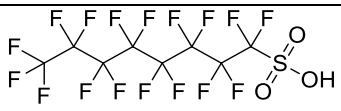
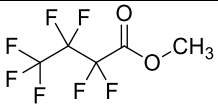
Additional File- Excel Document

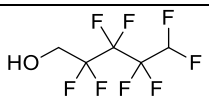
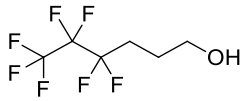
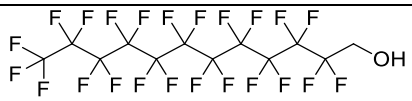
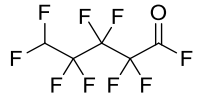
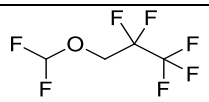
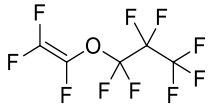
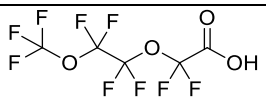
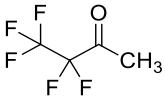
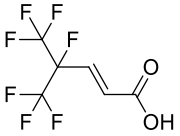
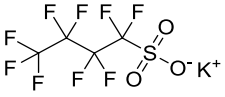
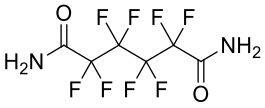
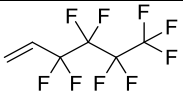
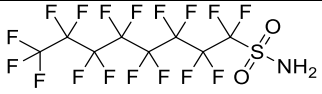
Table S1: Chemical information and structures of 74 PFAS from the U.S. EPA PFASs screening library.

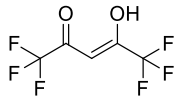
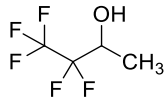
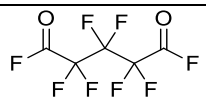
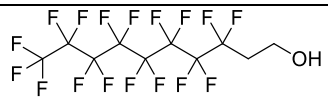
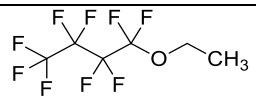
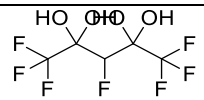
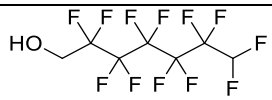
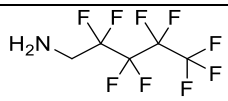
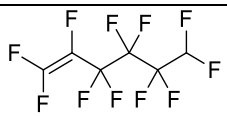
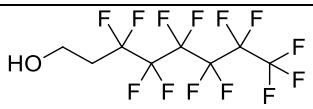
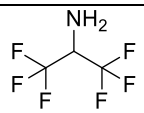
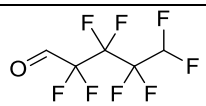
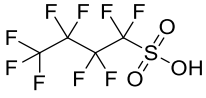
ID	CAS	Preferred Name	Abbreviation	Category	Vapor pressure[a]	Molecular Formula	Structure
1	58244-27-2	Tris(Trifluoroethoxy) methane		Ether	0.46	C7H7F9O3	
2	2144-53-8	6:2 Fluorotelomer methacrylate	6:2 FTMAC	Ester	0	C12H9F13O2	
3	28523-86-6	Sevoflurane		Ether	246.49	C4H3F7O	
4	679-12-9	4H-Perfluorobutanoic acid	H-PFBA	Carboxylate	0.91	C4H2F6O2	
5	1652-63-7	Perfluorooctanesulfonamido ammonium iodide	PFOSAmS	Sulfonamide	0	C14H16F17N2O2S	
6	2795-39-3	Potassium perfluorooctanesulfonate	Potassium PFOS	Sulfonate	0.01	C8F17KO3S	
7	55621-21-1	Perfluoro-3,6-dioxaoctane-1,8-dioic acid		Carboxylate	0	C6H2F8O6	
8	375-72-4	Perfluorobutanesulfonyl fluoride	PBSF	Others	3845.09	C4F10O2S	
9	1691-99-2	N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide	NEt-FOSE	Sulfonamide	0	C12H10F17NO3S	

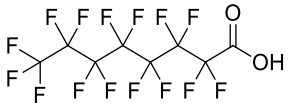
10	32971 0-76-1	2-(Trifluoromethoxy)ethyl trifluoromethanesulfonate		Ether	0.78	C4H4F6 O4S	
11	375-01-9	Heptafluorobutanol	HFB	Alcohol	39.35	C4H3F7 O	
12	375-22-4	Perfluorobutanoic acid	PFBA	Carboxylate	5.82	C4HF7O 2	
13	74427 -22-8	2,2-Difluoroethyl triflate		Others	19.36	C3H3F5 O3S	
14	91463 7-49-3	2H,2H,3H,3H-Perfluorooctanoic acid	5:3 FTCA	Carboxylate	0.08	C8H5F1 1O2	
15	75712 4-72-4	4:2 Fluorotelomer sulfonic acid	4:2 FTS	Sulfonate	0.02	C6H5F9 O3S	
16	31506 -32-8	N-Methylperfluorooctane sulfonamide	NMe-FOSA	Sulfonamide	0	C9H4F1 7NO2S	
17	375-95-1	Perfluorononanoic acid	PFNA	Carboxylate	0.07	C9HF17 O2	
18	15242 -17-8	Allyl perfluoroisopropyl ether		Ether	271.94	C6H5F7 O	
19	13485 -61-5	Nonafluoropentanamide		Carboxamide	3.07	C5H2F9 NO	
20	307-24-4	Perfluorohexanoic acid	PFHxA	Carboxylate	1.65	C6HF11 O2	
21	3825-26-1	Ammonium perfluorooctanoate	Ammonium PFOA	Carboxylate	0.34	C8H4F1 5NO2	

22	355-95-3	1-Propenylperfluoropropane		Others	2451.97	C6H5F7	
23	1763-28-6	3,3-Bis(trifluoromethyl)-2-propenoic acid		Carboxylate	1.64	C5H2F6O2	
24	4151-50-2	N-Ethylperfluorooctanesulfonamide	NEt-FOSA	Sulfonamide	0	C10H6F17NO2S	
25	239795-57-4	2-Vinylperfluorobutane		Others	2856.11	C6H3F9	
26	3871-99-6	Potassium perfluorohexanesulfonate	Potassium PFHxS	Sulfonate	0.02	C6F13KO3S	
27	333-36-8	Flurothyl		Ether	226.66	C4H4F6O	
28	863090-89-5	Perfluoro(4-methoxybutanoic) acid	PFMOBA	Carboxylate	0.46	C5HF9O3	
29	406-58-6	1,1,1,3,3-Pentafluorobutane	R365mfc	Others	2807.55	C4H5F5	
30	125070-38-4	3-(Perfluoro-2-butyl)propane-1,2-diol		Alcohol	0.04	C7H7F9O2	
31	662-50-0	Heptafluorobutyramide		Carboxamide	0.14	C4H2F7NO	
32	129301-42-4	1H,1H,8H,8H-Perfluoro-3,6-dioxaoctane-1,8-diol		Alcohol	0	C6H6F8O4	
33	31253-34-6	2-Aminohexafluoropropan-2-ol		Others	0.7	C3H3F6NO	
34	330562-41-9	Perfluoro-3,6,9-trioxatridecanoic acid		Carboxylate	0.01	C10HF19O5	

35	376-90-9	Hexafluoroamylene glycol		Alcohol	0.12	C5H6F6O2	
36	424-18-0	Methyl perfluorohexanoate	MePFOA	Ester	356.7	C7H3F11O2	
37	13252-13-6	Perfluoro-2-methyl-3-oxahexanoic acid	GenX	Carboxylate	0.06	C6HF11O3	
38	355-81-7	Perfluoropentanamide		Carboxamide	0.11	C5H3F8NO	
39	132424-36-3	Methyl 2H,2H,3H,3H-perfluoroheptanoate		Ester	152.32	C8H7F9O2	
40	3792-02-7	4:4 Fluorotelomer alcohol	4:4 FTOH	Alcohol	8.75	C8H9F9O	
41	2043-47-2	4:2 Fluorotelomer alcohol	4:2 FTOH	Alcohol	47.07	C6H5F9O	
42	375-02-0	Perfluorobutyraldehyde		Others	2080.3	C4HF7O	
43	356-42-3	Pentafluoropropanoic anhydride	PFPA	Others	534.29	C6F10O3	
44	163702-08-7	Perfluoroisobutyl methyl ether		Ether	352.29	C5H3F9O	
45	883498-76-8	Bis(1H,1H-perfluoropropyl)amine		Others	7.23	C6H5F10N	
46	1763-23-1	Perfluorooctanesulfonic acid	PFOS	Sulfonate	0.01	C8HF17O3S	
47	356-24-1	Methyl heptafluorobutyrate	MeHFB	Ester	288.29	C5H3F7O2	

48	355-80-6	1H,1H,5H-Perfluoropentanol		Alcohol	45.59	C5H4F8O	
49	679-02-7	3-(Perfluoropropyl)propanol		Alcohol	38.97	C6H7F7O	
50	423-65-4	11:1 Fluorotelomer alcohol	11:1 FTOH	Alcohol	0.02	C12H3F23O	
51	813-03-6	5H-Octafluoropentanoyl fluoride		Others	1572.91	C5HF9O	
52	56860-81-2	Difluoromethyl 1H,1H-perfluoropropyl		Ether	263.35	C4H3F7O	
53	1623-05-8	Heptafluoropropyl trifluorovinyl ether		Ether	212.15	C5F10O	
54	151772-58-6	Perfluoro-3,6-dioxaheptanoic acid	PDHA	Carboxylate	1.54	C5HF9O4	
55	374-41-4	Methyl perfluoroethyl ketone		Others	801.62	C4H3F5O	
56	243139-64-2	3-(Perfluoroisopropyl)-2-propenoic acid		Carboxylate	1.76	C6H3F7O2	
57	29420-49-3	Potassium perfluorobutanesulfonate	Potassium PFBS	Sulfonate	0.5	C4F9KO3S	
58	355-66-8	Octafluoroadipamide		Carboxamide	0	C6H4F8N2O2	
59	19430-93-4	1H,1H,2H-Perfluoro-1-hexene	PFH	Others	2133.94	C6H3F9	
60	754-91-6	Perfluorooctanesulfonamide	PFOSA	Sulfonamide	0.18	C8H2F17NO2S	

61	1694-30-0	3H-Perfluoro-4-hydroxy-3-penten-2-one		Alcohol	283.31	C5H2F6O2	
62	374-40-3	1-Pentafluoroethylethanol		Alcohol	39.48	C4H5F5O	
63	678-78-4	Perfluoroglutaryl difluoride		Others	4008.51	C5F8O2	
64	678-39-7	8:2 Fluorotelomer alcohol	8:2 FTOH	Alcohol	0.05	C10H5F17O	
65	16370 2-05-4	Ethyl perfluorobutyl ether		Ether	188.89	C6H5F9O	
66	77953-71-0	3H-Perfluoro-2,2,4,4-tetrahydroxypentane		Alcohol	0	C5H5F7O4	
67	335-99-9	Dodecafluoroheptanol	H-6:1 FTOH	Alcohol	6.31	C7H4F12O	
68	355-27-1	1H,1H-Perfluoropentylamine		Others	151.42	C5H4F9N	
69	1767-94-8	6H-Perfluorohex-1-ene		Others	358	C6HF11	
70	647-42-7	6:2 Fluorotelomer alcohol	6:2 FTOH	Alcohol	4.86	C8H5F13O	
71	1619-92-7	2-Amino-2H-perfluoropropane		Others	133.26	C3H3F6N	
72	2648-47-7	5H-Perfluoropentanal		Others	915.14	C5H2F8O	
73	375-73-5	Perfluorobutanesulfonic acid	PFBS	Sulfonate	0.5	C4HF9O3S	

74	335-67-1	Perfluorooctanoic acid	PFOA	Carboxylate	0.34	C8HF15O2	

[a]Vapor pressures were predicted by Open Structure-activity/property Relationship App (OPERA) developed by the U. S. EPA.

Table S2: Among 74 PFAS, 36 ionizable PFAS were subjected for BCF analysis and 25 PFAS were detectable in zebrafish larvae. 31 PFAS from five structural categories prone to metabolism were selected for metabolite profiling with non-targeted analysis.

ID	CAS	Ionizable[a]	BCF[b]	Metabolite profiling[c]	Number of metabolite features[d]	Representative metabolites[e]
1	58244-27-2	N	N	N	-	-
2	2144-53-8	N	N	Y	1	6:2 FTOH sulfate (See Figure S9)[f]
3	28523-86-6	N	N	N	-	-
4	679-12-9	Y	Y	N	-	-
5	1652-63-7	Y	Y	Y	74	Demethylated metabolites, PFOS (See Figure 2C)
6	2795-39-3	Y	Y	N	-	-
7	55621-21-1	Y	N	N	-	-
8	375-72-4	N	N	N	-	-
9	1691-99-2	N	N	Y	51	NEt-FOSA
10	329710-76-1	N	N	N	-	-
11	375-01-9	Y	N	Y	0	-
12	375-22-4	Y	Y	N	-	-
13	74427-22-8	N	N	N	-	-
14	914637-49-3	Y	Y	Y	5	Taurie conjugates (See Figure 6B)
15	757124-72-4	Y	Y	N	-	-
16	31506-32-8	Y	Y	Y	33	PFOS (See Figure S2)
17	375-95-1	Y	Y	N	-	-
18	15242-17-8	N	N	N	-	-
19	13485-61-5	N	N	Y	1	PFPeA (See Figure 3)
20	307-24-4	Y	Y	N	-	-
21	3825-26-1	Y	Y	N	-	-
22	355-95-3	N	N	N	-	-

23	1763-28-6	Y	Y	Y	0	-
24	4151-50-2	Y	Y	Y	72	PFOS (See Figure S2)
25	239795-57-4	N	N	N	-	-
26	3871-99-6	Y	Y	N	-	-
27	333-36-8	Y	N	N	-	-
28	863090-89-5	Y	Y	N	-	-
29	406-58-6	N	N	N	-	-
30	125070-38-4	N	N	Y	24	Sulfate, glucuronide and taurine conjugates, carboxylates (See Figure S8)
31	662-50-0	N	N	Y	1	PFBA (See Figure 3)
32	129301-42-4	Y	Y	Y	10	Sulfate and glucuronide conjugate, carboxylates (See Figure 4B)
33	31253-34-6	N	N	N	-	-
34	330562-41-9	Y	Y	N	-	-
35	376-90-9	Y	Y	Y	1	Sulfate conjugate
36	424-18-0	Y	N	Y	0	-
37	13252-13-6	Y	N	N	-	-
38	355-81-7	Y	Y	Y	1	1H-PFBA (See Figure 3)
39	132424-36-3	N	N	Y	46	Taurine conjugate (See Figure 6D)
40	3792-02-7	N	N	Y	72	Sulfate, glucuronide and taurine conjugates, carboxylates (See Figure 4D)
41	2043-47-2	N	N	Y	28	Sulfate, glucuronide and taurine conjugates, carboxylates

42	375-02-0	N	N	N	-	-
43	356-42-3	N	N	N	-	-
44	163702-08-7	N	N	N	-	-
45	883498-76-8	N	N	N	-	-
46	1763-23-1	Y	Y	N	-	-
47	356-24-1	N	N	Y	0	-
48	355-80-6	Y	N	Y	11	Sulfate, glucuronide conjugates
49	679-02-7	N	N	Y	57	Sulfate, glucuronide and taurine conjugates, carboxylates (See Figure S8)
50	423-65-4	Y	N	Y	9	Carboxylate, sulfate and glucuronide conjugates
51	813-03-6	N	N	N	-	-
52	56860-81-2	N	N	N	-	-
53	1623-05-8	N	N	N	-	-
54	151772-58-6	Y	Y	N	-	-
55	374-41-4	N	N	N	-	-
56	243139-64-2	Y	Y	Y	1	Taurine conjugate (See Figure S8)
57	29420-49-3	Y	Y	N	-	-
58	355-66-8	Y	N	Y	0	-
59	19430-93-4	N	N	N	-	-
60	754-91-6	Y	Y	Y	6	PFOS
61	1694-30-0	Y	N	Y	0	-
62	374-40-3	N	N	Y	0	-
63	678-78-4	N	N	N	-	-
64	678-39-7	N	N	Y	14	Sulfate, glucuronide and taurine conjugates,

						carboxylates (See Figure S6)
65	163702-05-4	N	N	N	-	-
66	77953-71-0	Y	N	Y	0	-
67	335-99-9	N	N	Y	3	Sulfate, glucuronide conjugates and carboxylates (See Figure S7)
68	355-27-1	Y	N	N	-	-
69	1767-94-8	N	N	N	-	-
70	647-42-7	N	N	Y	12	Sulfate, glucuronide and taurine conjugates, carboxylates
71	1619-92-7	N	N	N	-	-
72	2648-47-7	N	N	N	-	-
73	375-73-5	Y	Y	N	-	-
74	335-67-1	Y	Y	N	-	-

[a] The 36 ionizable PFAS detectable by LC-MS were highlighted as 'Y'.
[b] The 25 PFAS detectable in zebrafish larvae for BCF analysis were highlighted as 'Y'.
[c] The 31 PFAS selected for metabolite profiling were highlighted as 'Y'.
[d] The number of metabolite features detected for each PFAS. Note that the number of metabolite features might be overestimated for some PFASs as low-abundance features might be attributed to impurities of standards. Thus, high abundance metabolites were selected for structure prediction as described in the method section.
[e] The representative metabolites with high abundances.
[f] The structures of representative metabolites were shown in corresponding figures.

Table S3: Summary of 28 PFAS that were detectable in zebrafish larvae, including concentrations in medium (μM), recovery (%) and method detection limit (MDL) (ng/g).

ID	CAS	Preferred Name	Abbreviation	Category	Concentration in medium (μM)		Recovery (%)	MDL (ng/g)
					5μM	0.5μM		
4	679-12-9	4H-Perfluorobutanoic acid	H-PFBA	Carboxylates	3.8 ± 0.09	0.31 ± 0.02	95.86 ± 2.73	0.4
5	1652-63-7	Perfluorooctanesulfonamido ammonium iodide	PFOSAmS	Sulfonamides	4.51 ± 0.08	0.36 ± 0.01	94.96 ± 1.79	0.35
6	2795-39-3	Potassium perfluorooctanesulfonate	Potassium PFOS	Sulfonates	3.35 ± 0.03	0.32 ± 0.01	87.45 ± 3.88	0.1
12	375-22-4	Perfluorobutanoic acid	PFBA	Carboxylates	3.13 ± 0.08	0.31 ± 0.03	90.73 ± 17.88	0.58
14	914637-49-3	2H,2H,3H,3H-Perfluorooctanoic acid	5:3 FTCA	Carboxylates	4.03 ± 0.2	0.48 ± 0.02	99.13 ± 3.49	0.01
15	757124-72-4	4:2 Fluorotelomer sulfonic acid	4:2 FTS	Sulfonates	4.21 ± 0.07	0.31 ± 0.02	86.98 ± 1.64	0.1
16	31506-32-8	N-Methylperfluorooctanesulfonamide	NMe-FOSA	Sulfonamides	3.76 ± 0.49	0.35 ± 0.01	92.89 ± 10.35	0.74

17	375-95-1	Perfluorononanoic acid	PFNA	Carboxylates	3.65 ± 0.09	0.39 ± 0.01	93.89 ± 6.7	0.07
19	13485-61-5	Nonafluoropentanamide		Amides	4.77 ± 0.24	0.29 ± 0.05	85.02 ± 3.69	1.72
20	307-24-4	Perfluorohexanoic acid	PFHxA	Carboxylates	4.51 ± 0.11	0.34 ± 0.01	86.28 ± 5.65	0.11
21	3825-26-1	Ammonium perfluorooctanoate	Ammonium PFOA	Carboxylates	3.67 ± 0.06	0.38 ± 0.01	87.73 ± 2.27	0.1
23	1763-28-6	3,3-Bis(trifluoromethyl)-2-propenoic acid		Carboxylates	3.07 ± 0.07	0.33 ± 0.07	75.12 ± 9.59	0.42
24	4151-50-2	N-Ethylperfluorooctanesulfonamide	NEt-FOSA	Sulfonamides	4.01 ± 0.18	0.44 ± 0.01	79.1 ± 2.79	0.09
26	3871-99-6	Potassium perfluorohexanesulfonate	Potassium PFHxS	Sulfonates	4.37 ± 0.05	0.33 ± 0.03	94.27 ± 4.8	0.28
28	863090-89-5	Perfluoro(4-methoxybutanoic) acid	PFMOBA	Ethers	4.12 ± 0.09	0.31 ± 0.01	97.91 ± 8.33	0.09
31	662-50-0	Heptafluorobutyramide		Amides	4.79 ± 0.18	0.41 ± 0.04	86.91 ± 0.9	1.39
32	129301-42-4	1H,1H,8H,8H-Perfluoro-3,6-dioxaoctane-1,8-diol		Alcohols	3.2 ± 0.12	0.39 ± 0.03	81.14 ± 4.67	0.07

34	330562-41-9	Perfluoro-3,6,9-trioxatridecanoic acid		Ethers	4.16 ± 0.45	0.34 ± 0.02	82.46 ± 11.1	1.3
38	355-81-7	Perfluoropentanamide		Amides	4.41 ± 0.67	0.29 ± 0.01	75.25 ± 8.32	0.2
46	1763-23-1	Perfluorooctanesulfonic acid	PFOS	Sulfonates	3.46 ± 0.05	0.25 ± 0.06	71.49 ± 2.33	0.09
48	355-80-6	1H,1H,5H-Perfluoropentanol		Alcohols	5.67 ± 0.25	0.62 ± 0.04	111.16 ± 7.44	0.04
50	423-65-4	11:1 Fluorotelomer alcohol	11:1 FTOH	Alcohols	4.89 ± 0.78	0.56 ± 0.01	104.87 ± 8.15	0.04
54	151772-58-6	Perfluoro-3,6-dioxaheptanoic acid	PDHA	Ethers	3.71 ± 0.3	0.33 ± 0.02	77.02 ± 10.05	0.03
56	243139-64-2	3-(Perfluoroisopropyl)-2-propenoic acid		Carboxylates	3.39 ± 0.08	0.37 ± 0.01	78.08 ± 2.49	0.03
57	29420-49-3	Potassium perfluorobutanesulfonate	Potassium PFBS	Sulfonates	4.49 ± 0.5	0.32 ± 0.05	77.75 ± 2.42	0.32
58	355-66-8	Octafluoroadipamide		Amides	3.39 ± 0.36	0.25 ± 0.03	82.66 ± 4.7	0.82
60	754-91-6	Perfluorooctanesulfonamide	PFOSA	Sulfonamides	4.16 ± 0.08	0.4 ± 0.01	93.96 ± 4.28	0.46
61	1694-30-0	3H-Perfluoro-4-hydroxy-3-penten-2-one		Alcohols	3.61 ± 0.18	0.34 ± 0.07	92.81 ± 2.78	0.01

73	375-73-5	Perfluorobutanesulfonic acid	PFBS	Sulfonates	4.76 ± 0.17	0.36 ± 0.03	78.51 ± 4.6	0.29
74	335-67-1	Perfluorooctanoic acid	PFOA	Carboxylates	3.94 ± 0.08	0.42 ± 0.03	77.49 ± 1.8	0.09

Table S4: Bioaccumulations and toxicities of 74 PFAS in early life stage (ELS) of zebrafish. Bioconcentration factors (BCFs, L/kg) are shown for PFAS at both 0.5μM and 5μM. Mortality was only shown for higher concentrations of 5 μM, N=12-20.

ID	CAS	Category	Preferred Name	Abbreviation	BCF 0.5μM	BCF 5μM	Mortality[d] (%)	p-value
1	58244-27-2	Ether	tris(Trifluoroethoxy)methane		-[a]	-	0	0.5984
2	2144-53-8	Ester	6:2 Fluorotelomer methacrylate	6:2 FTMAC	-	-	0	0.4263
3	28523-86-6	Ether	Sevoflurane		-	-	1.1	0.857
4	679-12-9	Carboxylate	4H-Perfluorobutanoic acid	H-PFBA	3.4 ± 1.4[b]	1.9 ± 0.4	0	0.5984
5	1652-63-7	Sulfonamide	Perfluorooctanesulfonamido ammonium iodide	PFOSAmS	48 ± 6.0	56 ± 16	2.2	0.9968
6	2795-39-3	Sulfonate	Potassium perfluorooctanesulfonate	Potassium PFOS	288 ± 99	82 ± 9.2	2.2	0.9969
7	55621-21-1	Carboxylate	Perfluoro-3,6-dioxaoctane-1,8-dioic acid		ND[c]	ND	1.1	0.857
8	375-72-4	Others	Perfluorobutanesulfonyl fluoride	PBSF	-	-	2.2	0.9969

9	1691-99-2	Sulfonamide	N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide	NEt-FOSE	-	-	1.1	0.857
10	329710-76-1	Ether	2-(Trifluoromethoxy)ethyl trifluoromethanesulfonate		-	-	0	0.5984
11	375-01-9	Alcohol	Heptafluorobutanol	HFB	ND	ND	1.1	0.857
12	375-22-4	Carboxylate	Perfluorobutanoic acid	PFBA	2.6 ± 1.3	1.0 ± 0.28	4.4	0.6892
13	74427-22-8	Others	2,2-Difluoroethyl triflate		-	-	2.2	0.9968
14	914637-49-3	Carboxylate	2H,2H,3H,3H-Perfluorooctanoic acid	5:3 FTCA	6.7 ± 1.0	8.7 ± 2.1	1.1	0.857
15	757124-72-4	Sulfonate	4:2 Fluorotelomer sulfonic acid	4:2 FTS	5.7 ± 1.0	2.5 ± 0.13	0	0.5984
16	31506-32-8	Sulfonamide	N-Methylperfluorooctanesulfonamide	NMe-FOSA	292 ± 56	89 ± 9.4	**34.4[e]**	**<0.0001**
17	375-95-1	Carboxylate	Perfluorononanoic acid	PFNA	153 ± 6.0	73 ± 6.9	1.1	0.857

18	15242-17-8	Ether	Allyl perfluoroisopropyl ether		-	-	3.3	0.9238
19	13485-61-5	Carboxamide	Nonafluoropentanamide		-	-	1.1	0.857
20	307-24-4	Carboxylate	Perfluorohexanoic acid	PFHxA	6.6 ± 1.1	3.5 ± 0.64	0	0.9968
21	3825-26-1	Carboxylate	Ammonium perfluorooctanoate	Ammonium PFOA	43 ± 4.5	21 ± 0.42	0	0.5984
22	355-95-3	Others	1-Propenylperfluoropropane		-	-	3.3	0.9238
23	1763-28-6	Carboxylate	3,3-Bis(trifluoromethyl)-2-propenoic acid		1.8 ± 0.98	0.69 ± 0.29	2.2	0.4256
24	4151-50-2	Sulfonamide	N-Ethylperfluorooctanesulfonamide	NEt-FOSA	28 ± 7.8	24 ± 2.9	3.3	0.9238
25	239795-57-4	Others	2-Vinylperfluorobutane		-	-	1.1	0.857
26	3871-99-6	Sulfonate	Potassium perfluorohexanesulfonate	Potassium PFHxS	55 ± 6.3	30 ± 0.71	3.3	0.9238
27	333-36-8	Ether	Flurothyl		ND	ND	1.1	0.5984

28	863090-89-5	Carboxylate	Perfluoro(4-methoxybutanoic) acid	PFMOBA	5.2 ± 3.2	1.4 ± 0.17	1.1	0.857
29	406-58-6	Others	1,1,1,3,3-Pentafluorobutane	R365mfc	-	-	3.3	0.9243
30	125070-38-4	Alcohol	3-(Perfluoro-2-butyl)propane-1,2-diol		-	-	0	0.5984
31	662-50-0	Carboxamide	Heptafluorobutyramide		-	-	2.2	0.9968
32	129301-42-4	Alcohol	1H,1H,8H,8H-Perfluoro-3,6-dioxaoctane-1,8-diol		5.9 ± 0.08	8.4 ± 1.1	3.3	0.9969
33	31253-34-6	Others	2-Aminohexafluoropropan-2-ol		-	-	7.8	0.1014
34	330562-41-9	Carboxylate	Perfluoro-3,6,9-trioxatridecanoic acid		585 ± 174	93 ± 19	10	0.9243
35	376-90-9	Alcohol	Hexafluoroamylene glycol		1.6 ± 0.46	1.1 ± 0.09	0	0.5984
36	424-18-0	Ester	Methyl perfluorohexanoate	MePFOA	ND	ND	4.4	0.6892

37	13252-13-6	Carboxylate	Perfluoro-2-methyl-3-oxahexanoic acid	GenX	ND	ND	1.1	0.857
38	355-81-7	Carboxamide	Perfluoropentanamide		1.8 ± 0.31	1.9 ± 0.66	**17.8**	**<0.0001**
39	132424-36-3	Ester	Methyl 2H,2H,3H,3H-perfluoroheptanoate		-	-	1.1	0.9238
40	3792/2/7	Alcohol	4:4 Fluorotelomer alcohol	4:4 FTOH	-	-	0	0.5984
41	2043-47-2	Alcohol	4:2 Fluorotelomer alcohol	4:2 FTOH	-	-	0	0.1014
42	375-02-0	Others	Perfluorobutyraldehyde		-	-	0	0.5984
43	356-42-3	Others	Pentafluoropropanoic anhydride	PFPA	-	-	5.6	0.4263
44	163702-08-7	Ether	Perfluoroisobutyl methyl ether		-	-	1.1	0.857
45	883498-76-8	Others	Bis(1H,1H-perfluoropropyl)amine		-	-	2.2	0.857
46	1763-23-1	Sulfonate	Perfluorooctanesulfonic acid	PFOS	271 ± 69	91 ± 10	2.2	0.9968

47	356-24-1	Ester	Methyl heptafluorobutyrate	MeHFB	-	-	0	0.5984
48	355-80-6	Alcohol	1H,1H,5H-Perfluoropentanol		ND	ND	1.1	0.857
49	679-02-7	Alcohol	3-(Perfluoropropyl)propanol		-	-	1.1	0.857
50	423-65-4	Alcohol	11:1 Fluorotelomer alcohol	11:1 FTOH	ND	1.7 ± 0.23	1.1	0.857
51	813-03-6	Others	5H-Octafluoropentanoyl fluoride		ND	0.75 ± 0.15	0	0.5984
52	56860-81-2	Ether	Difluoromethyl 1H,1H-perfluoropropyl		-	-	2.2	0.9968
53	1623-05-8	Ether	Heptafluoropropyl trifluorovinyl ether		-	-	2.2	0.5984
54	151772-58-6	Carboxylate	Perfluoro-3,6-dioxaheptanoic acid	PDHA	2.1 ± 0.27	2.0 ± 0.40	2.2	0.9968
55	374-41-4	Others	Methyl perfluoroethyl ketone		-	-	2.2	0.1039

56	24313 9-64-2	Carboxyla te	3-(Perfluoroiso propyl)-2-propenoic acid		2.6 ± 0.1	1.6 ± 0.21	4.4	0.6892
57	29420 -49-3	Sulfonate	Potassium perfluorobut anesulfonate	Potassium PFBS	4.0 ± 0.9	3.0 ± 0.54	2.2	0.9968
58	355-66-8	Carboxam ide	Octafluoroad ipamide		ND	ND	6.7	0.2238
59	19430 -93-4	Others	1H,1H,2H-Perfluoro-1-hexene	PFH	-	-	4.4	0.6892
60	754-91-6	Sulfonami de	Perfluorooct anesulfonami de	PFOSA	501 ± 19	-	**100**	**<0.0001**
61	1694-30-0	Alcohol	3H-Perfluoro-4-hydroxy-3-penten-2-one		ND	7.7 ± 2.3	4.4	0.6884
62	374-40-3	Alcohol	1-Pentafluoroet hylethanol		-	-	6.7	0.2238
63	678-78-4	Others	Perfluoroglut aryl difluoride		-	-	5.6	0.4256
64	678-39-7	Alcohol	8:2 Fluorotelome r alcohol	8:2 FTOH	-	-	3.3	0.9238
65	16370 2-05-4	Ether	Ethyl perfluorobut yl ether		-	-	0	0.5984

66	77953-71-0	Alcohol	3H-Perfluoro-2,2,4,4-tetrahydroxypentane		ND	ND	1.1	0.857
67	335-99-9	Alcohol	Dodecafluoroheptanol	H-6:1 FTOH	-	-	0	0.5984
68	355-27-1	Others	1H,1H-Perfluoropentylamine		ND	ND	1.1	0.857
69	1767-94-8	Others	6H-Perfluorohex-1-ene		-	-	0	0.5984
70	647-42-7	Alcohol	6:2 Fluorotelomer alcohol	6:2 FTOH	-	-	0	0.5984
71	1619-92-7	Others	2-Amino-2H-perfluoropropane		-	-	3.3	0.9238
72	2648-47-7	Others	5H-Perfluoropentanal		-	-	3.3	0.9238
73	375-73-5	Sulfonate	Perfluorobutanesulfonic acid	PFBS	2.9 ± 0.36	2.8 ± 0.47	5.6	0.4256
74	335-67-1	Carboxylate	Perfluorooctanoic acid	PFOA	32 ± 4.4	17 ± 3.2	4.4	0.6892
Control					-	-	2.4	

[a] BCF was not determined as these PFAS were not ionizable under ESI as determined by high resolution mass spectrometry.
[b] The average and standard deviations of BCFs across three replicates. Corresponding to Figure S1.
[c] PFAS were not detected in ELS zebrafish.
[d] Toxicities were only shown for high dose treatment (5 μM) while no significant lethal effects were observed at 0.5 μM.

[e] Significant toxicities were labeled as bold. One-way analysis of variance (ANOVA) with Dunnett test was employed for the statistical test, $p < 0.05$ were deemed statistically significant.

Table S5: Information of nine PFAS considered as high affinity liver fatty acid binding protein (L-FABP) ligands (K_d < 20 µM) (Yang et al. 2020)

ID	Preferred Name	Abbreviations	CAS	Molecular fomula	Kd (µM)
6	Potassium FTCA perfluorooctanesulfonate	Potassium PFOS	2795-39-3	$C_8F_{17}KO_3S$	8.10
46	Perfluorooctanesulfonic acid	PFOS	1763-23-1	$C_8HF_{17}O_3S$	8.10
26	Potassium perfluorohexanesulfonate	Potassium PFHxS	3871-99-6	$C_6F_{13}KO_3S$	11.2
60	Perfluorooctanesulfonamide	PFOSA	754-91-6	$C_8H_2F_{17}NO_2S$	5.87
21	Ammonium perfluorooctanoate	Ammonium PFOA	3825-26-1	$C_8H_4F_{15}NO_2$	18.7
74	Perfluorooctanoic acid	PFOA	335-67-1	$C_8HF_{15}O_2$	18.7
34	Perfluoro-3,6,9-trioxatridecanoic acid	long-chain PFCA	330562-41-9	$C_{10}HF_{19}O_5$	8.22
17	Perfluorononanoic acid	PFNA	375-95-1	$C_9HF_{17}O_2$	4.30
24	N-Ethylperfluorooctanesulfonamide	NEt-FOSA	4151-50-2	$C_{10}H_6F_{17}NO_2S$	16.5

Table S6: Peak intensities of metabolites detected in zebrafish larvae exposed to 15 fluorotelomer alcohols (FTOHs) at 5 μM and 120 hpf.

FTOH	Sulfate	Glucuronide	Carboxylates	Shortened carboxylates [a]	Cysteine adduct	Taurine
FTOHs with 1 hydrocarbon						
1H-4:1 FTOH (**48**)	3.3×10^{5} [b]	2.3×10^{5}	× [c]	×	×	×
1H-6:1 FTOH (**67**)	4.5×10^{6}	2.7×10^{7}	4.2×10^{6}	×	×	×
35	1.7×10^{5}	×	×	×	×	×
11:1 FTOH (**50**)	3.2×10^{5}	1.9×10^{6}	8.2×10^{6}	×	×	×
32	3.4×10^{6}	1.9×10^{6}	6.4×10^{6}	×	×	×
3:1 FTOH (**11**)	×	×	×	×	×	×
FTOHs with 2 hydrocarbons						
4:2 FTOH (**41**)	1.0×10^{6}	1.2×10^{6}	8.3×10^{5}	1.9×10^{6}	×	4.2×10^{5}
6:2 FTOH (**70**)	1.3×10^{7}	2.3×10^{6}	×	1.0×10^{6} [d]	5.6×10^{4}	1.0×10^{5} [e]
8:2 FTOH (**64**)	6.3×10^{7}	1.9×10^{7}	×	2.3×10^{6}	2.9×10^{5}	1.4×10^{6}
FTOHs with more than 2 hydrocarbons						
4:4 FTOH (**40**)	4.2×10^{6}	4.6×10^{6}	5.4×10^{5}	2.0×10^{6}	3.4×10^{5}	6.9×10^{7}
3:3 FTOH (**49**)	1.1×10^{6}	4.6×10^{6}	1.5×10^{6}	5.1×10^{4}	9.4×10^{5}	1.8×10^{8}
30	2.2×10^{7}	5.0×10^{5}	2.9×10^{6}	1.3×10^{6}	×	1.6×10^{6}
Other FTOHs						
61	×	×	×	×	×	×
62	×	×	×	×	×	×
66	×	×	×	×	×	×

[a] Carboxylates with shorter carbon chain length, via β-oxidation.
[b] The average peak intensities of metabolites from three biological replicates.
[c] Not detected.
[d] Peak intensities were only shown for the most abundant carboxylates, *e.g.*, 5:3 FTUCA.
[e] Taurine conjugates were detected for shortened carboxylates, *e.g.*, 5:3 FTUCA.

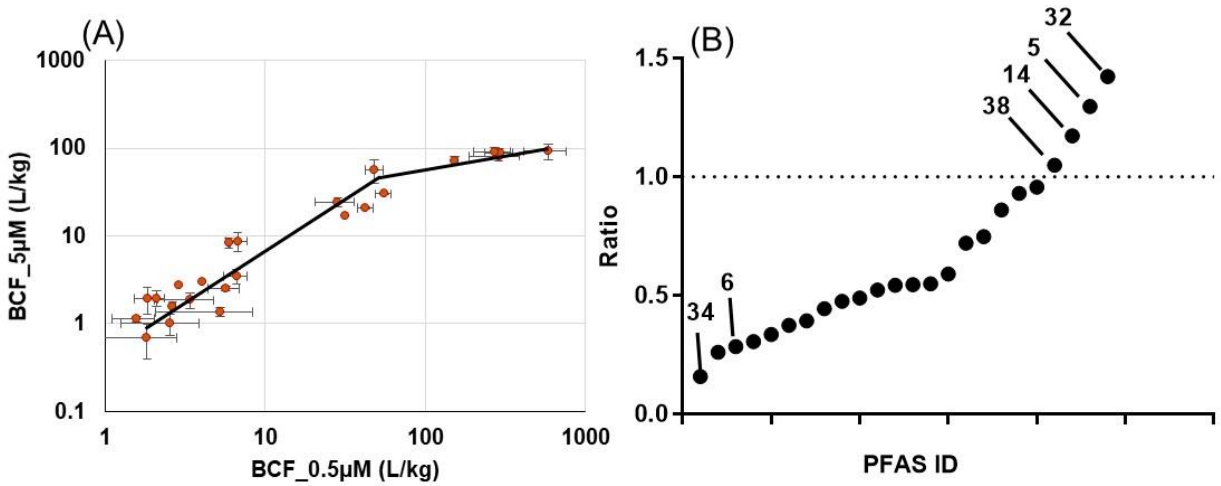


Figure S1: Relationships between BCFs and exposure concentrations. (A) Comparison of the BCFs of PFAS in zebrafish larvae at 120 hpf, at 0.5 μM and 5 μM. Dots represent mean ± SD (n=3). (B) The ratios of BCFs at 5 μM to 0.5 μM. Notes: PFAS, per- and polyfluoroalkyl substances; BCFs, bioconcentration factor. The summary data can be found in Table S3. The lines from panel A represent stepwise linear trends.

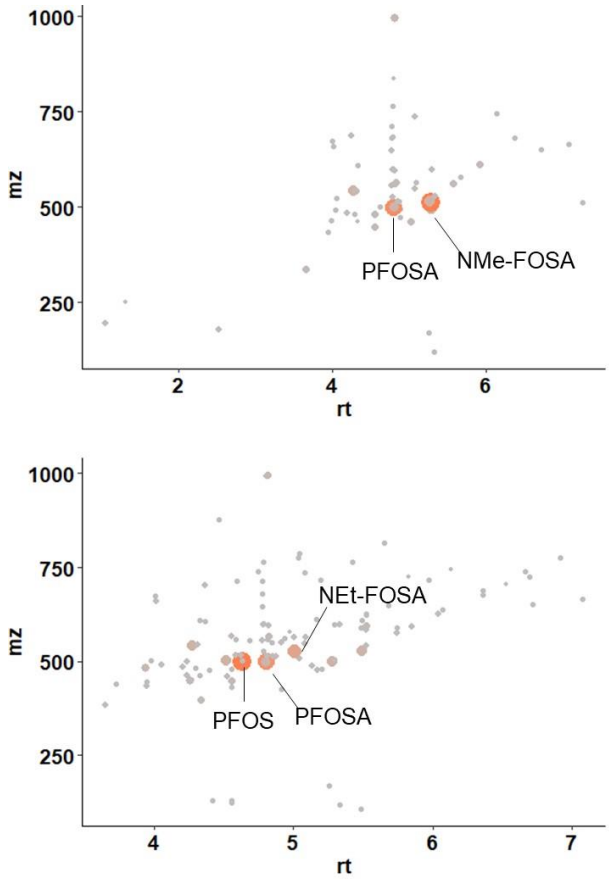


Figure S2: Metabolites of NMe-FOSA and NEt-FOSA. Nontargeted detection of metabolites in zebrafish larvae exposed to 5 µM of NMe-FOSA (top panel) and NEt-FOSA (bottom panel) was accomplished using the R scripts as detailed in method section. The sizes and colors of the dots are proportional to intensities. PFOS (**46**) and PFOSA (**60**) were confirmed with authentic standards (confidence level 1). Notes: NMe-FOSA, N-Methylperfluorooctanesulfonamide; NEt-FOSA, N-Ethylperfluorooctanesulfonamide; PFOSA, perfluorooctanesulfonamide; PFOS, perfluorooctanesulfonic acid.

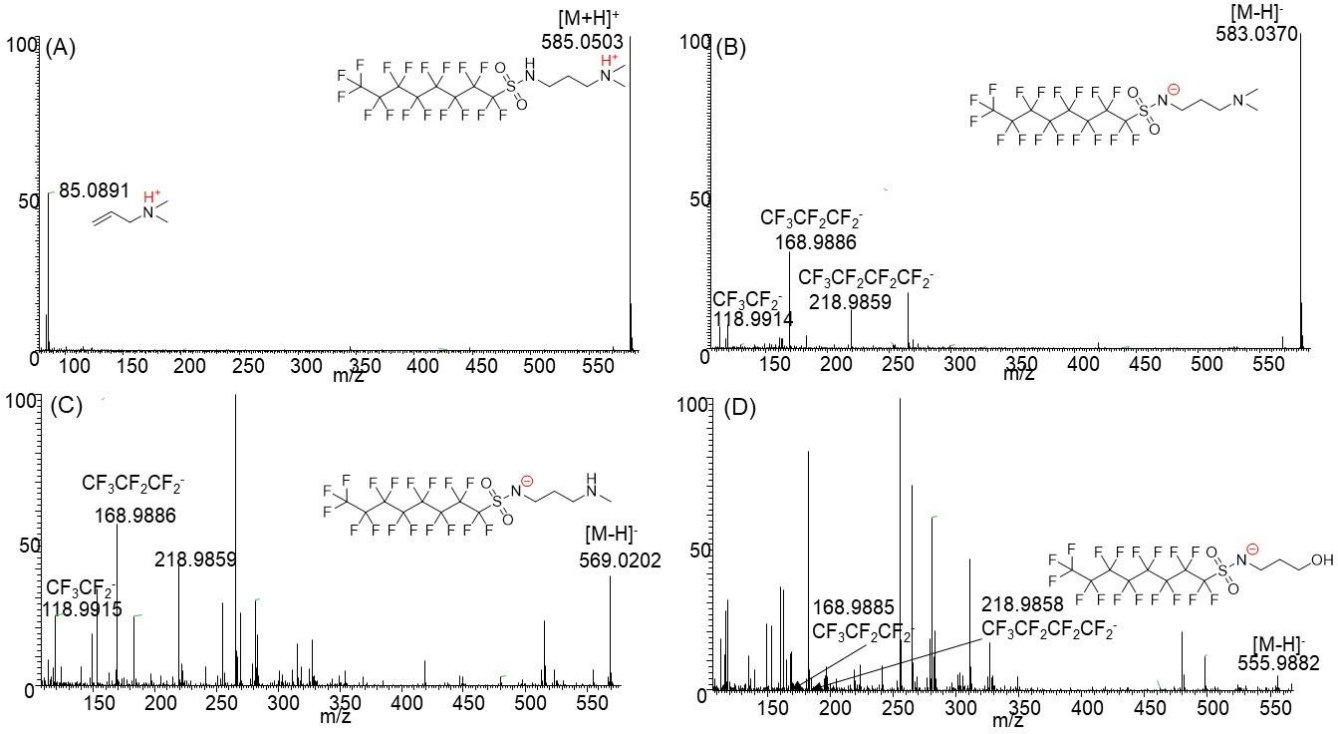


Figure S3: Metabolites of perfluorooctane sulfonamide quaternary ammonium salt (PFOSAmS, **5**). Tentative identification of metabolites from PFOSAmS was accomplished by interpreting the high-resolution MS^2 spectra of the three most abundant metabolite.

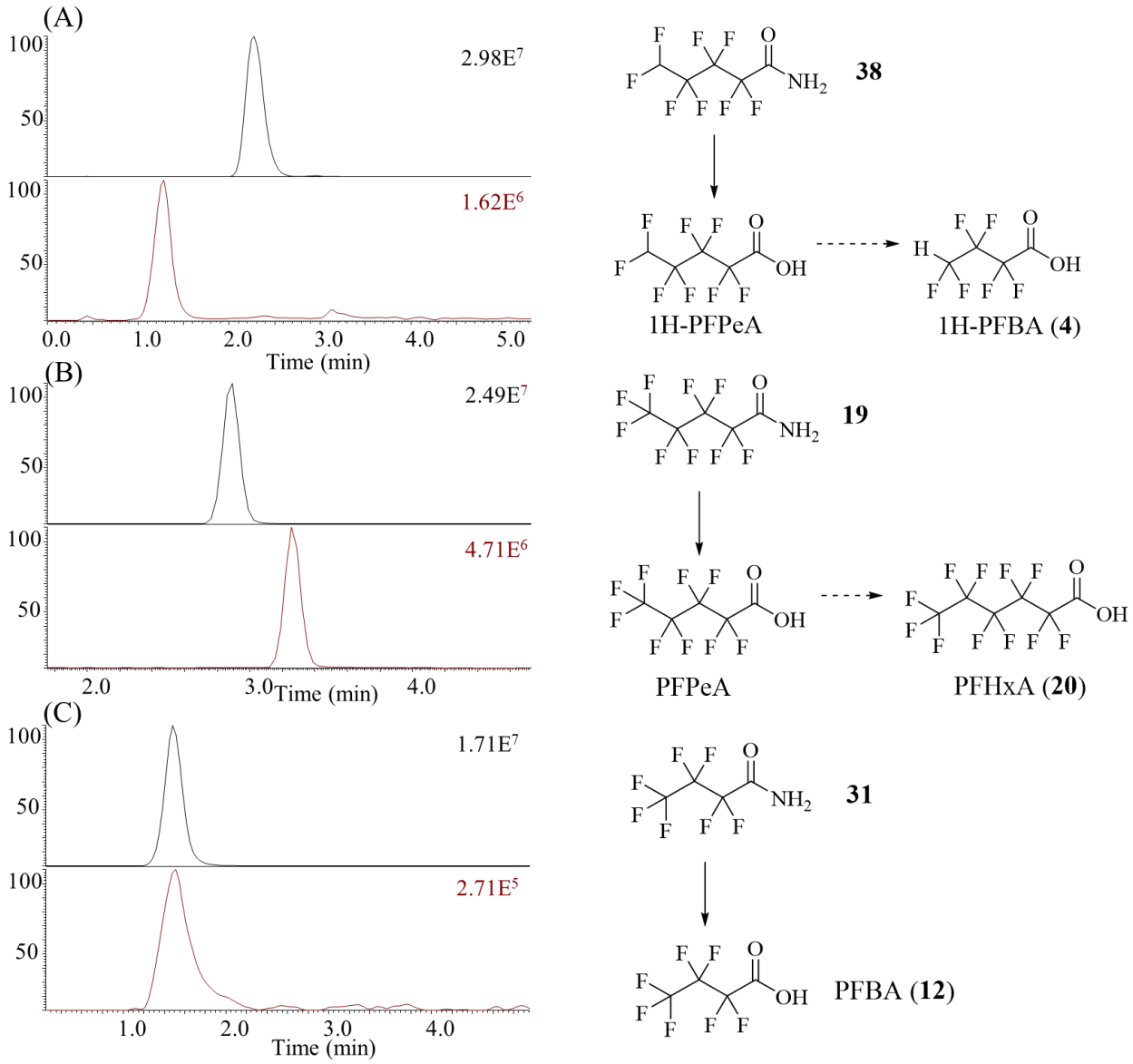


Figure S4: Representative chromatograms of shorter-chain PFCAs in zebrafish larvae metabolized from perfluoroalkyl carboxamides. (A) The chromatograms of 1H-PFPeA metabolized from amide **38** (top), and 1H-PFBA (bottom) directly exposed to zebrafish larvae. (B) The chromatograms of PFPeA metabolized from amide **19** (top), and PFHxA directly exposed to zebrafish larvae. (C) The chromatograms of PFBA metabolized from amide **38** (top), and PFBA directly exposed to zebrafish larvae. 1H-PFBA (**4**), PFHxA (**20**), PFBA (**12**) and PFPeA were confirmed with authentic standards (confidence level 1). The authentic standard of 1H-PFPeA was not available (confidence level 3). Note: PFBA, perfluorobutanoic acid; PFHxA, perfluorohexanoic acid; PFPeA, perfluoropentanoic Acid.

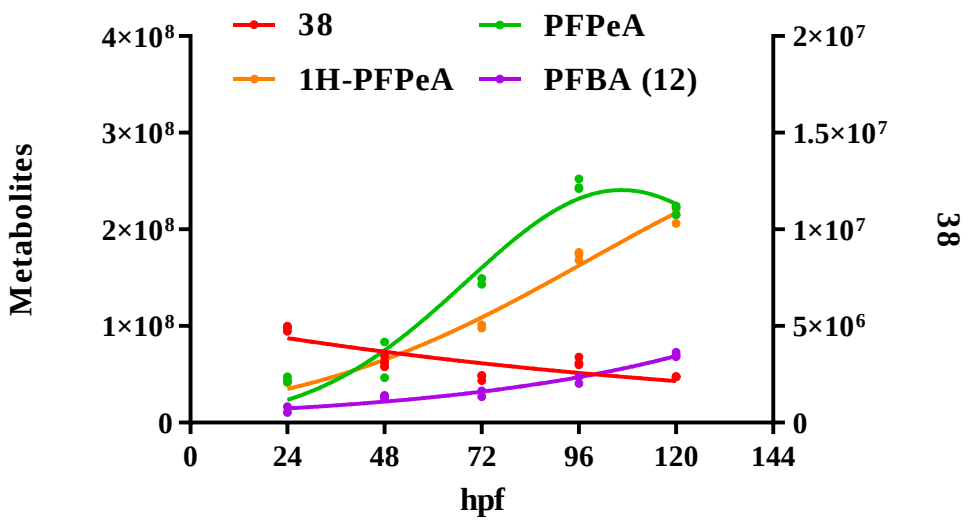


Figure S5. Time courses of carboxamides and polyfluoroalkyl carboxylic acids metabolites. Parent compound and carboxylic acids metabolites of **19**, **31** and **38** were monitored separately across development in zebrafish exposed to 5 μM of each parent carboxamides. The peak areas of polyfluoroalkyl carboxylic acid metabolites were plotted against the left y-axis, while the peak area of carboxamide 38 was plotted against the right y-axis. Perfluorobutanoic acid (PFBA, **12**) and perfluoropentanoic acid (PFPeA) were confirmed with authentic standards (confidence level 1). The authentic standard of 1H-PFPeA was not available (confidence level 3). The summary data can be found in Excel Table S8.

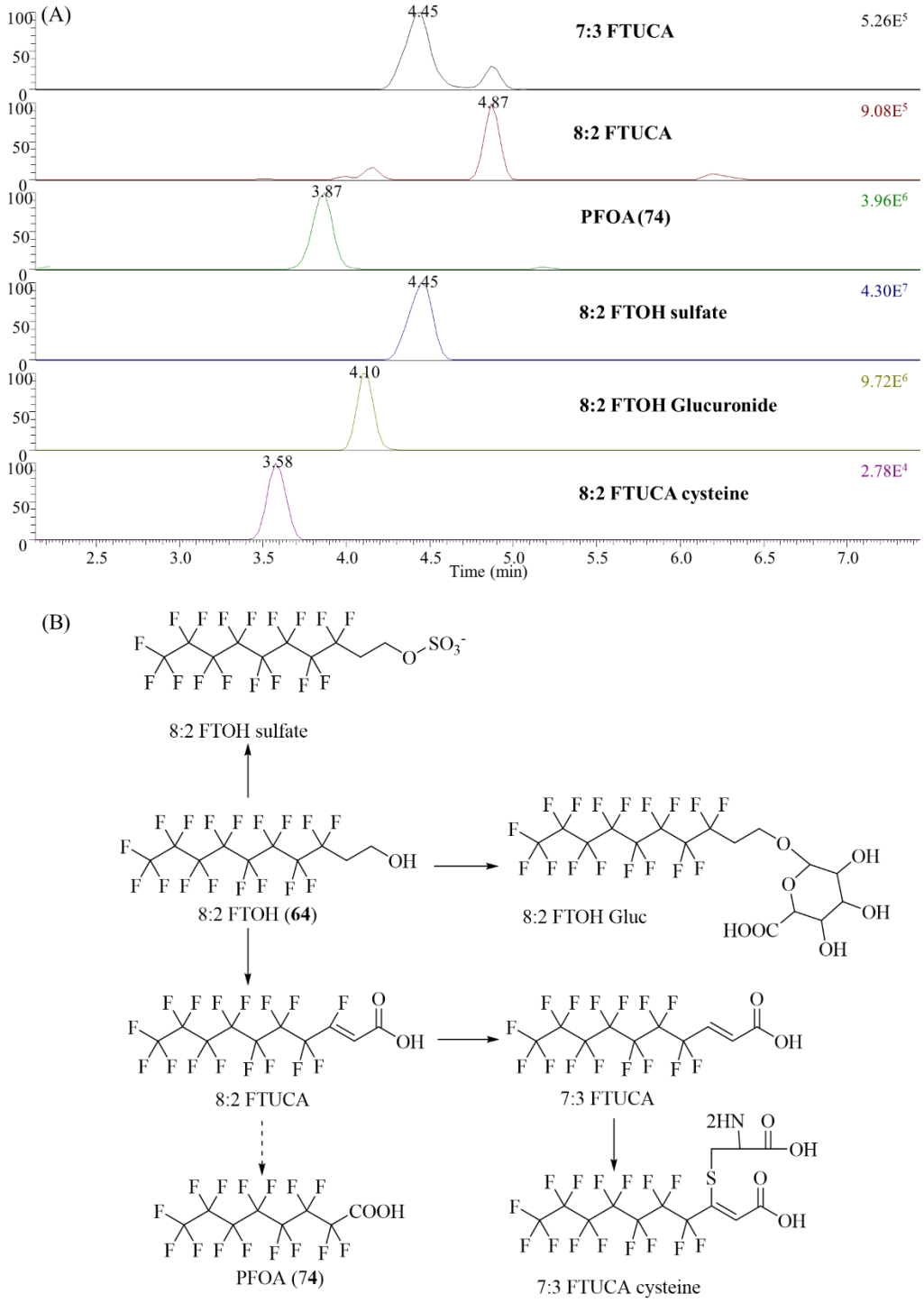


Figure S6: Hydrolysis products of 8:2 FTOH. Representative metabolites of 8:2 FTOH were detected in zebrafish larvae exposed to 5μM of 8:2 FTOH after 120h exposure. (A) Chromatograms of representative metabolites; (B) Proposed metabolism pathways. PFOA (**74**) was confirmed with authentic standards (confidence level 1). The authentic standards of 7:3 FTUCA, 8:2 FTUCA, 8:2 FTOH sulfate, 8:2 FTOH Gluc, 7:3 FTUCA cysteine were not available (confidence level 3). Note:

FTOHs, fluorotelomer alcohols; FTUCA, fluorotelomer unsaturated carboxylic acids; PFOA, perfluorooctanoic acid.

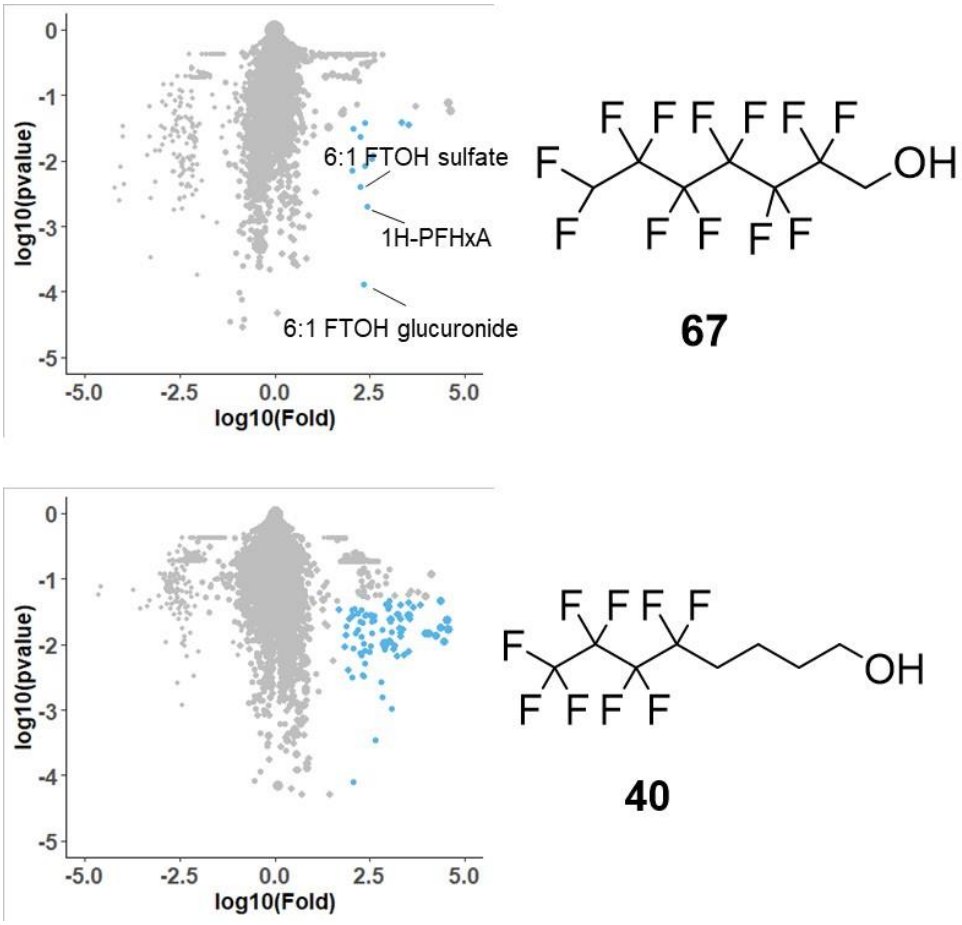


Figure S7: Metabolites of two FTOH. Metabolites detected in zebrafish larvae exposed to H-6:1 FTOH (**67)** and 4:4 FTOH (**40)** were plotted versus the intensities of metabolites from 8:2 FTOH. Blue dots represent metabolites showing significantly higher fold-changes (FC>20, p<0.05, student's t-test) relative to 8:2 FTOH. The authentic standards of 1H-PFHxA, 6:1 FTOH sulfate and 6:1 FTOH glucuronide were not available (confidence level 3). Note: FTOHs, fluorotelomer alcohols; PFHxA, perfluorohexanoic acid.

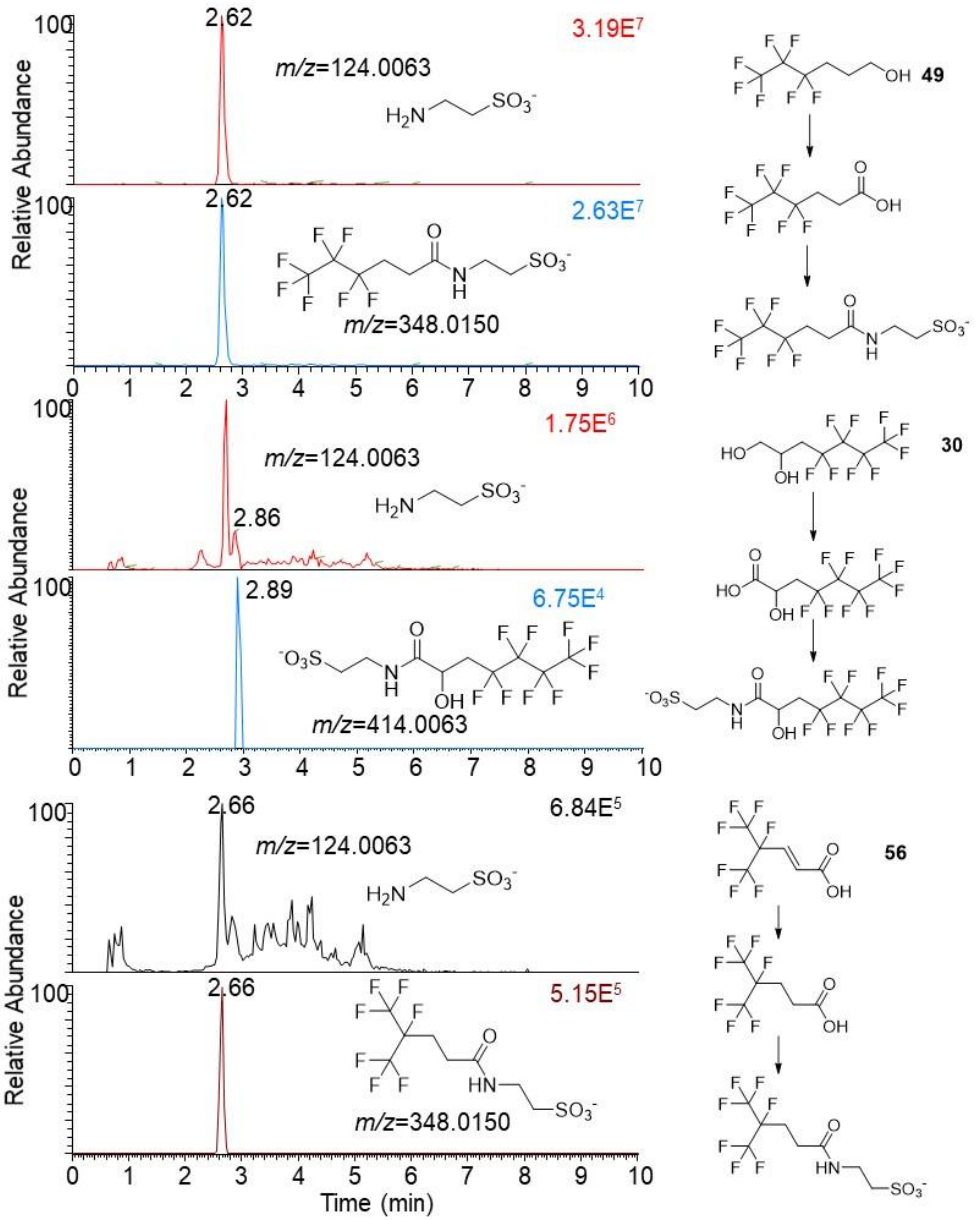


Figure S8. Taurine metabolites of PFAS **49**, **30**, and **56** in zebrafish. Taurine conjugates from PFAS were identified by employing high-resolution MS^2 spectra. The authentic standards of metabolites were not available, so they were tentatively identified at confidence level 3.

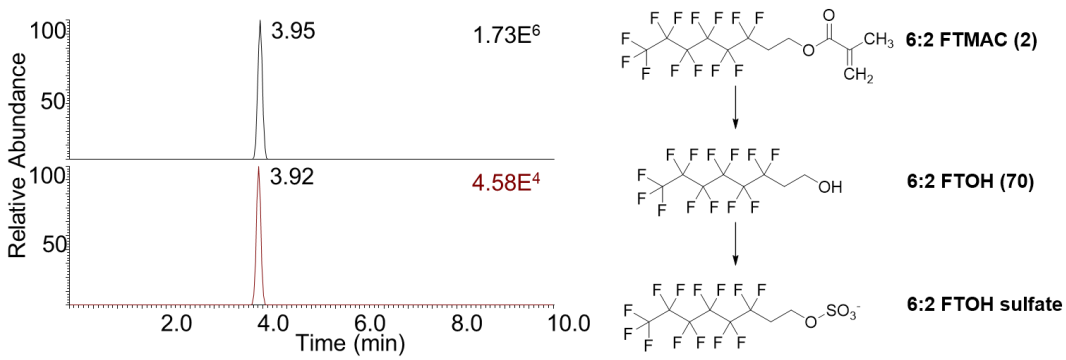


Figure S9. Metabolite of 6:2 FTMAC. 6:2 FTOH sulfate was detected in zebrafish larvae exposed to 5 µM of compound **2**. The chromatograms of 6:2 FTOH sulfate from compound 2 and the control are shown in the top and bottom panels. Note that minor background contamination was detected from the control. The proposed metabolism pathway of compound 2 is shown on the right. 6:2 FTOH (**70**) was confirmed with authentic standards (confidence level 1). The authentic standards of 6:2 FTOH sulfate was not available (confidence level 3). Note: FTOHs, fluorotelomer alcohols.

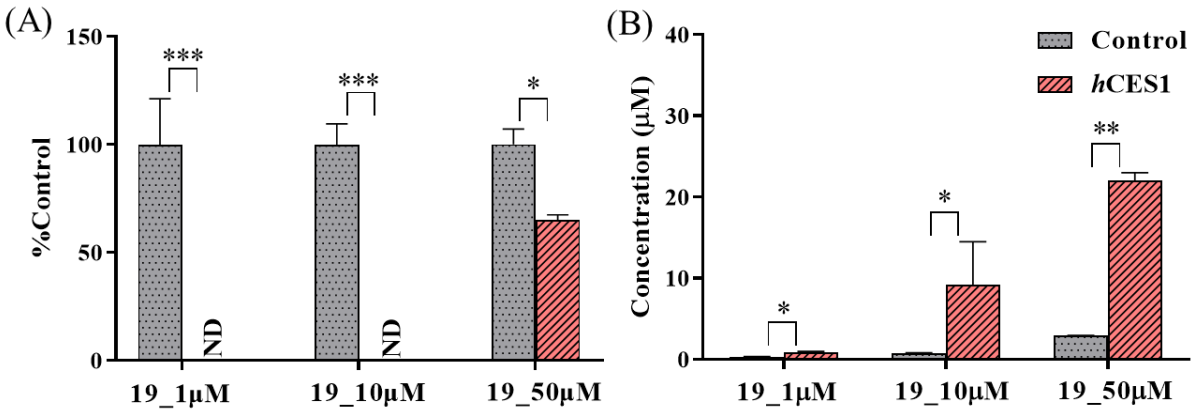


Figure S10. Hydrolysis of polyfluoroalkyl carboxamide **19** by hCES1. Reaction mixtures contained various concentrations **19** and 100 µg/L human recombinant human liver carboxylesterase 1 (*h*CES1) was incubated with 100 µL phosphate buffer at 37 °C for 1 hour, N=3. (A) The percentages of parent PFAS hydrolyzed by *h*CES1. (B) The concentrations of corresponding hydrolysis product perfluoropentanoic acid (PFPeA) detected. One-way ANOVA with Dunnett test was employed for the statistical test. Asterisk indicates *0.01<p<0.05, **0.01<p<0.001 and ***p<0.0001. Bars represent mean ± SD (n=3). Notes: The summary data can be found in Excel Tables S9 and S10.

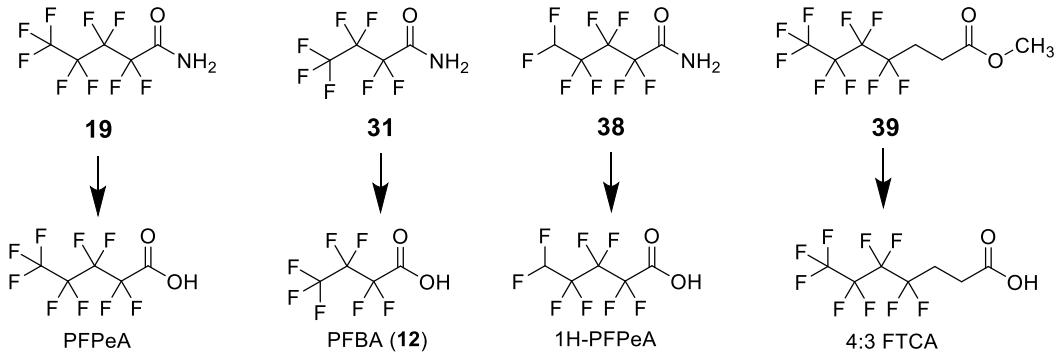


Figure S11. Structures of hydrolysis products detected in human recombinant human liver carboxylesterase 1 (*h*CES1) hydrolysis assay. Perfluorobutanoic acid (PFBA, **12**) and perfluoropentanoic acid (PFPeA) were confirmed with authentic standards, the confidence level was assigned to level 1. The authentic standards of 1H-PFPeA and 4:3 fluorotelomer carboxylic acid (FTCA) were not available, so they were confirmed with high resolution MS^1 and MS^2 spectra at confidence level 3.

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References

Yang D, Han J, Hall DR, Sun J, Fu J, Kutarna S, et al. 2020. Nontarget Screening of Per- and Polyfluoroalkyl Substances Binding to Human Liver Fatty Acid Binding Protein. Environmental science & technology 54(9): 5676-5686.