Ambient and Indoor Air Sampling for Per- and Poly-Fluorinated Alkyl Substances (PFAS)

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LECO



PFAS in Air – Outline

PFAS Background

• PFAS in Air Testing

Source Air Sampling

- OTM-45 overview
- ASE extraction

Ambient and Indoor Air

- Small volume sampler
- Breakthrough
- Fluorotelomer Alcohols by GC-MS/SIM





PFAS in Air – Outline

High Resolution GC-MSTOF analysis

- Deconvolution tools
- Library matching and mass accuracy
- EI and CI data



PFAS in Air Testing

- Source emissions can spread volatile and semi-volatile PFAS
 - PFAS can be dispersed in vapor phase or on particulates
- Combustion can create both short chain and large fluorinated molecules
 - Combustion and incineration processes can create short chain PFAS such as trifluoroacetic acid (TFA) and carbon tetrafluoride (CF₄)
 - At ≤ 800°C fluorinated dioxins and furans can be created





PFAS in Air Testing

Volatile PFAS are present in air

- Neutral PFAS such as fluorotelomer alcohols (FTOH), perfluorinated sulfonamides (FOSA) and sulfonamide ethanols (FOSE) are volatile and capable of long-range atmospheric transport
- Neutral PFAS are precursors to ionic PFAS compounds such as perfluoroalkyl carboxylates (PFCA) and perfluoroalkane sulfonates (PFSA)



Annika Jahnke, Urs Berger, Trace analysis of per- and polyfluorinated alkyl substances in various matrices—How do current methods perform?, Journal of Chromatography A, Volume 1216, Issue 3, 2009, Pages 410-421





PFAS in Air Testing

• PFAS can be present in indoor air

- Off gassing of volatile PFAS from consumer products
- Airborne dust containing PFAS from product wear and tear



Kerstin Winkens et al, Perfluoroalkyl acids and their precursors in floor dust of children's bedrooms – Implications for indoor exposure, Environmental International, Volume 119, 2018, Pages 493-502





Source Air Sampling – OTM-45

- Combines filter, XAD-2, and liquid impingers
- Suitable for C₄ to C₁₈ PFAS compounds
- Many different PFAS classes (PFCA, PFSA, FOSA, FOSE, etc.)





OTM-45 – ASE Extraction

- OTM-45 sample prep for XAD-2 fraction is two rounds of 16-hour shakeouts using 360 mL total solvent
 - 32-hour extraction plus time for solvent blowdown
- Accelerated Solvent Extraction (ASE) advantages
 - Reduced time ~45 minutes/sample
 - Reduced solvent use <100mL solvent/sample
 - Higher extraction efficiency 1.4 to 55 times more response on ASE





OTM-45 – ASE Extraction

ASE:SHAKE AREA





Pure Chromatography

OTM-45 – MDL

Name	OTM-45 MDL	Restek MDL	Name	OTM-45 MDL	Restek MDL	Name	OTM-45 MDL	Restek MDL
PFBA	2.08	0.06	FHEA		0.09	FDEA		0.07
PF40PeA		0.02	ADONA	0.14	0.02	PFUnA	0.33	0.08
3:3 FTCA		0.05	PFeCHS		0.03	11CI-PF3OUdS	0.18	0.04
PFPeA	0.2	0.03	6-2 FTS	0.29	0.02	FOSA-I	0.27	0.13
PFBS	0.17	0.07	PFHpS	0.08	0.03	10:2 FTS		0.04
PF5OHxA		0.01	PFOA	0.43	0.22	PFDoA	0.12	0.10
PFEESA		0.01	PFOS	0.35	0.04	PFDoS		0.06
3,6-OPFHpA		0.02	FOUEA		0.07	N-MeFOSA-M		0.07
4-2 FTS	0.20	0.02	PFNA	0.15	0.06	N-Me-FOSE-M		0.07
PFHxA	0.31	0.02	FHpPA		0.14	N-MeFOSAA	0.4	0.05
PFPeS	0.14	0.02	FOEA		0.18	PFHxDA		0.05
HFPO-DA	2.77	0.22	9CI-PF3ONS	0.17	0.03	N-EtFOSA-M		0.17
PFHpA	0.21	0.10	PFNS	0.14	0.18	N-EtFOSE-M		0.05
5:3 FTCA		0.07	PFDA	0.13	0.05	N-EtFOSAA	0.39	0.08
FHUEA		0.06	8-2 FTS	0.27	0.07	PFODA		0.05
PFHxS	0.17	0.06	PFDS	0.17	0.32	PFTrDA	0.12	0.8
		MDL values in	ng/m3 air			PFTA	0.19	0.05



RESTEK

- Resin sampling from OTM-45 can be adapted to ambient and indoor air
- 8 g of Ultra-Clean Resin was packed into a small volume air sampler
- 20 µm frit to catch particulates
- TD tube used to catch any potential breakthrough compounds





- Small volume sampler can be fit into a 100 mL ASE cell for cleaning and extraction
- Removes the need to separately clean and extract resin, frits, and glass holder







Pure Chromatography

- Initial testing shows no breakthrough for OTM-45 compounds
- FTOH also tested and showed no breakthrough when spiked on resin
- Sample spiked and air pulled through for 24 hours at 300
 mL/min
- 432 L/0.432 m³ of air sampled





FTOH by GC-MS SIM

- Agilent 7890B
- Rtx 624Sil-MS 60 x 0.25 x 1.4
- Inlet
 - 250C
 - 5:1 split
 - 2 mL/min flow
- Oven
 - 80C hold 3min
 - 15C/min to 300C, hold 5 minutes
- MSD transfer line
 - 250C



- Agilent 5977
- Mass Spec SIM mode
 - SIM
 - m/z 45, 69, 95, 119, 131
 - Dwell time 50
 - MS Source
 - 350C
- MS Quad
 - 200C



FTOH by GC-MS SIM



- 4:2 FTOH 7.391 min
- 6:2 FTOH 8.889 min
- 8:2 FTOH 10.187 min
- 10:2 FTOH 11.317 min





FTOH by GC-MS SIM

- Calibration from 400-5000 ppb in solution
- 0.9-4.5 ng/ m³ at 432 L of air sampled

Name	% RSE	MDL (ng/m3)	Avg. Recovery (@ 1.4 ng/m3)	% RSD (@ 1.4 ng/m3)
4:2 FTOH	20%	0.25	90%	7%
6:2 FTOH	16%	0.23	102%	5%
8:2 FTOH	19%	0.38	92%	10%
10:2 FTOH	21%	0.31	111%	7%



- Real world samples from a residential home
- Downstairs dining room, upstairs office, basement, and outside porch
- Sampled at 200 mL/min for 24 hours, 288 L or 0.288 m³









No PFAS present in targeted GC-MS SIM or LC-MS/MS analysis





High-Resolution GC-TOFMS

LECO Pegasus[®] HRT+ 4D



- Mass Accuracy: 1 PPM
- Resolution: Up to 50,000
- Acquisition Speed: up to 200 sps
- Ionization: EI, PCI, ECNI

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₽	Maximum molecular weight allowed: 1500
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- ✓ Deconvolution
- ✓ Spectral Database Comparisons
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High-Resolution GC-TOFMS





Pure Chromatography

Deconvolution of Spectra



Pure Chromatography

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Library Similarity and Mass Accuracy



Hit	Name	CAS	Formula	m/z calc	m/z obs	PPM	Similarity
1	Heneicosane	629-94-7	C21H44	296.3438	306.1826	N/A	863
2	Eicosane	112-95-8	C20H42	282.3281	282.328	-0.39	855
3	Docosane	629-97-0	C22H46	310.3594	306.1826	N/A	845
4	Heneicosane	629-94-7	C21H44	296.3438	306.1826	N/A	844
5	Octadecane	593-45-3	C18H38	254.2968	253.288	N/A	842
6	Octadecane	593-45-3	C18H38	254.2968	253.288	N/A	839
7	Hexadecane	544-76-3	C16H34	226.2655	226.2599	-24.77	835
8	Eicosane	112-95-8	C20H42	282.3281	282.328	-0.39	834
9	Hexadecane	544-76-3	C16H34	226.2655	226.2599	-24.77	833
10	Heptadecane	629-78-7	C17H36	240.2812	240.2767	-18.53	833

- Library similarity alone can lead to misidentifications
- Presence of molecular ion and confirmation by mass accuracy improves confidence in matches



Complementary El and Cl Data





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•••••••••••••••••••••••••••••	668 11 3-Ethylbenzoic add 3.00 PPM 696.175 s) 702.425 s) 100 15 12 n-Decanoic add 3.00 PPM 696.175 s) 702.425 s) 100 15 13* 4-Ethylbenzoic add 3.00 PPM 705.876 s) 710.924 s) 100 15 14 (c) -4 (But -1 en -1 -Y)gualacol 3.00 PPM 763.997 s) 767.803 s) 100 15 15 4-Acctylbenzoic add 3.00 PPM 929.23 s) 932.97 s) 100 15 16 Benzoic add, phenyl ester 3.00 PPM 1016.43 s) 1020.37 s) 100 15 18 2-Propanol, 1-chloro-, phosphate (3:1) 3.00 PPM 1016.25 s) 1056.44 s) 100 15 20 Pyrene, 4,5-dilydro- 3.00 PPM 1062.56 s) 100 15 21 Methyl palmitate 3.00 PPM 1086.99 s) 1090.61 s) 100 15 22 Palmi		10	m-Ethylacetophenone	ļ	3.00	PPM	631.64 s	635.56 s	100 !5	Library
12 n-becanok add 3.00 PPM 704.889 s 709.111 s 100 15 11dex 14 (E)-4 (But-1-en-1-yl)gualacol 3.00 PPM 763.997 s 767.803 s 100 15 15 4 Acetylbenzok add 3.00 PPM 763.997 s 767.803 s 100 15 15 4 Acetylbenzok add 3.00 PPM 838.055 s 846.945 s 100 15 15 4 Acetylbenzok add 3.00 PPM 838.055 s 846.945 s 100 15 16 Benzok add, penyl ester 3.00 PPM 1016.42 s 1021.98 s 100 15 17 Phenanthrene 3.00 PPM 1016.22 s 1021.98 s 100 15 19 Caffeine 3.00 PPM 1061.92 s 1025.85 s 100 15 20 Pyrene, 4,5-dihydro- 3.00 PPM 1065.99 s 1090.61 s 100 15 21 Methyl palmitzte 3.00 PPM 1106.24 s 1100 15 22	12 n-becanoc acid 3.00 PPM 704.889 5 709.111 s 100 15 11 4 Fttylbenzoic acid 3.00 PPM 705.876 s 710.924 s 100 15 14 (E)-4-(But-1-en-1-yl)guaiacol 3.00 PPM 763.997 s 767.803 s 100 15 15 4-Acctylbenzoic acid 3.00 PPM 838.055 s 846.945 s 100 15 16 Benzoic acid, phenylester 3.00 PPM 1016.43 s 102.037 s 100 15 17 Phenanthrene 3.00 PPM 1016.43 s 102.037 s 100 15 18 2-Propanol, 1-chloro-, phosphate (3:1) 3.00 PPM 1016.25 s 1006.44 s 100 15 20 Pyrene, 4,5-dihydro- 3.00 PPM 1062.56 s 1006.15 100 15 21 Methyl palmitze 3.00 PPM 1062.45 s 100 15 22 Palmitiz add <td>668</td> <td>11</td> <td>3-Ethylbenzoic acid</td> <td></td> <td>3.00</td> <td>PPM</td> <td>696.175 s</td> <td>702.425 s</td> <td>100 !5</td> <td>-</td>	668	11	3-Ethylbenzoic acid		3.00	PPM	696.175 s	702.425 s	100 !5	-
13 4*EthMoBiLOU add 3.00 PPM 703.975 710.924* 100 15 14 (E)-4 (Bt1-1en1-1y)guaiacol 3.00 PPM 703.975 710.924* 100 15 15 4 Acctylbenzok add 3.00 PPM 838.055 \$ 846.945 \$ 100 15 16 Benzok add, phenyl ester 3.00 PPM 929.23 \$ 932.97 \$ 100 15 17 Phenanthrene 3.00 PPM 101.423 \$ 1021.93 \$ 100 15 18 2-Propanol, 1-chloro-, phosphate (3:1) 3.00 PPM 101.92 \$ 1021.93 \$ 100 15 20 Pyrene, 4,5-dihydro- 3.00 PPM 106.25 \$ 106.64 \$ 100 15 21 Palantita 3.00 PPM 106.25 \$ 106.64 \$ 100 15 22 Palantita 3.00 PPM 106.25 \$ 106.64 \$ 100 15 21 Methyl palmitate 3.00 </td <td>13 4*EuNiverzity au 3.00 PPM 705.878 710.728 710.918 100 15 14 (E) + (But 1-en 1-yl)gualacol 3.00 PPM 765.978 710.728 100 15 15 4 - Accetylbenzoic acid 3.00 PPM 838.055 s 846.945 s 100 15 16 Benzoic acid, phenyl ester 3.00 PPM 929.23 s 932.97 s 100 15 17 Phenanthrene 3.00 PPM 1016.43 s 100.15 15 16 Benzoic acid, phenyl ester 3.00 PPM 1016.43 s 100.15 15 17 Phenanthrene 3.00 PPM 1016.43 s 100.15 15 10 Caffeine 3.00 PPM 1062.56 s 1066.44 s 100 15 20 Prene, 4,5-dihydro- 3.00 PPM 1064.45 s 110.76 s 100 15 21 Methyl palmitate 3.00 PPM 1064.45</td> <td>etention</td> <td>12</td> <td>n-Decanoic acid</td> <td></td> <td>3.00</td> <td>PPM</td> <td>704.889 s</td> <td>709.111 s</td> <td>100 !5</td> <td>Shift RTs</td>	13 4*EuNiverzity au 3.00 PPM 705.878 710.728 710.918 100 15 14 (E) + (But 1-en 1-yl)gualacol 3.00 PPM 765.978 710.728 100 15 15 4 - Accetylbenzoic acid 3.00 PPM 838.055 s 846.945 s 100 15 16 Benzoic acid, phenyl ester 3.00 PPM 929.23 s 932.97 s 100 15 17 Phenanthrene 3.00 PPM 1016.43 s 100.15 15 16 Benzoic acid, phenyl ester 3.00 PPM 1016.43 s 100.15 15 17 Phenanthrene 3.00 PPM 1016.43 s 100.15 15 10 Caffeine 3.00 PPM 1062.56 s 1066.44 s 100 15 20 Prene, 4,5-dihydro- 3.00 PPM 1064.45 s 110.76 s 100 15 21 Methyl palmitate 3.00 PPM 1064.45	etention	12	n-Decanoic acid		3.00	PPM	704.889 s	709.111 s	100 !5	Shift RTs
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29 Tris(2,4-di-tert-butylphenyl) phosphate 3.00 PPM 2078.65 s 2089.75 s 100 !5	29 Tris(2,4-di-tert-butylphenyl) phosphate 3.00 PPM 2078.65 s 2089.75 s 100 !5 Library	77	28	Cholesterol		3.00	PPM	1686.68 s	1692.12 s	100 !5	
	Jibrary	44	29	Tris(2,4-di-tert-butylphenyl) phosphate		3.00	PPM	2078.65 s	2089.75 s	100 !5	
	Library										

Input Masses For Target Analyte Finding

Analyte: 4-Ethylbenzoic acid

#	Formula	Isotope	M/Z	Tolerance	Units	Required
1*			105.06989	3.00	PPM	
2			135.04400	3.00	PPM	
3	C9H10O2	150.06808		3.00	PPM	

- In addition to library search, a targeted search can be done
- Based on retention time HRAM target ions, and mass accuracy



Library and Target Search Results

Name	Formula	R.T. (s)	Similarity	PPM
3-Penten-2-one, 4-methyl-	C6H10O	237	867	-0.23
2,5-Hexanedione	C6H10O2	336	851	-0.81
Benzene, 1-ethyl-4-methyl-	C9H12	373	806	-1.46
Pyridine, 2,4,6-trimethyl-	C8H11N	393	907	-1.52
Phenol, 2,4,6-trimethyl-	C9H12O	424	805	-1.14
Benzene, 1-ethenyl-3-ethyl-	C10H12	478	885	-0.99
1,3-Benzenediol, 4-ethyl-	C8H10O2	483	801	-1.18
Benzene, 1-ethenyl-4-ethyl-	C10H12	485	739	-0.81
3-Hexen-2-one	C6H10O	531	710	-0.52
Benzene, 1-methyl-4-(1-propynyl)-	C10H10	538	805	-1.92
Naphthalene	C10H8	545	808	-1.06
Benzoic acid	C7H6O2	548	944	-1.37
Ethanone, 1-(4-ethylphenyl)-	C10H12O	633	877	-0.85
Ethanone, 1-(2,4,5-trimethylphenyl)-	C11H14O	667	708	-1.82
3-Ethylbenzoic acid	C9H10O2	700	858	-1.23
4-Ethylbenzoic acid	C9H10O2	709	830	-1.39
1-Tetracosene	C24H48	1008	774	N/A
Octadecane	C18H38	1012	911	-1.82
Phenanthrene	C14H10	1019	859	-1.32
Naphthalene, 1,2-dihydro-4-phenyl-	C16H14	1024	901	-1.62
Pyrene, 4,5-dihydro-	C16H12	1065	858	-1.97
4,4'-Diisopropylbiphenyl	C18H22	1085	745	-0.88
Methyl palmitate	C17H34O2	1089	846	-1.02
n-Hexadecanoic acid	C16H32O2	1109	907	-1.27
1-Hexacosene	C26H52	1128	872	N/A
1(2H)-Naphthalenone, 3,4-dihydro-4-phenyl-	C16H14O	1145	860	-1.48
Octadecanenitrile	C18H35N	1193	710	N/A
Methyl stearate	C19H38O2	1202	800	-1.52
Docosane	C22H46	1240	741	-0.53
1,2-Benzenediol, o-(4-ethylbenzoyl)-	C15H14O3	1302	866	N/A
Tris(1,3-dichloroisopropyl)phosphate	C9H15Cl6O4P	1320	810	N/A
9-Octadecenamide, (Z)-	C18H35NO	1327	906	-1.91
Cyclohexane, 1,3,5-triphenyl-	C24H24	1378	848	-0.99
Palmitoleamide	C16H31NO	1425	786	N/A
13-Docosenamide, (Z)-	C22H43NO	1516	747	-1.82
Supraene	C30H50	1536	828	-0.47
Tris(2.4-di-tert-butylphenyl) phosphate	C42H63O4P	2085	861	N/A

Name	R.T. (s)	Lab 1	Lab 2	Upstairs	Downstairs	Outside	Basement	Blank
Pyridine, 2,5-dimethyl-	345	152949	16654			7217	370398	
Mesitylene	374	850291	104510	2996001	786923	430791	7996627	49229
Pyridine, 2,4,6-trimethyl-	394	10250356		42859146	4227280	373437	88331	1561
Phenol, 2,4,6-trimethyl-	425	806941	141350	2812204	672453	132962	183903	143247
Phenol, 2,3,5-trimethyl-	425	806941	141350	2812204	672453	132962	47723	143247
Benzene, 1-ethenyl-4-ethyl-	478	382052	26405	293687	1355856	44611	1037596	14995
Benzoic acid	545	12117211	5320053	21778833	28381572	4042177	31377717	4515978
Naphthalene	546	178096	5711	124945	1194741	8659	443537	3677
Benzaldehyde, 4-ethyl-	548	257890	35837	196560	356496	48843	234340	59949
m-Ethylacetophenone	634	505941	128638	602296	560632	241158	4056399	230196
3-Ethylbenzoic acid	699	1805288	404727	2709814	4429110	217204	2822753	323275
n-Decanoic acid	707	1012552	265392	1634600	758017	489958	865613	43746
4-Ethylbenzoic acid	708	2226809		3840128	4752473		3613152	
(E)-4-(But-1-en-1-yl)guaiacol	766	1441133	5053	778220	3831205	4510	1262971	5541
4-Acetylbenzoic acid	843	422298	53772	1303643	844192			9881
Benzoic acid, phenyl ester	931	555034	16255	314132	1642299	16429	433918	14146
Phenanthrene	1018	244292	12300	515466	167733	40478	4108111	7313
2-Propanol, 1-chloro-, phosphate (3:1)	1020	66447	26159	143475	59798	41356	31687	13018
Caffeine	1054	27276	28565	55134	36719	18786	20575	3951
Pyrene, 4,5-dihydro-	1065	235908	2227	91788	298062	3424	183903	
Methyl palmitate	1089	2789689	3538808	4667398	3383883	18094834	243214	1413054
Palmitic acid	1109	2840142	1018703	13345980	4553202	536493	602303	48421
1(2H)-Naphthalenone, 3,4-dihydro-4-phenyl-	1145	149901	5283	77243	529167	8144	371440	5759
Methyl stearate	1202	1747912	2322300	2786688	2324708	8582380	5186465	4669389
Hexadecanamide	1232	3175375	4568609	11102206	8127365	5603988	135611	9672632
13-Docosenamide, (Z)-	1516	7988159	7452341	21331950	13134242	11127936	3644943	4269155
Supraene	1536	428097	5456202	32728565	12283024	5595007	19823	441696
Cholesterol	1689	205753	306701	1554775	507339	320107	375233	19106
Tuis (2, 4, s) as an heat shall be seen by the second state	2004	2554660	2527640	7252720	4450700	2200602	6007056	6437507

Despite all these powerful tools, no untargeted PFAS detected





Final Results – No Detectable PFAS

- Many studies of indoor PFAS exposure point to dust as a major contributor
 - Samplers were in out of the way places that may not generate airborne dust
- Other studies show that volatile FTOH can be present in air at low or sub ng/m³
 - Larger sampling volumes or more sensitive instrumentation may be needed to properly identify and quantify PFAS in indoor air



Conclusions

- Lab-based testing shows small volume SDVB resin samplers can be used for a wide variety PFAS, including FTOH
- GC-MS can be used for volatile PFAS analysis, and GC-HRTOFMS can facilitate non-target characterization
- Real-world samples taken from a home show collection of many VOCs, but no presence of PFAS compounds
- Further work to increase sensitivity is needed to reach PFAS levels seen in some studies





Questions?



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Pure Chromatography