

-SUPPORTING INFORMATION-

Biotransformation of 6:2 fluorotelomer sulfonate (6:2 FTS) in sulfur-rich media by *Trametes cervina*

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Table S1. Reported 6:2 FTS concentrations at sites impacted with PFAS containing aqueous film forming foams (AFFF).

Study location	Contamination Source	Media	6:2 FTS Concentration		Reference
			individual (µg/L)	site average (ppm)	
Tyndall AFB, USA	Aqueous Film Forming Foam	groundwater well 1	14600.0	6.85	<i>Schultz et. al 2004</i>
		groundwater well 2	7100.0		
		groundwater well 3	4630.0		
		groundwater well 4	1080.0		
Wurtsmith AFB, USA	Aqueous Film Forming Foam	groundwater well 1	2.9	0.05	<i>Schultz et. al 2004</i>
		groundwater well 2	88.0		
		groundwater well 3	95.0		
		groundwater well 4	2.0		
		groundwater well 5	42.0		
		groundwater well 6	53.0		
		groundwater well 7	66.0		
		groundwater well 8	7.2		
		groundwater well 9	27.0		
		groundwater well 10	16.0		
		groundwater well 11	173.0		
		groundwater well 12	139.0		
		groundwater well 13	8.7		
		groundwater well 14	1.0		
		groundwater well 15	0.9		
Flesland Airport, Sweden	Aqueous Film Forming Foam	soil sample 1	612 (ng/g)	1.36	<i>Karrman et. al 2011</i>
		soil sample 2	2101 (ng/g)		

Table S2. Description of PFAS analytes mentioned in this study.

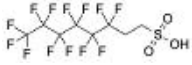
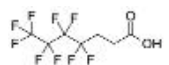
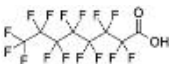



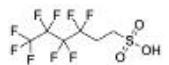
Name	CAS	Formula	Mass (Da)	Structure	Canonical SMILES
6:2 FTS	27619-97-2	C8H5F13O3S	428.16		<chem>C(CS(=O)(=O)O)C(C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)(F)(F)(F)F</chem>
6:2 FTCA	53826-12-3	C8H3F13O2	378.09		<chem>C(=O)O)C(C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)(F)(F)F</chem>
6:2 FTuCA	70887-88-6	C8H2F12O2	358.08		<chem>C(=C(C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)(F)(F)F)C(=O)O</chem>
5:3 FTCA	914637-49-3	C8H5F11O2	342.11		<chem>CC(C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)(F)(F)C(=O)O</chem>
4:3 FTCA	80705-13-1	C7H5F9O2	292.10		<chem>CC(C(C(C(C(F)(F)(F)(F)(F)(F)(F)C(=O)O</chem>
PFHxA	307-24-4	C6HF11O2	314.05		<chem>C(=O)(C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)F)F)O</chem>
PFPeA	2706-90-3	C5HF9O2	264.05		<chem>C(=O)(C(C(C(C(F)(F)(F)(F)(F)F)F)F)O</chem>
PFBA	375-22-4	C4HF7O2	214.04		<chem>C(=O)(C(C(C(F)(F)(F)F)F)F)O</chem>
5:2 sFTOH	914637-05-1	C7H5F11O	314.10		<chem>CC(C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)F)F)F)O</chem>
5:2 Ketone	2708-07-8	C7H3F11O	312.08		<chem>CC(=O)C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)F)F)F</chem>
PFOA	335-67-1	C8HF15O2	414.07		<chem>C(=O)(C(C(C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)(F)(F)F)F)F)F)O</chem>
PFHpA	375-85-9	C7HF13O2	364.06		<chem>C(=O)(C(C(C(C(C(C(F)(F)(F)(F)(F)(F)(F)F)F)F)F)F)O</chem>
PFBS	375-73-5	C4HF9O3S	300.10		<chem>C(C(C(F)S(=O)(=O)O)(F)F)(C(F)(F)F)F</chem>
PFPeS	2706-91-4	C5HF11O3S	372.09		<chem>C(C(C(F)F)F)F)(C(C(F)S(=O)(=O)O)(F)F)F</chem>
PFHxS	355-46-4	C6HF13O3S	400.12		<chem>C(C(C(C(F)S(=O)(=O)O)(F)F)(F)F)(C(C(F)F)F)F)F</chem>
4:2 FTS	757124-72-4	C6H5F9O3S	350.14		<chem>C(CS(=O)(=O)O)C(C(C(C(F)F)F)F)F)F)F</chem>

Table S3. Instrumental method parameters and method quantification limits in the LC-QTOF/MS quantitative analysis.

Instrument:	SCIEX X500R High Performance Liquid Chromatograph with a SCIEX Quadrupole Time-of-Flight Mass Spectrometer equipped with an electrospray source. The mass spectrometer was operated in the negative ion multiple reaction-monitoring mode.		
Analytical Column:	Phenomenex Gemini (Gemini 3 μ m C18, 110 Å, LC Column 100mm x 3mm, PRD-621757)		
Column Temperature:	30 °C		
Mobile Phases:	A: 5mM ammonium acetate in HPLC grade water B: 5mM ammonium acetate in methanol		
Gradient Profile:	<u>Time (min)</u>	<u>Flow (mL/min)</u>	<u>B Conc (%)</u>
	0.00	0.6000	10.0
	1.50	0.6000	65.0
	8.00	0.6000	95.0
	8.10	0.6000	99.0
	12.00	0.6000	99.0
	12.50	0.6000	10.0
	15.50	0.6000	10.0
Injection Volume:	50 μ L		
Estimated Instrument Detection Limit (IDL):	$IDL \left(\frac{ng}{mL} \right) = \frac{\text{Concentration of lowest used calibration standard} \left(\frac{ng}{mL} \right)}{\left(\frac{S}{N} \text{ of analyte peak} \div 3 \right)}$		

Calibration
Standard
Concentrations:

S/N and concentration used for IDL calculation								
Analyte	std 8	std 7	std 6	std 5	std 4	std 3	std 2	std 1
(ng/mL)								
PFBA	0.009	0.027	0.08	0.25			6.7	
PFPeA		0.027	0.08	0.25	0.74			20
PFHxA		0.027	0.08	0.25			6.7	20
PFHxA_2		0.027	0.08	0.25			6.7	20
PFHpA	0.009	0.027	0.08	0.25	0.74	2.2		
PFHpA_2	0.009	0.027	0.08	0.25	0.74	2.2		
PFOA	0.009	0.027	0.08	0.25	0.74	2.2	6.7	
PFOA_2	0.009	0.027	0.08	0.25	0.74	2.2	6.7	
PFBS	0.009	0.027	0.08	0.25	0.74	2.2	6.7	
PFBS_2	0.009	0.027	0.08	0.25	0.74	2.2	6.7	
PFPeS		0.027	0.08	0.25	0.74	2.2		
PFPeS_2		0.027	0.08	0.25	0.74	2.2		
PFHxS Linear	0.009	0.027	0.08		0.74	2.2	6.7	
PFHxS_2 Linear	0.009	0.027	0.08		0.74	2.2	6.7	
4:2 FTS	0.009	0.027	0.08	0.25	0.74	2.2		
4:2 FTS_2	0.009	0.027	0.08	0.25	0.74	2.2		
6:2 FTS						2.2	6.7	20
6:2 FTS_2						2.2	6.7	20
4:3 FTCA	0.009	0.027		0.25	0.74	2.2		
4:3 FTCA_2	0.009	0.027		0.25	0.74	2.2		
6:2 FTuCA	0.009	0.027	0.08	0.25	0.74	2.2		
6:2 FTuCA_2	0.009	0.027	0.08	0.25	0.74	2.2		
5:2 Ketone			0.8	2.5	7.4	22		
5:2 Ketone_2			0.8	2.5	7.4	22		
6:2 FTCA	0.009	0.027	0.08	0.25	0.74	2.2	6.7	20
6:2 FTCA_2	0.009	0.027	0.08	0.25	0.74	2.2	6.7	20
5:3 FTCA	0.009	0.027	0.08	0.25	0.74	2.2	6.7	20
5:3 FTCA_2	0.009	0.027	0.08	0.25	0.74	2.2	6.7	20
5:2 sFTOH	0.09	0.27	0.8	2.5	7.4	22		
5:2 sFTOH_2	0.09	0.27	0.8	2.5	7.4	22		

Monitored Ion
Transitions:

Analyte	Group Name	Ion transition (Da > Da)	Declustering Potential (V)	Collision Energy (V)	IDL (ng/mL)
PFBA	PFBA	212.98 > 168.9889	-25	-12	0.006632751
PFPeA	PFPeA	262.98 > 218.9859	-20	-12	0.024072282
PFHxA	PFHxA	312.97 > 268.9827	-25	-12	0.059551479
PFHxA_2	PFHxA	312.97 > 118.9926	-25	-28	
PFHpA	PFHpA	362.97 > 318.9788	-25	-12	0.030933694
PFHpA_2	PFHpA	362.97 > 168.9892	-25	-20	
PFOA	PFOA	412.97 > 368.9755	-25	-14	0.017537841
PFOA_2	PFOA	412.97 > 168.9893	-25	-22	
PFBS	PFBS	298.94 > 79.9568	-55	-58	0.019194286
PFBS_2	PFBS	298.94 > 98.9553	-55	-40	
PFPeS	PFPeS	348.94 > 79.9573	-60	-66	0.793552099
PFPeS_2	PFPeS	348.94 > 98.9555	-60	-45	
PFHxS Linear	PFHxS	398.94 > 79.9573	-60	-74	0.059129009

PFHxS_2 Linear	PFHxS	398.94 > 98.9557	-60	-50	
4:2 FTS	4:2 FTS	327 > 306.97	-42	-25	0.054783168
4:2 FTS_2	4:2 FTS	327 > 79.9587	-42	-49	
6:2 FTS	6:2 FTS	427 > 406.9613	-33	-31	2.809486045
6:2 FTS_2	6:2 FTS	427 > 80.9645	-33	-40	
4:3 FTCA	4:3 FTCA	291.01 > 166.9943	-50	-25	0.029908792
4:3 FTCA_2	4:3 FTCA	291.01 > 187.0007	-50	-15	
6:2 FTuCA	6:2 FTuCA	356.98 > 292.9857	-55	-20	0.043306933
6:2 FTuCA_2	6:2 FTuCA	356.98 > 242.9882	-55	-45	
5:2 Ketone	5:2 Ketone	310.99 > 268.9858	-110	-15	0.950724774
5:2 Ketone_2	5:2 Ketone	310.99 > 118.9939	-110	-30	
6:2 FTCA	6:2 FTCA	377 > 292.9866	-25	-25	0.064240042
6:2 FTCA_2	6:2 FTCA	377 > 62.9899	-25	-10	
5:3 FTCA	5:3 FTCA	341 > 236.9981	-25	-15	0.042856991
5:3 FTCA_2	5:3 FTCA	341 > 216.9917	-25	-30	
5:2 sFTOH	5:2 sFTOH	313.01 > 293.005	-40	-10	0.305773089
5:2 sFTOH_2	5:2 sFTOH	313.01 > 268.9849	-40	-10	
13C4_PFBA	PFBA	216.99 > 171.9994	-25	-12	NA (IS)
13C5_PFPeA	PFPeA	267.99 > 222.9996	-20	-12	NA (IS)
13C5_PFHxA	PFHxA	317.99 > 273	-25	-12	NA (IS)
13C4_PFHpA	PFHpA	366.98 > 321.9912	-25	-12	NA (IS)
13C8_PFOA	PFOA	420.99 > 376.0001	-25	-14	NA (IS)
13C9_PFNA	PFNA	471.99 > 427	-25	-14	NA (IS)
13C6_PFDA	PFDA	519 > 474	-25	-16	NA (IS)
13C7_PFUdA	PFUdA	570 > 525	-25	-18	NA (IS)
13C2_PFDoA	PFDoA	615 > 570	-25	-18	NA (IS)
M3_PFBs	PFBs	302 > 98.9558	-55	-58	NA (IS)
M3_PFHxS	PFHxS	402 > 98.9558	-60	-50	NA (IS)
13C8_PFOS	PFOS	507 > 98.9558	-65	-108	NA (IS)
13C8_PFOsA	PFOSa	506 > 77.9655	-60	-85	NA (IS)
d3-MeFOSAA	MeFOSAA	573 > 419	-75	-28	NA (IS)

M2 4:2 FTS	4:2 FTS	329 > 308.9748	-42	-25	NA (IS)
M2 6:2 FTS	6:2 FTS	429 > 408.9684	-33	-31	NA (IS)
M2 8:2 FTS	8:2 FTS	529 > 508.962	-150	-37	NA (IS)
M2PFTeDA	PFTeDA	715 > 669.9608	-90	-19	NA (IS)
d5-N- EtFOSAA	N-EtFOSAA	589 > 418.9734	-75	-22	NA (IS)

LC/MS/MS

Parameters:

Ion Source:

Curtain gas (psi): 30; Ion source gas 1 (psi): 60; Ion source gas 2 (psi): 60; Temperature (°C): 450

Experiment:

Scan type: MRMhr; Polarity: Negative; Ionspray voltage (V): -4500; CAD gas: 10

TOFMS:

Time bins to sum: 4; Channels 1-4: True; TOF start (Da): 100; TOF stop (Da): 1000; Accumulation time (s): 0.05; Declustering potential (V): -50; Declustering potential spread (V): 0; Collision energy (V): -5; Collision energy spread (V): 0

TOFMSMS:

Enhance dynamic range: True

Table S4. Instrumental method parameters for the LC-QTOF/MS non-target analysis.

Instrument:	SCIEX X500R High Performance Liquid Chromatograph with a SCIEX Quadrupole Time-of-Flight Mass Spectrometer equipped with an electrospray source. The mass spectrometer was operated in negative ion multiple reaction-monitoring mode.																								
Analytical Column:	Phenomenex Gemini (Gemini 3 μ m C18, 110 Å, LC Column 100mm x 3mm, PRD-621757)																								
Column Temperature:	30 °C																								
Mobile Phases:	A: 5mM ammonium acetate in HPLC grade water B: 5mM ammonium acetate in methanol																								
Gradient Profile:	<table><thead><tr><th><u>Time (min)</u></th><th><u>Flow (mL/min)</u></th><th><u>B Conc (%)</u></th></tr></thead><tbody><tr><td>0.00</td><td>0.6000</td><td>10.0</td></tr><tr><td>1.50</td><td>0.6000</td><td>65.0</td></tr><tr><td>8.00</td><td>0.6000</td><td>95.0</td></tr><tr><td>8.10</td><td>0.6000</td><td>99.0</td></tr><tr><td>12.00</td><td>0.6000</td><td>99.0</td></tr><tr><td>12.50</td><td>0.6000</td><td>10.0</td></tr><tr><td>15.50</td><td>0.6000</td><td>10.0</td></tr></tbody></table>	<u>Time (min)</u>	<u>Flow (mL/min)</u>	<u>B Conc (%)</u>	0.00	0.6000	10.0	1.50	0.6000	65.0	8.00	0.6000	95.0	8.10	0.6000	99.0	12.00	0.6000	99.0	12.50	0.6000	10.0	15.50	0.6000	10.0
<u>Time (min)</u>	<u>Flow (mL/min)</u>	<u>B Conc (%)</u>																							
0.00	0.6000	10.0																							
1.50	0.6000	65.0																							
8.00	0.6000	95.0																							
8.10	0.6000	99.0																							
12.00	0.6000	99.0																							
12.50	0.6000	10.0																							
15.50	0.6000	10.0																							
Injection Volume:	50 μ L																								
QTOF/MS Parameters:	SCIEX SWATH Acquisition; Number of scan windows: 13; Lower m/z limit: 100; Upper m/z limit: 2500																								
QTOF/MS Parameters:	Ion Source: Curtain gas (psi): 30; Ion source gas 1 (psi): 40; Ion source gas 2 (psi): 60; Temperature (°C): 450 Experiment: Scan type: SWATH; Polarity: Negative; Ionspray voltage (V): -4500; CAD gas: 10 TOFMS: Time bins to sum: 4 Channel 1-4: True TOF start mass (Da): 100 TOF stop mass (Da): 2500 Accumulation time (s): 0.1																								

Declustering potential (V): -20 Declustering potential spread (V): 0 Collision energy (V): -5 Collision energy spread (V): 0 TOFMSMS: TOF start mass (Da): 50 TOF stop mass (Da): 2500 Accumulation time (s): 0.05 Dynamic collision energy: False Charge State: 1 Enhance dynamic range: False
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Table S5. Figure 1 data						
sample	group	compound	day	mean	max	min
CS0	control	6:2 FTS+products	0	87.8%	90.9%	84.6%
CS10	control	6:2 FTS+products	10	92.8%	102.7%	83.0%
CS20	control	6:2 FTS+products	20	95.7%	100.1%	91.3%
CS30	control	6:2 FTS+products	30	98.8%	103.8%	93.7%
SP1S0	SP1	6:2 FTS+products	0	94.4%	100.5%	88.3%
SP1S10	SP1	6:2 FTS+products	10	100.6%	104.6%	96.5%
SP1S20	SP1	6:2 FTS+products	20	90.1%	92.2%	87.9%
SP1S30	SP1	6:2 FTS+products	30	93.0%	95.4%	90.7%
SP2S0	SP2	6:2 FTS+products	0	97.0%	109.6%	84.5%
SP2S10	SP2	6:2 FTS+products	10	89.9%	98.5%	81.3%
SP2S20	SP2	6:2 FTS+products	20	71.5%	77.1%	65.8%
SP2S30	SP2	6:2 FTS+products	30	75.0%	76.6%	73.4%
CS0	control	PFOA	0	119.1%	120.6%	117.6%
CS10	control	PFOA	10	116.7%	118.0%	115.5%
CS20	control	PFOA	20	132.6%	154.3%	110.8%
CS30	control	PFOA	30	101.4%	124.7%	78.1%
SP1S0	SP1	PFOA	0	123.5%	145.3%	101.7%
SP1S10	SP1	PFOA	10	116.6%	128.1%	105.1%
SP1S20	SP1	PFOA	20	103.9%	109.8%	97.9%
SP1S30	SP1	PFOA	30	113.5%	115.3%	111.8%
SP2S0	SP2	PFOA	0	116.6%	125.4%	107.8%
SP2S10	SP2	PFOA	10	107.8%	115.4%	100.1%
SP2S20	SP2	PFOA	20	116.7%	137.5%	95.9%
SP2S30	SP2	PFOA	30	145.8%	149.9%	141.8%

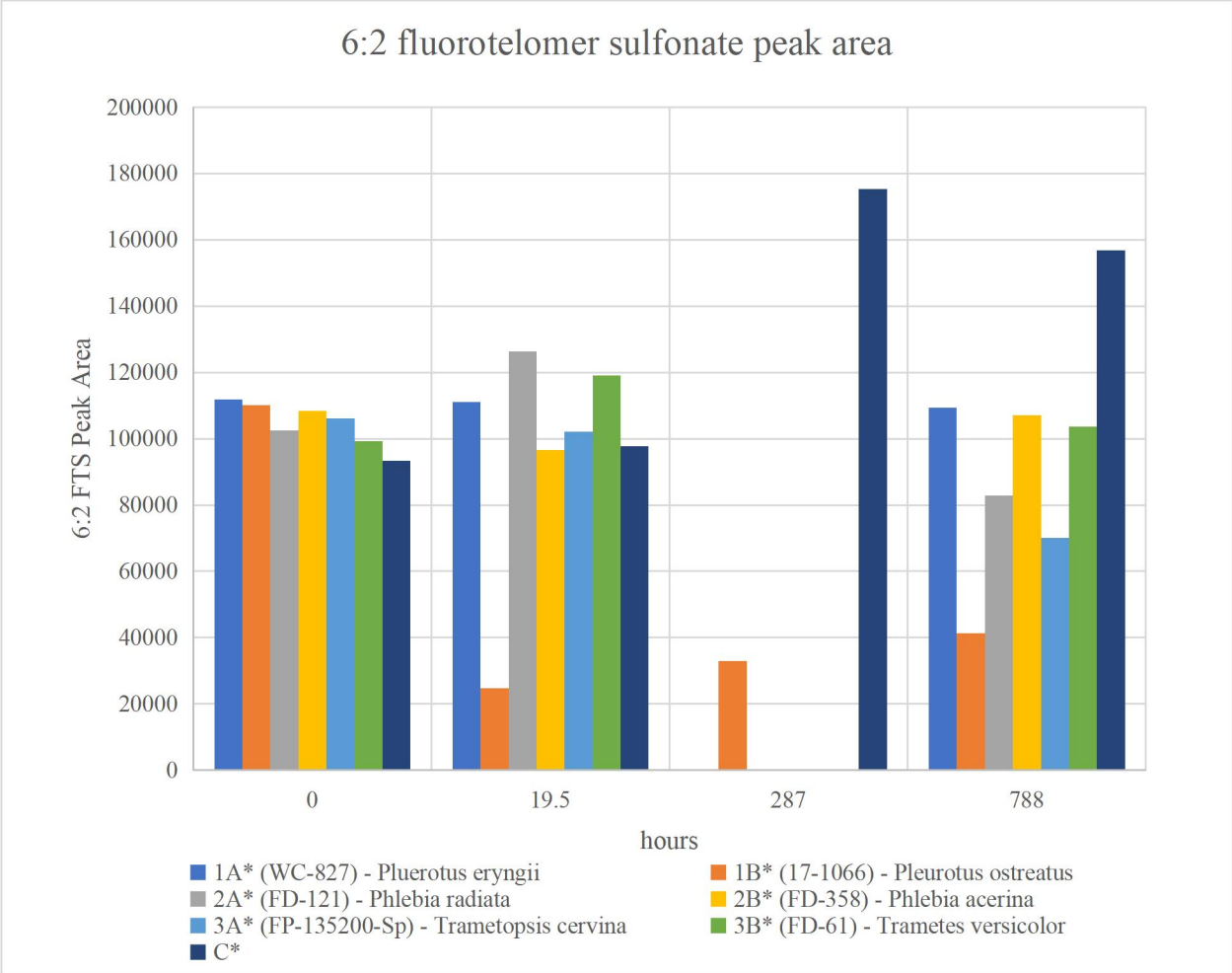
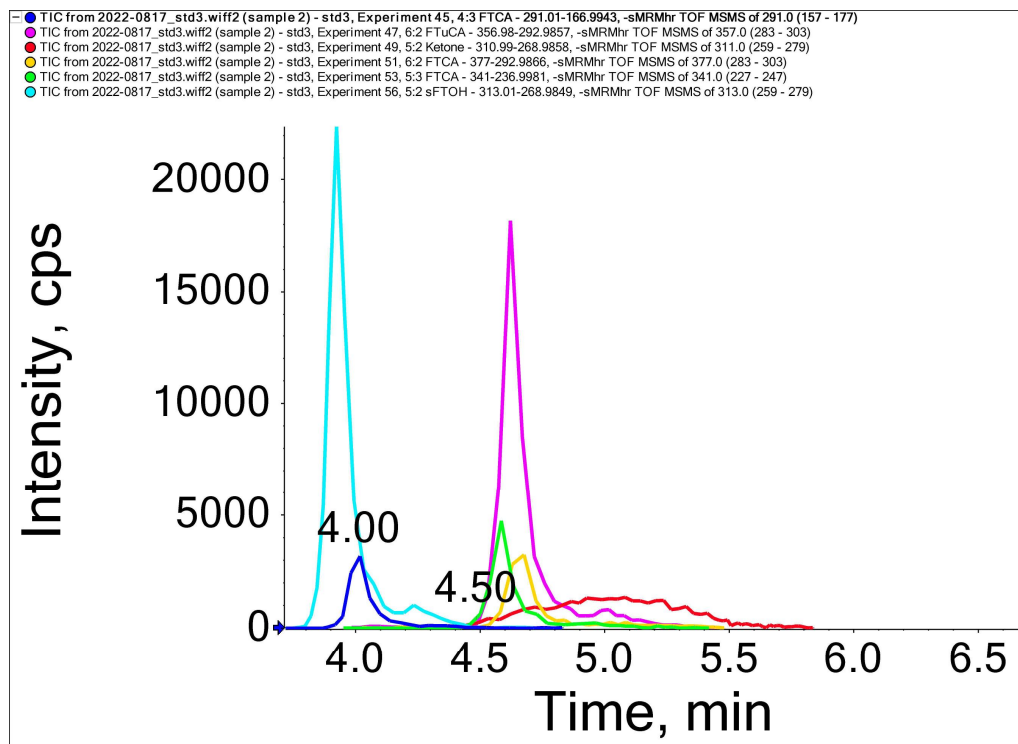
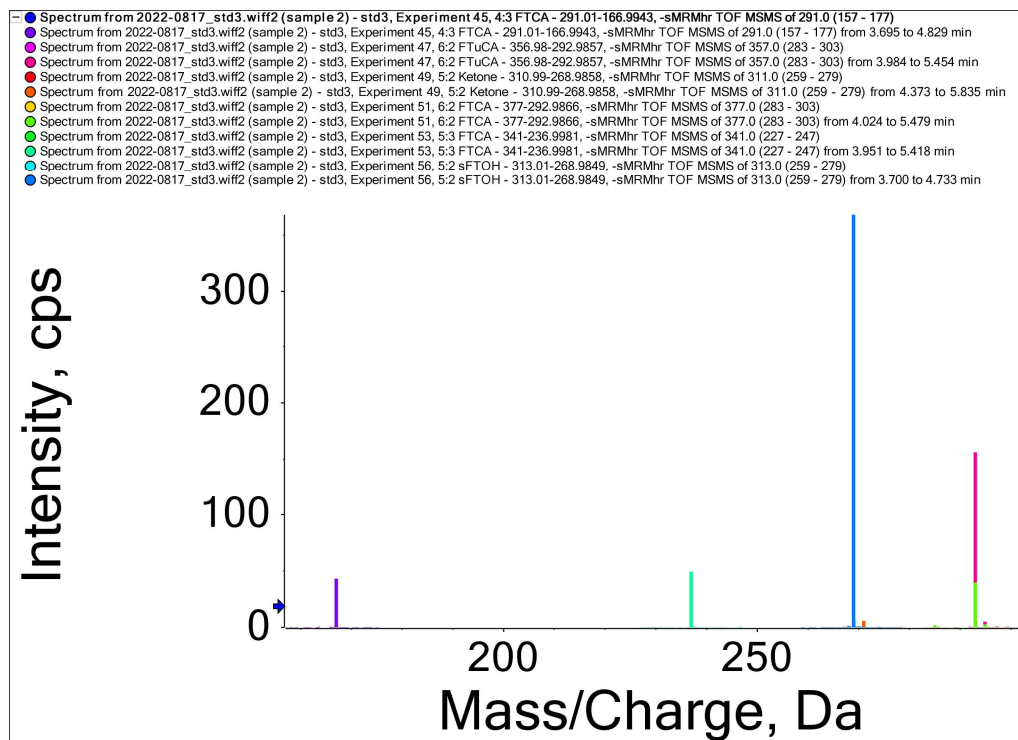


Figure S1. Preliminary screening for 6:2 FTS degrading fungi.



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Figure S2. TIC spectra for 6:2 FTS degradation products 4:3 FTuCA, 6:2 FTuCA, 5:2 ketone, 5:2 sFTOH, 6:2 FTCA, and 5:3 FTCA.



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Figure S3. XIC spectra for 6:2 FTS degradation products 4:3 FTuCA, 6:2 FTuCA, 5:2 ketone, 5:2 sFTOH, 6:2 FTCA, and 5:3 FTCA.