



PFAS NON-TARGETED ANALYSIS AND METHODS INTERIM REPORT

Process and Non-Process Wastewater and Stormwater

Prepared by

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ACRONYMS AND ABBREVIATIONS

CFRW – Cape Fear River Watch

DEQ - Department of Environmental Quality

NCCW – non-contact cooling water

PFAS – per- and polyfluoroalkyl substances

Q-TOF-MS – quadrupole time of flight mass spectrometry

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1 INTRODUCTION

This report has been prepared by The Chemours Company FC, LLC (Chemours) to provide an update on the characterization of previously unidentified (additional) per- and polyfluoroalkyl substances (PFAS) in aqueous samples collected from process wastewater, non-process wastewater (i.e., non-contact cooling water [NCCW]) and stormwater at the Chemours Fayetteville Works, North Carolina site (the Facility; Figure 1). The purpose of the work is to identify previously unknown PFAS that may be present in samples of collected water and to develop standards and methods to facilitate the quantitative analysis of these PFAS. The work described in this report was conducted according to the PFAS Non-Targeted Analysis and Methods Development Plan, Version 2 (the Development Plan, Chemours and Geosyntec, 2019). This work is intended to address requirements specified in Paragraph 11 subpart (a) in the Consent Order executed 25 February 2019 between Chemours and the North Carolina Department of Environmental Quality (DEQ) with the Cape Fear River Watch (CFRW) as intervenor. Other parts of the Consent Order will be addressed separately by Chemours.

Non-targeted analysis refers to a procedure that searches for unknown compounds in a sample following analysis of the sample by a given analytical method; the compounds are considered to be unknown because the analytical method has not been calibrated for them (for example, because authentic standards do not exist). Analytical methods do, however, contain data (such as mass spectral data) that can be used to provide some information on unknown compounds despite the lack of calibration.

Non-targeted analysis for unknown PFAS can be conducted using liquid chromatography coupled to high resolution quadrupole time of flight mass spectrometry (Q-TOF-MS). Q-TOF-MS accurately measures the mass-to-charge ratio of unknown PFAS facilitating the determination of their chemical formulas. Relevant structural information can then be interpreted by fragmenting ions via tandem mass spectrometry, where candidates that do not fit the fragmentation requirements for a particular structure are eliminated so that the tentative structure for the molecule can be assigned. After tentative identification, the structural identity of an analyte can be further assessed by comparing the analyte's chromatographic retention time and mass spectrometry fragmentation patterns to those of an authentic standard.

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The remainder of this report consists of:

- Section 2: Methods
- Section 3: Results
- Section 4: Discussion and Next Steps



2 METHODS

2.1 Sample Collection

Samples were collected from 7 locations (Figure 2). Five sampling locations (Locations 4, 8, 9, 20 and 42) represent a combination of stormwater, treated non-Chemours process wastewater and/or non-contact cooling water. Two locations (16 and 17B) represent Chemours process wastewater. Some locations were sampled more than once; a total of 18 samples were collected. Samples were collected according to the methods outlined in the May 2019 PFAS Characterization Sampling Plan (Geosyntec, 2019) along with modifications to the sampling program to collect stormwater samples as outlined in Version 2 of the *PFAS Non-Targeted Analysis and Method Development Plan* (Chemours, 2019). Samples from locations 4, 9 and 42 were stormwater samples, and were collected during rain events.

2.2 <u>Sample Preparation and Analysis</u>

Samples were prepared for non-targeted analysis by filtration through a 0.2-micrometer filter and were not diluted. Following filtration, the samples were injected directly into the analytical instrument for analysis by liquid chromatography followed by Q-TOF-MS (Agilent).

Known PFAS (i.e., compounds on the analytical lists for EPA Method 537 Modified and Table 3+ Standard Operating Procedure (SOP)) were identified and removed from consideration. Unknown PFAS¹ were identified from the remaining, unidentified chromatographic peaks with a signal-to-noise level of greater than 6 using the mass defect of fluorine as the molecular feature². The empirical formula of the unknown PFAS was then determined based on the accurate mass from the mass spectral data. Results are provided in Tables 2 through 8 for Locations 4, 8, 9, 16, 17B, 20 and 42, respectively.

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¹ Trifluoroacetic acid (TFA) and hexafluoropropylene oxide-trimer acid (HFPO-TA) are known PFAS compounds which have been definitively identified and for which authentic standards exist. TFA and HFPO-TA are not included on the analytical lists for EPA Method 537 Modified and Table 3+ SOP, and thus were identified as an "unknown" compound in the initial assessment.

² A mass defect occurs when the mass of an atom is different from the sum of the masses of its subatomic particles. In this case, fluorine is well-known to have a negative mass defect and when LC-QToF is operated in the negative mode, one can select F-containing features and empirical formulas using available software provided by the instrument vendor. The exact procedures utilized followed closely to what was outlined in the McCord & Strynar 2019 which consists of using a software workflow of Agilent ProFinder, MassHunter, and Mass Profile.



3 RESULTS

To identify the most relevant unknown PFAS, the non-targeted results were assessed in two groups:

- General Facility Discharge samples: samples from locations that may reach the Cape Fear River (Locations 4, 8, 9, 20 and 42). Water from these locations consists of stormwater, treated non-Chemours process wastewater and/or non-contact cooling water discharging to the Cape Fear River; and
- Chemours Process Wastewater samples: samples from these locations (Locations 16 and 17B) consist of process wastewater from Chemours manufacturing areas.

Grouping the results in this way allows for the assessment of the most relevant unknown PFAS at the Facility and prioritization of which unknown PFAS should be advanced for synthesis of authentic standards.

In the General Facility Discharge samples, there were 21 unknown PFAS ranging in ion abundance from 1.8E9 to 5.5E6 (Table 9). The most abundant "unknown" PFAS was later identified as TFA. In the Chemours Process Wastewater samples, there were 250 unknown PFAS ranging in ion abundance from 7.1E8 to 5.3E6 (Table 10). Fourteen of the 21 unknown PFAS from the General Facility Discharge samples were also found in the Chemours Process Wastewater samples.



4 DISCUSSION AND NEXT STEPS

Non-targeted analysis has identified 21 unknown PFAS present in General Facility Discharge samples and 250 unknown PFAS present in Chemours Process Wastewater samples, with a total of 257 potential unique unknown PFAS (14 unknown PFAS were present in both types of samples). Empirical formulas were determined for all unknown PFAS. This work represents the first part of the Initial Assessment step in the Development Plan. The second part of the Development Plan, the Enhanced Assessment is to develop tentative molecular structures and subsequently for the highest priority detected samples, develop authentic standards (i.e. synthesize samples of the compounds to facilitate traditional targeted analysis.

To prioritize developing authentic standards for the most abundant unknown PFAS for each grouping of samples (General Facility Discharge and Chemours Process Wastewater), the 5 most abundant unknown PFAS from each group will be advanced to the Enhanced Assessment step. This is an adjustment from Chemours's prior proposal to carry the 5 most abundant unknown PFAS from each sample from the Initial Assessment step forward to the Enhanced Assessment step. This adjustment ensures that this program retains focus on unknown PFAS which were most abundant overall, whereas the 5 most abundant unknown PFAS in any given sample do not necessarily represent the most abundant unknown PFAS overall.

The 5 most abundant unknown PFAS in the General Facility Discharge samples (excluding TFA, which has been definitively identified and for which an authentic standard exists) consists of the following list:

- C₄H₅F₃O₂
- C₄H₂F₄O₂
- C₆H₆F₆O₂
- C₈H₇F₉O₂
- C₁₀H₈F₁₂O₂

The 5 most abundant unknown PFAS in the Chemours Process Wastewater samples consists of the following list:

- C₈H₂F₁₄O₇S
- C₈HF₁₃O₄
- C8H5F13O6S
- C9H2F14O6
- C₆HF₁₁O₄





None of the 5 most abundant unknown PFAS in the General Facility Discharge samples are represented in the 5 most abundant unknown PFAS in the Chemours Process Wastewater samples, and vice versa. Therefore, the 10 unknown PFAS in the two lists are unique.

During the Enhanced Assessment step, authentic standards will be prepared and analyzed for the unknown PFAS carried forward from the Initial Assessment step. Following this, the Development Plan states that a test method will be developed for these unknown PFAS. The timeline for the Enhanced Assessment and the Test Method Development is provided in Figure 3.

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5 REFERENCES

- Chemours and Geosyntec, 2019. PFAS Non-Targeted Analysis and Methods Development Plan. Version 2. December 5, 2019.
- Geosyntec Consultants, 2019. PFAS Characterization Sampling Plan. Chemours Fayetteville Works. May 1, 2019.
- McCord, J. and Strynar, M., 2019. Identification of per-and polyfluoroalkyl substances in the Cape Fear river by high resolution mass spectrometry and nontargeted screening. Environmental science & technology, 53(9), pp.4717-4727.

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TABLE 1 DESCRIPTION OF SAMPLING LOCATIONS Chemours Fayetteville Works, North Carolina

			Location	on Type		Sample	Category	
Sample Number	Sample Location Description	Sampling Method	Process Wastewater	General Facility Discharge	Outfall	Process Wastewater	Non-process wastewater (i.e., NCCW)	Stormwater
4*	Combined stormwater discharge from Kuraray northern leased area and Chemours PPA area	Temporal Composite		~				✓
8	Outfall 001 non-Chemours treated process wastewater discharge to open channel to Outfall 002	Temporal Composite		✓		✓	✓	
9*	Chemours Monomers IXM NCCW and stormwater discharge including stormwater from Vinyl Ethers South and Vinyl Ethers North	Temporal Composite		✓			✓	✓
16**	Chemours Monomers IXM Area combined process wastewater	Grab	✓			✓		
17B	Chemours PPA Area combined process wastewater	Grab	✓			✓		
20	Outfall 002 to Cape Fear River	Temporal Composite		√	✓			
42*	Stormwater from rooftop gutters from the Chemours Monomers IXM area going to the Cooling Water Channel	Grab		✓				√

Notes

Sample numbers 4, 8, 9, 16, 17, and 20 refer to locations identified in Figure 2 and correspond to locations identified in the May 2019 PFAS Characterization Sampling Plan (Geosyntec, 2019a). Sample number 42 refers to the location identified in Figure 2 and corresponds to the location identified in the September 2019 Stormwater Grab Sampling Workplan (Geosyntec, 2019b).

NCCW - non-contact cooling water

PPA - polymer processing aid

- * Locations 4, 9, and 42 were sampled during a rain event
- ** Location 16 was sampled during dry and rain events

		Mass to	Sample Collected 12/20/2019
Empirical Formula	Mass (amu)	Charge Ratio (m/z)	Ion Abundance
C6H6F6O2	224.0275	223.0200	2.7E+07
C4H2F4O2	157.9980	156.9909	5.6E+07

Notes:

amu - atomic mass units

C - carbon

F - fluorine

H - hydrogen

O - oxygen

PFAS - per- and polyfluoroalkyl substances

		Mass to	Sample Collected 6/21/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019
Empirical Formula	Mass (amu)	Charge Ratio (m/z)		Ion Abundance	•
C4H5F3O2	142.0241	141.0168	6.3E+08		
C2H3F3SO4	179.9706	178.9633		1.6E+07	
C6H6F6O2	224.0273	223.0201	5.1E+07		
C4HF9O2S	283.9544	282.9471		2.1E+07	1.9E+07
C8H7F9O2	306.0287	305.0213	2.4E+07		3.3E+07
C10H8F12O2	388.0314	387.0240	9.8E+06		1.4E+07
C8H2F15SO2	447.9599	446.9519	7.6E+06	7.6E+06	8.4E+06
C12H9F15O2	470.0329	469.0252			7.3E+06
C10HF19O3	529.9623	528.9549	5.4E+06		6.8E+06

Notes:

-- - not detected

amu - atomic mass units

		Mass to	Sample Collected 12/20/2019
Empirical Formula	Mass (amu)	Charge Ratio (m/z)	Ion Abundance
C2HF3O2 (TFA)	113.9928	112.9856	4.0E+07
C3H3F3O3	144.0033	142.9960	1.6E+07
C4H2F4O2	157.9982	156.9910	4.9E+07
C3H3F3O4	159.9973	158.9901	5.5E+06
C6H6F6O2	224.0275	223.0203	9.4E+07
C6H3F7O2	240.0005	238.9936	6.0E+06
C8H7F9O2	306.0307	305.0234	5.8E+07
C8H4F10O2	322.0043	320.9969	1.1E+07
C10H8F12O2	388.0339	387.0264	2.0E+07
C8HF13O4	407.9668	406.9596	1.5E+07

Notes:

amu - atomic mass units

C - carbon

F - fluorine

H - hydrogen

O - oxygen

PFAS - per- and polyfluoroalkyl substances

TFA - trifluoroacetic acid

		Mass to	Sample Collected 6/27/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019	Sample Collected 12/20/2019	Sample Collected 1/29/2020	Sample Collected 4/28/2020
Empirical Formula	Mass (amu)	Charge Ratio (m/z)			Ion Ab	undance		
C2HF3O2 (TFA)	113.9928	112.9856	2.0E+07	3.5E+07	5.3E+08	3.0E+07	3.0E+07	7.5E+07
C3H3F3O3	144.0024	142.9959	2.0E+07	3.3E+07	5.5E+06	3.0E+07	1.1E+07	1.4E+07
C4H2F4O2	157.9981	156.9908				2.0E+07		
C2H3F3SO4	179.9700	178.9628				4.4E+07		
C3HF5O4	195.9794	194.9722			1.2E+07	4.4E±07		6.1E+06
C4H2F6O2	195.9955	194.9882		5.9E+06	2.1E+07			0.1E+00
C4H2F0O2 C6H8F4O3	204.0399	203.0326		3.9E+00	2.1E+07			6.5E+06
C3HF5O3S	211.9566	210.9493		2.8E+07				0.3E+00
C4H2F6O3	211.9904	210.9831		5.8E+06	7.0E+06			
C6H6F6O2	224.0272	223.0199		1.2E+07	1.3E+07			
C5H2F6O4	239.9858	238.9786		1.2E±0/ 	8.0E+06			
C5H6F6O4	244.0170	243.0097		1.0E+07	8.0E±00		7.5E+06	
C5H2F8O2		243.0097						
	245.9919		1.7E+07	2.4E+08	4.9E+07	6.8E+07	5.5E+07	1.5E+07
C3H2F6O4S	247.9579	246.9506	2.1E+08	3.3E+08	1.5E+08	9.9E+06	7.9E+06	1.6E+07
C6H2F8O2	257.9928	256.9855	 4.2E+07	 4.2E+07		0.0E+00		6.2E+06
C6H5F7O3	258.0127	257.0054	4.2E+07	4.2E+07				
C4H2F6O4S	259.9577	258.9504						8.9E+06
C4HF7SO3	261.9535	260.9463		6.2E+06				
C5H2F8O3	261.9875	260.9803	5.2E+07	3.2E+07	1.4E+09	2.6E+07	1.9E+07	1.2E+07
C6HF9O2	275.9831	274.9759	2.1E+07	1.4E+07	1.4E+07			3.0E+07
C6H4F8O3	276.0035	274.9962		7.7E+06				
C4HF7SO4	277.9478	276.9413		1.4E+07				2.6E+07
C4H3F7SO4	279.9645	278.9572						3.1E+07
C4HF9O2S	283.9548	282.9476		1.8E+07		7.0E+06		
C6H2F10O2	295.9895	294.9822	1.2E+07	1.0E+07	7.9E+06			
C8H7F9O2	306.0302	305.0229			9.5E+06		7.2E+06	
C4H2F6O7S	307.9416	306.9345			6.4E+06			
C5H2F8O4S	309.9543	308.9470						8.6E+06
C6H2F10O3	311.9844	310.9775	1.4E+07	4.6E+07	9.8E+07	3.7E+08	4.4E+07	2.9E+07
C5H2F10SO2	315.9622	314.9550		5.3E+06				
C7H2F10O3	323.9844	322.9769	6.5E+06	-	5.6E+07	1.2E+07		
C7H5F9O4	324.0045	322.9974	7.4E+06	-				
C5H2F8SO5	325.9519	324.9446		2.9E+07				
C6H2F10O4	327.9800	326.9724			8.6E+06		1.0E+07	
C7H3F11O2	327.9939	326.9867		4.6E+07	1.1E+07	9.6E+06	7.0E+06	
C7H6F6SO6	331.9799	330.9726				6.9E+06		
C7H2F10O4	339.9790	338.9717			6.2E+06			
C8H6F10O3	340.0156	339.0083	7.7E+06	9.0E+06				
C5H2F8O6S	341.9446	340.9374	1.3E+07	4.9E+07				1.4E+07
C7H4F10O4	341.9945	340.9872	4.0E+07		3.0E+08	8.7E+06		
C5HF9O5S	343.9395	342.9322	9.9E+06	3.0E+07	3.8E+07			1.5E+07
C7H3F11O3	343.9903	342.9830	6.1E+06					
C4H2F8SO7	345.9389	344.9316		1.0E+07				
C6H6F4S2O8	345.9486	344.9374			8.7E+06			
C6HF11O4	345.9693	344.9620			2.6E+07		3.8E+09	1.8E+08
C5H2F10O4S	347.9516	346.9442	4.3E+07	5.9E+07	3.7E+07	6.4E+07	5.0E+07	2.4E+08
C8H3F9O5	349.9834	348.9761		5.5E+07 	1.4E+07		5.0E+07	
C8H4F10O4	353.9954	352.9882	1.6E+07		1.4E+07			
C7HF11O4 / C7H4F10SO3	357.9704	356.9633	1.0E+07					
C7H3F11O4	359.9855	358.9782			5.4E+06			7.0E+06
C7H2F11O4 C7H2F12O3	361.9813	360.9740	8.7E+07	3.4E+07	8.6E+08	4.2E+07	2.0E+07	2.4E+07
C4HF9SO7	363.9269	362.9196	1.7E+07	3.4E+07 4.6E+07	6.0E±08	4.2ETU/	2.0E±07	7.8E+06

Empirical Formula C5H2F10O5S C5HF11SO4 C7H2F8O6S C6H2F12O2S	Mass (amu) 364.9487	Charge Ratio (m/z)						
C5H2F10O5S C5HF11SO4 C7H2F8O6S	364.9487				Ion Ab	undance		
C5HF11SO4 C7H2F8O6S		363.9415				8.4E+06		
C7H2F8O6S	365.9419	364.9346	6.9E+06		4.7E+07	9.9E+07	3.4E+07	2.4E+07
	365.9449	181.9651	0.9E+00	6.2E+06	4./E+0/	9.9E+07	3.4E+07	2.4E±07
C01121 12O23	365.9582	364.9510		1.5E+07	5.0E+06			
C10H15F5O5S2	374.0288	373.0214		1.5E+07				
C7H3F1105	375.9790	374.9717					2.25:07	1.1E+07
C8H7F11SO2	375.9998	374.9927	 2.50.05				2.3E+07	
C6HF11SO4	377.9420	376.9350	2.7E+07	5.8E+06				
C7H2F12O4	377.9766	376.9693	1.3E+07	6.4E+06	5.9E+08	1.2E+07		1.1E+07
C7HF13O3	379.9676	378.9645	1.2E+07		1.6E+07	3.3E+07	1.6E+07	
C6H2F12SO3	381.9515	380.9441		1.0E+07	4.5E+07			
C6H9F5O9S2	383.9622	382.9547				-		7.6E+06
C5H6F6S2O9	387.9353	386.9280			6.4E+06			6.0E+06
C10H8F12O2	388.0339	387.0265			6.0E+06			
C8HF13O3	391.9715	390.9643	1.3E+07	7.8E+06		-		-
C7H2F12O5 / C7H5F11SO4	393.9712	392.9640		-	3.1E+07	1	1.1E+07	-
C8H8F6SO9	393.9801	392.9728				6.9E+06		
C8H3F13O3	393.9873	392.9797	6.4E+06					
C6H3F11SO5	395.9497	394.9433			1.2E+07	-	1.4E+07	
C7HF13O4	395.9641	394.9594		9.8E+06	1.2E+07	3.0E+07		2.7E+07
C8H3F11O6	403.9753	402.9685	7.8E+07	2.0E+07	1.3E+09	1.0E+08	5.3E+07	4.3E+07
C8HF13O4	407.9670	406,9598	4.2E+09	7.1E+08		4.1E+09	2.6E+09	3.4E+07
C7H5F11O5S	409.9677	408.9605	7.0E+07	7.1E+00				5.1E-07
C8H3F13O4	409.9822	408.9749	1.2E+07		1.3E+07	-		
C9H4F14O2	409.9980	408.9908	1.2L+07	1.2E+07	1.5E+07			
C7HF13O5	411.9620	410.9544		1.2E+07	1.3E+07		1.8E+08	5.9E+07
C8H7F7SO9	411.9713	410.9627			1.4E+07		1.6E±06	3.9E±07
C8H2F14O3	411.9780	410.9707	6.4E+06		1.4E+07	1.3E+07		
				1.3E+07			1.5E+07	
C6H2F12SO5	413.9435	412.9362	3.2E+08	4.1E+08	4.9E+08	6.3E+07	5.8E+06	1.1E+08
C7H3F13SO3	413.9562	412.9503		1.6E+07		1.4E+07	1.4E+07	1.5E+07
C6HF13SO4	415.9352	414.9341	1.6E+07		2.4E+07	1.1E+07		
C9H2F12O3S	417.9532	416.9444			9.5E+06			
C9H2F12O5	417.9711	416.9638			4.2E+07	-		
C8H5F11SO5	421.9657	420.9584			1.4E+07			
C9H6F12O5 / C9H9F11SO4	422.0026	420.9953	7.9E+06					
C7H3F11O6S	423.9475	422.9404	7.6E+06	-		-		-
C8HF13O5	423.9615	422.9557		8.0E+06		-		
C7H3F11O8	423.9652	422.9589			2.1E+07			
C9H5F13O4	423.9950	422.9881	1.7E+07		2.5E+07			
C7H2F12O5S	425.9438	424.9365	2.9E+07			-		
C8H3F13SO3	425.9567	424.9500			2.9E+07	5.6E+06		
C9H4F14O3	425.9931	424.9858			9.7E+06	-		
C7HF13O4S	427.9392	426.9319	3.6E+07	3.6E+07		-		
C7H3F13SO4	429,9524	428.9451				-	1.3E+07	
C8HF15O3	429.9685	428.9613	3.3E+08	6.0E+07	1.4E+09	2.2E+07	1.3E+07	4.1E+07
C6H7F7S2O10	435.9351	434.9279	3.3E±08	0.0E⊤07 	1.4E±09	6.6E+06	1.3E±0/	4.1E±0/
C8H3F11SO6	435.9475	434.9402						
			 (7E+0(6.8E+06				
C10H4F14O3	437.9949	436.9877	6.7E+06		 1 (E+07			
C9H6F12O6 / C9H9F11SO5	437.9975	436.9902			1.6E+07			
C9H2F14O4	439.9731	438.9661	6.6E+07			7.7E+06		
C10H3F15O2 C9H5F13O5	439.9895 439.9930	438.9821 438.9858	1.9E+07 8.1E+08	 2.0E+07	 1.2E+09	8.5E+07	1.3E+07	2.0E+07

		Mass to	Sample Collected 6/27/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019	Sample Collected 12/20/2019	Sample Collected 1/29/2020	Sample Collected 4/28/2020
Empirical Formula	Mass (amu)	Charge Ratio (m/z)			Ion Ab	undance		
C9HF15O3	441.9692	440.9619	4.1E+07					
C9H4F14O4	441.9885	440.9813	4.1E±07		8.1E+06			
C8HF15O4	445.9634	444.9530	3.4E+07	2.7E+07			3.1E+07	1.9E+07
C8H5F9S2O7	447.9334	446.9261	7.6E+06	2./E+0/			3.1E+07	1.9E+07
C7H2F14SO4	447.9446	446.9376	5.6E+06	1.1E+07				
C8H3F15O2S	447.9616	446.9542	5.0E+00	7.9E+06				
C8H51107S	449.9248	448.9184	2.7E+07	1.5E+07	5.9E+06		9.1E+06	
C8H2F12O6S	453.9380	452.9308	2./E+0/	2.1E+07	2.2E+07		9.1E+00	1.8E+07
C6H2F10SO10	455.9208	454.9136	1.6E+07	2.7E+08	2.2E+07			1.8E±07
C9H2F10SO10 C9H2F14O5	455.9678	454.9605	1.6E+07	5.8E+06	1.6E+07		+	
				1.3E+08				
C9H5F13O4S	455.9709	454.9636						
C6H4F10O8S2	457.9194	456.9119		2.7E+07				
C7H2F12O7S / C7H5F11S2O7	457.9331	456.9260	4.1E+07	1.4E+07	 5 1E+07	9.5E+06		0.75+06
C9HF15O4 / C9H4F14SO3	457.9638	456.9565	3.3E+08	5.6E+07	5.1E+07	1.6E+07		9.7E+06
C9H4F14O5	457.9822	456.9750	 2.1E+07		3.3E+07			
C9H3F15O4	459.9777	458.9712	2.1E+07		2.6E+07	8.3E+06		
C9HF11O7S	461.9245	460.9173			3.2E+07			
C8HF15SO3	461.9407	460.9356			3.1E+07			
C9H2F16O3	461.9746	460.9673			5.9E+07			
C8H3F15SO3	463.9542	462.9469			6.8E+06			
C10H12F10O7S	466.0147	465.0075		1.1E+07				
C7H8F8S2O10	467.9446	466.9372				8.4E+06		
C10H4F14O5	469.9832	468.9759	5.1E+06		7.7E+06			
C10H7F13O6	470.0032	468.9959			1.1E+07			
C7H3F11S2O7	471.9127	470.9054		6.0E+06				
C9H2F14O6	471.9630	470.9556	4.8E+07	1.2E+09	3.9E+09	7.1E+07	3.8E+07	6.1E+07
C8H3F13O6S	473.9448	472.9374		1.5E+07				
C10H2F16O3	473.9715	472.9671	2.6E+07	1.6E+07	6.4E+06			1.2E+07
C10H2F16O3	473.9744	472.9671			1.2E+07			1.2E+07
C8H5F13O6S	475.9587	474.9515	4.1E+09	1.3E+08	6.8E+07	4.7E+08	3.6E+07	8.4E+06
C9H2F16O4	477.9222	476.9629		6.7E+06				
C9H2F16O4	477.9698	476.9637	5.8E+06	6.9E+06	1.0E+08			
C9HF17O3	479.9605	478.9574	1.3E+07	9.4E+06	3.1E+07			1.8E+07
C8H2F16SO3	481.9448	480.9377	7.3E+06					
C8H3F13SO7	489.9389	488.9316	2.3E+07	5.9E+06	7.4E+06	1.1E+07		
C8H6F12SO8	489.9608	488.9536			6.1E+06			
C10H5F15O5 / C10H8F14SO4	489.9894	488.9821	2.0E+07		3.3E+07			
C8HF15SO5	493.9297	492.9224		1.8E+07				
C9H2F16O3S	493.9449	492.9379	6.9E+06					
C8H3F15SO5	495.9439	494.9366					6.3E+06	
C9HF17O4 (HFPO-TA)	495.9607	494.9557	1.1E+07	8.6E+06	3.3E+07		6.3E+07	1.1E+07
C8HF17O5	499.9549	498.9477			3.8E+07			
C10H3F15O6 / C10H6F14SO5	503.9669	502.9596	3.6E+07		1.2E+08			
C9H7F13SO7 / C9H4F14O8	505.9701	504.9629			5.5E+06			
C8H2F14O7S	507.9302	506.9229	2.2E+09	4.5E+09	4.1E+09	4.6E+07	2.6E+07	1.7E+07
C10H4F16O5	507.9775	506.9715			7.5E+06			
C8HF15O8 / C8H4F14SO7	509.9430	508.9367			6.4E+06	1.8E+07		
C10H3F17O4	509.9736	508.9664			1.0E+07			
C8H3F15SO6	511.9390	510.9317			9.0E+06			
C8H2F16SO5	513.9344	512.9272		1.1E+07	1.4E+07		2.7E+07	

		Mass to	Sample Collected 6/27/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019	Sample Collected 12/20/2019	Sample Collected 1/29/2020	Sample Collected 4/28/2020
	Mass	Charge Ratio			Ion Ab	undance		
Empirical Formula	(amu)	(m/z)		T.				1
C9H3F17SO3	513.9512	512.9445			6.3E+06			
C12H11F13O7	514.0289	513.0219			6.2E+06			2.6E+07
C11H5F15O6 / C11H8F14SO5	517.9846	516.9773			7.7E+06			
C9H5F13O6S2 / C9H2F14SO7	519.9326	518.9249		1.6E+07	 5 2E : 05			
C10H2F16O6 / C10H5F15SO5	521.9590	520.9523			5.3E+07			
C7H3F13O8S2	525.9057	524.8984	1.0E+07	2.4E+07				
C10HF13O8S	527.9139	526.9066	3.5E+07	4.1E+07		1.5E+07	8.2E+06	
C7H2F14O9S	527.9202	526.9130			9.1E+06			
C8H3F15SO7 / C9HF17SO4	527.9325	526.9252	8.6E+07	3.4E+08	1.6E+07			
C10HF19O3	529.9619	528.9545				6.5E+06		
C9HF19O2S	533.9375	532.9302		1.5E+07	8.8E+06			
C11H5F15O7 / C11H8F14SO6	533.9778	532.9705	4.1E+07		6.7E+07			
C11HF17O5	535.9529	534.9457	7.3E+06	1.1E+07	7.6E+06			
C9H4F14SO8	537.9428	536.9354		1.5E+07				
C9H3F15O7S / C9H6F14S2O6	539.9359	538.9285	1.7E+07					
C11H2F18O4 / C11H5F17SO3	539.9656	538.9584						8.8E+06
C11H5F17O5 / C11H8F16SO4	539.9843	538.9770	2.0E+07		7.1E+06			
C7H3F13O9S2	541.9016	540.8965	1.2E+07	5.7E+06				
C9H2F16SO6	541.9312	540.9240	1.9E+08	2.6E+07	9.3E+06	5.6E+07		9.2E+06
C9H5F15O7S	541.9522	540.9450	6.8E+06	4.0E+07	7.3E+06			
C10H3F17O6 / C10H6F16SO5	541.9658	540.9584						9.4E+06
C10H4F18O5	545.9775	544.9703			9.6E+06			
C10HF15O5S2	549.9015	548.8933	6.7E+06					
C12H9F15SO5 / C11H8F14O9 / C11H11F13SO8	549.9956	548.9883		8.2E+06	2.7E+07			5.6E+07
C11H3F17O6	553.9658	552.9586	1.8E+07		7.1E+07			
C8HF17SO7	563.9146	562.9073	5.5E+07					
C10H7F13O8S2	565.9382	564.9309		3.3E+07				
C11H5F15O9	565.9679	564.9605			6.1E+06			
C13H6F18O4	567.9969	566.9899			5.9E+06			
C11H3F17SO5	569.9473	568.9401	1.9E+07					
C11H3F17O7 / C11H6F16SO6	569.9585	568.9512			1.3E+08			1.4E+07
C11H2F18O6 / C11H5F17SO5	571.9564	570.9492			4.1E+07			
C11H3F19O5	575.9692	286.9774	4.1E+07					
C10HF19SO4	577.9266	576.9196		6.4E+06				
C11H2F20O4	577.9627	576.9550	2.7E+07	1.8E+07	2.8E+07			
C10H3F19SO4	579.9416	578.9343	2.7E+07	4.0E+07	2.7E+07	5.4E+06		
C11H4F16O9 / C11H7F15SO8	583.9587	582.9514	6.5E+06	1.4E+07				
C10H4F16O6S2	587.9196	586.9121		8.3E+06				
C11H2F18O7	587.9478	586.9405		1.0E+07				
C11H2F18O7 / C12H3F19SO3	587.9507	586.9434		1.2E+08	4.5E+07			
C10H3F17SO7 / C10H6F16S2O6	589.9338	588.9264	9.5E+06					
C9HF17SO8 / C9H4F16S2O7	591.9071	590.9063	J.5E-00	1.0E+07				
C11H3F19O6 / C11H6F18SO5	591.9625	590.9552	2.1E+07	1.0L+07		2.9E+07	1.3E+07	
C9H3F17O8S	593.9277	592.9226	9.7E+06	1.6E+07	1.5E+07	2.)L10/	1.5E+07	
C11H2F20O5	593.9580	592.9507		1.3E+07	1.1E+08			
C11H4F20SO3	595.9576	594.9504		1.5L+07			1.3E+07	
C13H6F18O6	599.9839	598.9767	6.5E+06				1.5E+07	
C12H2F20O6	621.9543	620.9463	3.5E+07		5.2E+07	8.5E+06		
C10H2F20SO6	629.9259	628.9176	2.1E+07	7.1E+07	1.3E+07	6.5E+00		
C13H2F20O7 / C13H5F19SO6	649.9490	648.9408	1.1E+07	7.1E+07	2.1E+07			
C11H5F19S2O7 / C11H2F20SO8	673.9165	672.9100	1.1E+0/	1.1E+07	2.1E+0/			

		Mass to	Sample Collected 6/27/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019	Sample Collected 12/20/2019	Sample Collected 1/29/2020	Sample Collected 4/28/2020
Empirical Formula	Mass (amu)	Charge Ratio (m/z)	Ion Abundance					
C14H3F23O7	719.9479	718.9446	1.3E+08	3.2E+07	5.2E+08	3.3E+07		
C12H7F19S2O10	735.9173	734.9104	5.5E+06	1.7E+07		-		
C16H6F24SO8	813.9388	812.9308	2.4E+08	1.3E+07	2.2E+08	6.4E+06		
C18H9F27S2O7	913.9324	912.9235			5.5E+06	-		

Notes:

-- - not detected

amu - atomic mass units

C - carbon

F - fluorine

H - hydrogen

HFPO-TA - hexafluoropropylene oxide trimer acid

O - oxygen

PFAS - per- and polyfluoroalkyl substances

TFA - trifluoroacetic acid

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		Mass to	Sample Collected 6/27/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019	
Empirical Formula	Mass (amu)	Charge Ratio (m/z)	Ion Abundance			
C2HF3O2 (TFA)	113.9928	112.9856	5.5E+07	8.0E+07	3.0E+08	
C4H5F3O2	142.0241	141.0168	2.5E+07	==		
C3H3F3O3	144.0033	142.9960		1.0E+07	2.3E+07	
C3H2F4O2	145.9977	144.9905	2.1E+07	1.0E+07	2.4E+07	
C4H2F4O2	157.9982	156.9909	7.1E+08	4.4E+08	5.6E+08	
C3H3F3O4	159.9978	158.9906			8.3E+07	
C4H2F6O2	195.9960	194.9888	6.5E+06		5.3E+07	
C5H3F5O3	206.0002	204.9929			1.7E+07	
C4H2F6O3	211.9908	210.9835			9.5E+06	
C5HF7O3	241.9803	240.9730		5.8E+06	1.0E+07	
C5H2F8O2	245.9927	244.9854			1.5E+07	
C3H2F6O4S	247.9580	246.9507	6.4E+07	3.2E+08	1.9E+09	
C5H2F4O5S	249.9534	248.9461			7.8E+07	
C6H2F10O2	295.9899	294.9826	3.5E+07	6.7E+06		
C7H4F8O5	319.9918	318.9842			7.3E+06	
C8H6F10O2	324.0181	323.0109			1.3E+07	
C7H7F5O9	330.0022	328.9948			1.4E+07	
C7H2F12O2	345.9868	344.9795			2.1E+07	
C5H7F5S2O8	353.9522	352.9447	3.2E+07	1.2E+07	1.2E+07	
C8H2F12O4	389.9760	388.9687			1.6E+07	
C8H4F12O4	391.9919	390.9830	5.7E+08	1.9E+08	3.6E+09	
C8H2F14O2	395.9831	394.9758		6.9E+06	3.8E+07	
C5H3F9S2O7	409.9187	408.9111	1.2E+07	9.8E+06	1.1E+07	
C8H2F14O3	411.9781	410.9708	7.2E+06	6.5E+06		
C8H10F6O10S / C9H11F7S2O6	411.9895	410.9821			9.2E+06	
C7H3F13SO3	413.9572	412.9505	1.6E+07			
C9HF13O4	419.9643	418.9575			7.9E+06	
C9H4F12O5	419.9869	418.9795			1.9E+07	

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		Mass to	Sample Collected 6/27/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019
Empirical Formula	Mass (amu)	Charge Ratio (m/z)		Ion Abundance	
C9H12F6O10S / C10H13F7S2O6	426.0045	424.9977		==	5.9E+06
C8HF15O3	429.9688	428.9616			7.7E+06
C7H5F9S2O8	451.9280	450.9214	1.9E+07	5.7E+06	7.3E+06
C10HF15O3	453.9658	452.9586	7.4E+06		7.2E+06
C11H5F15O2	454.0033	452.9960	2.2E+07		2.4E+08
C10H14F6S2O9	455.9976	454.9904			2.3E+07
C6H4F10S2O8	457.9210	456.9130	8.8E+06		1.2E+07
C9H2F16O3	461.9749	460.9677			1.3E+07
C8H3F15SO3	463.9536	462.9463			1.6E+07
C11H2F16O2	469.9794	468.9694			1.7E+07
C7H6F10S2O8	471.9310	470.9258			6.8E+06
C10H5F15O4	473.9950	472.9877			1.3E+07
C10H4F16O3	475.9884	474.9818			1.0E+07
C12H16F8S2O7	488.0217	487.0144			1.6E+07
C10H2F16O4	489.9702	488.9630			7.3E+07
C10H14F8S2O9	493.9944	492.9871			6.9E+06
C9HF17O4 (HFPO-TA)	495.9609	494.9537	3.7E+08	3.4E+08	2.8E+08
C10H2F18O2	495.9763	494.9690	1.0E+07	5.6E+06	2.4E+07
C8H2F14O7S	507.9308	506.9236	7.5E+06	9.0E+06	2.3E+08
C11H4F18O2	509.9890	508.9819			8.7E+06
C9H2F14SO7	519.9256	518.9207			7.9E+06
C10HF19O3	529.9611	528.9542		6.1E+06	8.6E+07
C13H6F18O2	536.0051	534.9980		2.3E+07	4.6E+07
C11H2F18O4	539.9668	538.9596			2.1E+07
C12H15F9O10S2	553.9946	552.9871			4.6E+07
C15H12F14O6 / C15H15F13SO5	554.0429	553.0355			7.7E+06
C13H7F19O2	556.0112	555.0041	5.4E+06	-	1.3E+08
C14H4F20O	567.9928	566.9855			4.8E+07

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		Mass to	Sample Collected 6/27/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019
Empirical Formula	Mass (amu)	Charge Ratio (m/z)		Ion Abundance	
C11H8F12O13	575.9767	574.9694			1.0E+07
C11H2F20O4	577.9636	576.9562	9.7E+06	7.1E+06	2.7E+07
C10H3F19SO4	579.9429	578.9360	3.6E+07	8.6E+06	2.8E+07
C13H15F13O9S	594.0231	593.0159			4.7E+07

Notes:

-- - not detected

amu - atomic mass units

C - carbon

F - fluorine

H - hydrogen

HFPO-TA - hexafluoropropylene oxide trimer acid

O - oxygen

PFAS - per- and polyfluoroalkyl substances

S - sulfur

TFA - trifluoroacetic acid

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		Mass to	Sample Collected 6/27/2019	Sample Collected 8/21/2019	Sample Collected 10/9/2019
Empirical Formula	Mass (amu)	Charge Ratio (m/z)		Ion Abundance	
C8H4F10O2	322.0041	320.9968		7.8E+06	6.8E+06
C4H2F4O2	157.9978	156.9906	2.3E+07	8.3E+06	2.3E+07
C10H8F12O2	388.0331	387.0258	3.6E+07		4.0E+07
C8H7F9O2	306.0302	305.0230	7.7E+07	8.8E+07	8.7E+07
C6H6F6O2	224.0272	223.0199	1.1E+08	1.2E+08	1.0E+08
C4H5F3O2	142.0241	141.0168	8.1E+08	8.6E+08	8.5E+08
C2H3F3SO4	179.9704	178.9631	7.2E+06	8.0E+06	

Notes:

-- - not detected

amu - atomic mass units

C - carbon

F - fluorine

H - hydrogen

O - oxygen

PFAS - per- and polyfluoroalkyl substances

S - sulfur

		Mass to	Sample Collected 12/20/2019
Empirical Formula	Mass (amu)	Charge Ratio (m/z)	Ion Abundance
C2HF3O2 (TFA)	113.9928	112.9856	1.8E+09
C4H2F4O2	157.9983	156.9910	2.6E+08
C4H2F6O2	195.9956	194.9884	2.8E+07
C6H6F6O2	224.0272	223.0199	3.2E+07
C6H3F7O2	240.0010	238.9937	1.8E+07
C8H7F9O2	306.0307	305.0232	1.1E+07
C8H4F10O2	322.0044	320.9968	1.2E+07
C7HF13SO2	395.9501	394.9428	5.8E+06
C8HF13O4	407.9670	406.9596	2.3E+07
C9HF17O4 (HFPO-TA)	495.9638	494.9564	2.5E+07
C8HF15O8	509.9432	508.9357	3.3E+07
C9HF17SO4	527.9332	526.9259	7.1E+06

Notes:

amu - atomic mass units

C - carbon

F - fluorine

H - hydrogen

HFPO-TA - hexafluoropropylene oxide trimer acid

O - oxygen

PFAS - per- and polyfluoroalkyl substances

S - sulfur

TFA - trifluoroacetic acid

TABLE 9
UNKNOWN PFAS IN SAMPLES FROM GENERAL FACILITY DISCHARGE SAMPLING LOCATIONS
Chemours Fayetteville Works, North Carolina

		Mass to	
	Mass	Charge Ratio	Ion
Empirical Formula	(amu)	(m/z)	Abundance
C2HF3O2 (TFA)	113.9928	112.9856	1.8E+09
C4H5F3O2	142.0241	141.0168	8.6E+08
C4H2F4O2	157.9983	156.9910	2.6E+08
C6H6F6O2	224.0272	223.0199	1.2E+08
C8H7F9O2	306.0302	305.0230	8.8E+07
C10H8F12O2	388.0331	387.0258	4.0E+07
C8HF15O8	509.9432	508.9357	3.3E+07
C4H2F6O2	195.9956	194.9884	2.8E+07
C9HF17O4 (HFPO-TA)	495.9638	494.9564	2.5E+07
C8HF13O4	407.9670	406.9596	2.3E+07
C4HF9O2S	283.9544	282.9471	2.1E+07
C6H3F7O2	240.0010	238.9937	1.8E+07
C2H3F3SO4	179.9706	178.9633	1.6E+07
C3H3F3O3	144.0033	142.9960	1.6E+07
C8H4F10O2	322.0044	320.9968	1.2E+07
C8H2F15SO2	447.9599	446.9519	8.4E+06
C12H9F15O2	470.0329	469.0252	7.3E+06
C9HF17SO4	527.9332	526.9259	7.1E+06
C10HF19O3	529.9623	528.9549	6.8E+06
C7HF13SO2	395.9501	394.9428	5.8E+06
C3H3F3O4	159.9973	158.9901	5.5E+06

Notes:

amu - atomic mass units

C - carbon

F - fluorine

H - hydrogen

HFPO-TA - hexafluoropropylene oxide trimer acid

O - oxygen

PFAS - per- and polyfluoroalkyl substances

S - sulfur

TFA - trifluoroacetic acid

TABLE 10
UNKNOWN PFAS IN SAMPLES FROM CHEMOURS PROCESS WASTEWATER SAMPLING LOCATIONS
Chemours Fayetteville Works, North Carolina

	Mass	Mass to Charge Ratio	Ion
Empirical Formula		(m/z)	Abundance
Empirical Formula C8H2F14O7S	(amu) 507.9302	506.9229	4.5E+09
C8HF13O4	407.9670	406.9598	4.3E+09 4.2E+09
C8H5F13O6S	475.9587	474.9515	4.2E+09 4.1E+09
C8H3F13O68 C9H2F14O6			
	471.9630	470.9556 344.9620	3.9E+09
C6HF11O4	345.9693 391.9919		3.8E+09
C8H4F12O4		390.9830	3.6E+09
C3H2F6O4S	247.9580	246.9507	1.9E+09
C8HF15O3	429.9685	428.9613	1.4E+09
C5H2F8O3	261.9875	260.9803	1.4E+09
C8H3F1106	403.9753	402.9685	1.3E+09
C9H5F13O5	439.9930	438.9858	1.2E+09
C7H2F12O3	361.9813	360.9740	8.6E+08
C4H2F4O2	157.9982	156.9909	7.1E+08
C7H2F12O4	377.9766	376.9693	5.9E+08
C2HF3O2 (TFA)	113.9928	112.9856	5.3E+08
C14H3F23O7	719.9479	718.9446	5.2E+08
C6H2F12SO5	413.9435	412.9362	4.9E+08
C9HF17O4 (HFPO-TA)	495.9609	494.9537	3.7E+08
C6H2F10O3	311.9844	310.9775	3.7E+08
C8H3F15SO7 / C9HF17SO4	527.9325	526.9252	3.4E+08
C9HF15O4 / C9H4F14SO3	457.9638	456.9565	3.3E+08
C7H4F10O4	341.9945	340.9872	3.0E+08
C6H2F10SO10	455.9208	454.9136	2.7E+08
C5H2F8O2	245.9919	244.9847	2.4E+08
C11H5F15O2	454.0033	452.9960	2.4E+08
C16H6F24SO8	813.9388	812.9308	2.4E+08
C5H2F10O4S	347.9516	346.9442	2.4E+08
C9H2F16SO6	541.9312	540.9240	1.9E+08
C7HF13O5	411.9620	410.9544	1.8E+08
C9H5F13O4S	455.9709	454.9636	1.3E+08
C11H3F17O7 / C11H6F16SO6	569.9585	568.9512	1.3E+08
C13H7F19O2	556.0112	555.0041	1.3E+08
C10H3F15O6 / C10H6F14SO5	503.9669	502.9596	1.2E+08
C11H2F18O7 / C12H3F19SO3	587.9507	586.9434	1.2E+08
C11H2F20O5	593.9580	592.9507	1.1E+08
C9H2F16O4	477.9698	476.9637	1.0E+08
C5HF11SO4	365.9419	364.9346	9.9E+07
C10HF19O3	529.9611	528.9542	8.6E+07
C3H3F3O4	159.9978	158.9906	8.3E+07
C5H2F4O5S	249.9534	248.9461	7.8E+07
C10H2F16O4	489.9702	488.9630	7.3E+07

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TABLE 10
UNKNOWN PFAS IN SAMPLES FROM CHEMOURS PROCESS WASTEWATER SAMPLING LOCATIONS
Chemours Fayetteville Works, North Carolina

	Mass	Mass to Charge Ratio	Ion
Empirical Formula	(amu)	(m/z)	Abundance
C11H3F17O6	553.9658	552.9586	7.1E+07
C10H2F20SO6	629.9259	628.9176	7.1E+07
C7H5F11O5S	409.9677	408.9605	7.0E+07
C11H5F15O7 / C11H8F14SO6	533.9778	532.9705	6.7E+07
C9H2F14O4	439.9731	438.9661	6.6E+07
C9H2F16O3	461.9746	460.9673	5.9E+07
C7H2F10O3	323.9844	322.9769	5.6E+07
C12H9F15SO5 / C11H8F14O9 / C11H11F13SO8	549.9956	548.9883	5.6E+07
C8HF17SO7	563.9146	562.9073	5.5E+07
C4H2F6O2	195.9960	194.9888	5.3E+07
C10H2F16O6 / C10H5F15SO5	521.9590	520.9523	5.3E+07
C12H2F20O6	621.9543	620.9463	5.2E+07
C5H2F8O6S	341.9446	340.9374	4.9E+07
C14H4F20O	567.9928	566.9855	4.8E+07
C13H15F13O9S	594.0231	593.0159	4.7E+07
C7H3F11O2	327.9939	326.9867	4.6E+07
C4HF9SO7	363.9269	362.9196	4.6E+07
C13H6F18O2	536.0051	534.9980	4.6E+07
C12H15F9O10S2	553.9946	552.9871	4.6E+07
C6H2F12SO3	381.9515	380.9441	4.5E+07
C2H3F3SO4	179.9700	178.9628	4.4E+07
C6H5F7O3	258.0127	257.0054	4.2E+07
С9Н2F12O5	417.9711	416.9638	4.2E+07
C9HF15O3	441.9692	440.9619	4.1E+07
C7H2F12O7S / C7H5F11S2O7	457.9331	456.9260	4.1E+07
C10HF13O8S	527.9139	526.9066	4.1E+07
C11H2F18O6 / C11H5F17SO5	571.9564	570.9492	4.1E+07
C11H3F19O5	575.9692	286.9774	4.1E+07
C10H3F19SO4	579.9416	578.9343	4.0E+07
C9H5F15O7S	541.9522	540.9450	4.0E+07
C5HF9O5S	343.9395	342.9322	3.8E+07
C8HF17O5	499.9549	498.9477	3.8E+07
C8H2F14O2	395.9831	394.9758	3.8E+07
C7HF13O4S	427.9392	426.9319	3.6E+07
C6H2F10O2	295.9899	294.9826	3.5E+07
C8HF15O4	445.9634	444.9530	3.4E+07
C9H4F14O5	457.9822	456.9750	3.3E+07
C7HF13O3	379.9676	378.9645	3.3E+07
C10H7F13O8S2	565.9382	564.9309	3.3E+07
C10H5F15O5 / C10H8F14SO4	489.9894	488.9821	3.3E+07
C9HF11O7S	461.9245	460.9173	3.2E+07

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TABLE 10
UNKNOWN PFAS IN SAMPLES FROM CHEMOURS PROCESS WASTEWATER SAMPLING LOCATIONS
Chemours Fayetteville Works, North Carolina

	Mass	Mass to Charge Ratio	Ion
Empirical Formula	(amu)	(m/z)	Abundance
C5H7F5S2O8	353.9522	352.9447	3.2E+07
C8HF15SO3	461.9407	460.9356	3.1E+07
C4H3F7SO4	279.9645	278.9572	3.1E+07
C7H2F12O5 / C7H5F11SO4	393.9712	392.9640	3.1E+07
C9HF17O3	479.9605	478.9574	3.1E+07
C7HF13O4	395.9641	394.9594	3.0E+07
C6HF9O2	275.9831	274.9759	3.0E+07
C8H3F13SO3	425.9567	424.9500	2.9E+07
C5H2F8SO5	325.9519	324.9446	2.9E+07
C7H2F12O5S	425.9438	424.9365	2.9E+07
C11H3F19O6 / C11H6F18SO5	591.9625	590.9552	2.9E+07
C3HF5O3S	211.9566	210.9493	2.8E+07
C11H2F20O4	577.9627	576.9550	2.8E+07
C6H4F10O8S2	457.9194	456.9119	2.7E+07
C8H2F16SO5	513.9344	512.9272	2.7E+07
C8HF11O7S	449.9248	448.9184	2.7E+07
C6HF11SO4	377.9420	376.9350	2.7E+07
C10H2F16O3	473.9715	472.9671	2.6E+07
C9H3F15O4	459.9777	458.9712	2.6E+07
C4HF7SO4	277.9478	276.9413	2.6E+07
C12H11F13O7	514.0289	513.0219	2.6E+07
C9H5F13O4	423.9950	422.9881	2.5E+07
C4H5F3O2	142.0241	141.0168	2.5E+07
C10H2F18O2	495.9763	494.9690	2.4E+07
C3H2F4O2	145.9977	144.9905	2.4E+07
C6HF13SO4	415.9352	414.9341	2.4E+07
C7H3F13O8S2	525.9057	524.8984	2.4E+07
C10H14F6S2O9	455.9976	454.9904	2.3E+07
C8H7F11SO2	375.9998	374.9927	2.3E+07
C3H3F3O3	144.0033	142.9960	2.3E+07
C8H3F13SO7	489.9389	488.9316	2.3E+07
C8H2F12O6S	453.9380	452.9308	2.2E+07
C13H2F20O7 / C13H5F19SO6	649.9490	648.9408	2.1E+07
C11H2F18O4	539.9668	538.9596	2.1E+07
C7H3F11O8	423.9652	422.9589	2.1E+07
C7H2F12O2	345.9868	344.9795	2.1E+07
C11H5F17O5 / C11H8F16SO4	539.9843	538.9770	2.0E+07
C7H5F9S2O8	451.9280	450.9214	1.9E+07
C10H3F15O2	439.9895	438.9821	1.9E+07
C9H4F12O5	419.9869	418.9795	1.9E+07
C11H3F17SO5	569.9473	568.9401	1.9E+07

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TABLE 10
UNKNOWN PFAS IN SAMPLES FROM CHEMOURS PROCESS WASTEWATER SAMPLING LOCATIONS
Chemours Fayetteville Works, North Carolina

	Mass	Mass to Charge Ratio	Ion
Empirical Formula	(amu)	(m/z)	Abundance
C8HF15O8 / C8H4F14SO7	509.9430	508.9367	1.8E+07
C8HF15SO5	493.9297	492.9224	1.8E+07
C4HF9O2S	283.9548	282.9476	1.8E+07
C11H2F16O2	469.9794	468.9694	1.7E+07
C9H3F15O7S / C9H6F14S2O6	539.9359	538.9285	1.7E+07
C5H3F5O3	206.0002	204.9929	1.7E+07
C12H7F19S2O10	735.9173	734.9104	1.7E+07
C9H2F14O5	455.9678	454.9605	1.6E+07
C7H3F13SO3	413.9562	412.9503	1.6E+07
C8H2F12O4	389.9760	388.9687	1.6E+07
C8H4F10O4	353.9954	352.9882	1.6E+07
C9H6F12O6 / C9H9F11SO5	437.9975	436.9902	1.6E+07
C9H5F13O6S2 / C9H2F14SO7	519.9326	518.9249	1.6E+07
C12H16F8S2O7	488.0217	487.0144	1.6E+07
C9H3F17O8S	593.9277	592.9226	1.6E+07
C8H3F15SO3	463.9536	462.9463	1.6E+07
C9HF19O2S	533.9375	532.9302	1.5E+07
C10H15F5O5S2	374.0288	373.0214	1.5E+07
C8H2F14O3	411.9780	410.9707	1.5E+07
C9H4F14SO8	537.9428	536.9354	1.5E+07
C8H3F13O6S	473.9448	472.9374	1.5E+07
C6H2F12O2S	365.9582	364.9510	1.5E+07
C11H4F16O9 / C11H7F15SO8	583.9587	582.9514	1.4E+07
C8H3F9O5	349.9834	348.9761	1.4E+07
C7H7F5O9	330.0022	328.9948	1.4E+07
C6H3F11SO5	395.9497	394.9433	1.4E+07
C8H5F11SO5	421.9657	420.9584	1.4E+07
C8H7F7SO9	411.9713	410.9627	1.4E+07
C10H5F15O4	473.9950	472.9877	1.3E+07
C7H3F13SO4	429.9524	428.9451	1.3E+07
C8H3F13O4	409.9822	408.9749	1.3E+07
C8HF13O3	391.9715	390.9643	1.3E+07
C8H6F10O2	324.0181	323.0109	1.3E+07
C11H4F20SO3	595.9576	594.9504	1.3E+07
C6H6F6O2	224.0272	223.0199	1.3E+07
C6H4F10S2O8	457.9210	456.9130	1.2E+07
C7H3F13O9S2	541.9016	540.8965	1.2E+07
C9H4F14O2	409.9980	408.9908	1.2E+07
C3HF5O4	195.9794	194.9722	1.2E+07
C5H3F9S2O7	409.9187	408.9111	1.2E+07
C7H2F14SO4	447.9446	446.9376	1.1E+07

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TABLE 10
UNKNOWN PFAS IN SAMPLES FROM CHEMOURS PROCESS WASTEWATER SAMPLING LOCATIONS
Chemours Fayetteville Works, North Carolina

	Mass	Mass to Charge Ratio	Ion
Empirical Formula	(amu)	(m/z)	Abundance
C10H12F10O7S	466.0147	465.0075	1.1E+07
C11H5F19S2O7 / C11H2F20SO8	673.9165	672.9100	1.1E+07
C10H7F13O6	470.0032	468.9959	1.1E+07
C11HF17O5	535.9529	534.9457	1.1E+07
C7H3F11O5	375.9790	374.9717	1.1E+07
C7HF11O4 / C7H4F10SO3	357.9704	356.9633	1.0E+07
C10H3F17O4	509.9736	508.9664	1.0E+07
C9HF17SO8 / C9H4F16S2O7	591.9071	590.9063	1.0E+07
C5H6F6O4	244.0170	243.0097	1.0E+07
C5HF7O3	241.9803	240.9730	1.0E+07
C6H2F10O4	327.9800	326.9724	1.0E+07
C4H2F8SO7	345.9389	344.9316	1.0E+07
C10H4F16O3	475.9884	474.9818	1.0E+07
C11H8F12O13	575.9767	574.9694	1.0E+07
C11H2F18O7	587.9478	586.9405	1.0E+07
C9H4F14O3	425.9931	424.9858	9.7E+06
C10H4F18O5	545.9775	544.9703	9.6E+06
C8H7F9O2	306.0302	305.0229	9.5E+06
C10H3F17SO7 / C10H6F16S2O6	589.9338	588.9264	9.5E+06
C9H2F12O3S	417.9532	416.9444	9.5E+06
C4H2F6O3	211.9908	210.9835	9.5E+06
C10H3F17O6 / C10H6F16SO5	541.9658	540.9584	9.4E+06
C8H10F6O10S / C9H11F7S2O6	411.9895	410.9821	9.2E+06
C7H2F14O9S	527.9202	526.9130	9.1E+06
C8H6F10O3	340.0156	339.0083	9.0E+06
C8H3F15SO6	511.9390	510.9317	9.0E+06
C4H2F6O4S	259.9577	258.9504	8.9E+06
C11H2F18O4 / C11H5F17SO3	539.9656	538.9584	8.8E+06
C11H4F18O2	509.9890	508.9819	8.7E+06
C6H6F4S2O8	345.9486	344.9374	8.7E+06
C5H2F8O4S	309.9543	308.9470	8.6E+06
C7H8F8S2O10	467.9446	466.9372	8.4E+06
C5H2F10O5S	364.9487	363.9415	8.4E+06
C10H4F16O6S2	587.9196	586.9121	8.3E+06
C9H4F14O4	441.9885	440.9813	8.1E+06
C5H2F6O4	239.9858	238.9786	8.0E+06
C8HF13O5	423.9615	422.9557	8.0E+06
C9H2F14SO7	519.9256	518.9207	7.9E+06
C9H6F12O5 / C9H9F11SO4	422.0026	420.9953	7.9E+06
C9HF13O4	419.9643	418.9575	7.9E+06
C8H3F15O2S	447.9616	446.9542	7.9E+06

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TABLE 10
UNKNOWN PFAS IN SAMPLES FROM CHEMOURS PROCESS WASTEWATER SAMPLING LOCATIONS
Chemours Fayetteville Works, North Carolina

	Mass	Mass to Charge Ratio	Ion
Empirical Formula	(amu)	(m/z)	Abundance
C10H4F14O5	469.9832	468.9759	7.7E+06
C15H12F14O6 / C15H15F13SO5	554.0429	553.0355	7.7E+06 7.7E+06
C13H12F14O6 / C13H13F13SO3 C11H5F15O6 / C11H8F14SO5	517.9846	516.9773	7.7E+06 7.7E+06
C6H4F8O3	276.0035	274.9962	7.7E+06 7.7E+06
	447.9334		
C8H5F9S2O7		446.9261	7.6E+06
C7H3F1106S	423.9475	422.9404	7.6E+06
C6H9F5O9S2	383.9622	382.9547	7.6E+06
C10H4F16O5	507.9775	506.9715	7.5E+06
C10HF15O3	453.9658	452.9586	7.4E+06
C7H5F9O4	324.0045	322.9974	7.4E+06
C7H4F8O5	319.9918	318.9842	7.3E+06
C8H2F16SO3	481.9448	480.9377	7.3E+06
C4H2F6O3	211.9904	210.9831	7.0E+06
C7H3F11O4	359.9855	358.9782	7.0E+06
C10H14F8S2O9	493.9944	492.9871	6.9E+06
C7H6F6SO6	331.9799	330.9726	6.9E+06
C8H8F6SO9	393.9801	392.9728	6.9E+06
C9H2F16O3S	493.9449	492.9379	6.9E+06
C7H6F10S2O8	471.9310	470.9258	6.8E+06
C8H3F11SO6	435.9475	434.9402	6.8E+06
C10HF15O5S2	549.9015	548.8933	6.7E+06
C10H4F14O3	437.9949	436.9877	6.7E+06
C6H7F7S2O10	435.9351	434.9279	6.6E+06
C6H8F4O3	204.0399	203.0326	6.5E+06
C13H6F18O6	599.9839	598.9767	6.5E+06
C4H2F6O7S	307.9416	306.9345	6.4E+06
C8H3F13O3	393.9873	392.9797	6.4E+06
C10HF19SO4	577.9266	576.9196	6.4E+06
C5H6F6S2O9	387.9353	386.9280	6.4E+06
C8H3F15SO5	495.9439	494.9366	6.3E+06
C9H3F17SO3	513.9512	512.9445	6.3E+06
C7H2F10O4	339.9790	338.9717	6.2E+06
C4HF7SO3	261.9535	260.9463	6.2E+06
C6H2F8O2	257.9928	256.9855	6.2E+06
C7H2F8O6S	365.9449	181.9651	6.2E+06
C7H3F11O3	343.9903	342.9830	6.1E+06
C11H5F15O9	565.9679	564.9605	6.1E+06
C8H6F12SO8	489.9608	488.9536	6.1E+06
C7H3F11S2O7	471.9127	470.9054	6.0E+06
C10H8F12O2	388.0339	387.0265	6.0E+06
C9H12F6O10S / C10H13F7S2O6	426.0045	424.9977	5.9E+06

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TABLE 10
UNKNOWN PFAS IN SAMPLES FROM CHEMOURS PROCESS WASTEWATER SAMPLING LOCATIONS
Chemours Fayetteville Works, North Carolina

	Mass	Mass to Charge Ratio	Ion
Empirical Formula	(amu)	(m/z)	Abundance
C13H6F18O4	567.9969	566.9899	5.9E+06
C9H7F13SO7 / C9H4F14O8	505.9701	504.9629	5.5E+06
C18H9F27S2O7	913.9324	912.9235	5.5E+06
C5H2F10SO2	315.9622	314.9550	5.3E+06

Notes:

amu - atomic mass units

C - carbon

F - fluorine

H - hydrogen

HFPO-TA - hexafluoropropylene oxide trimer acid

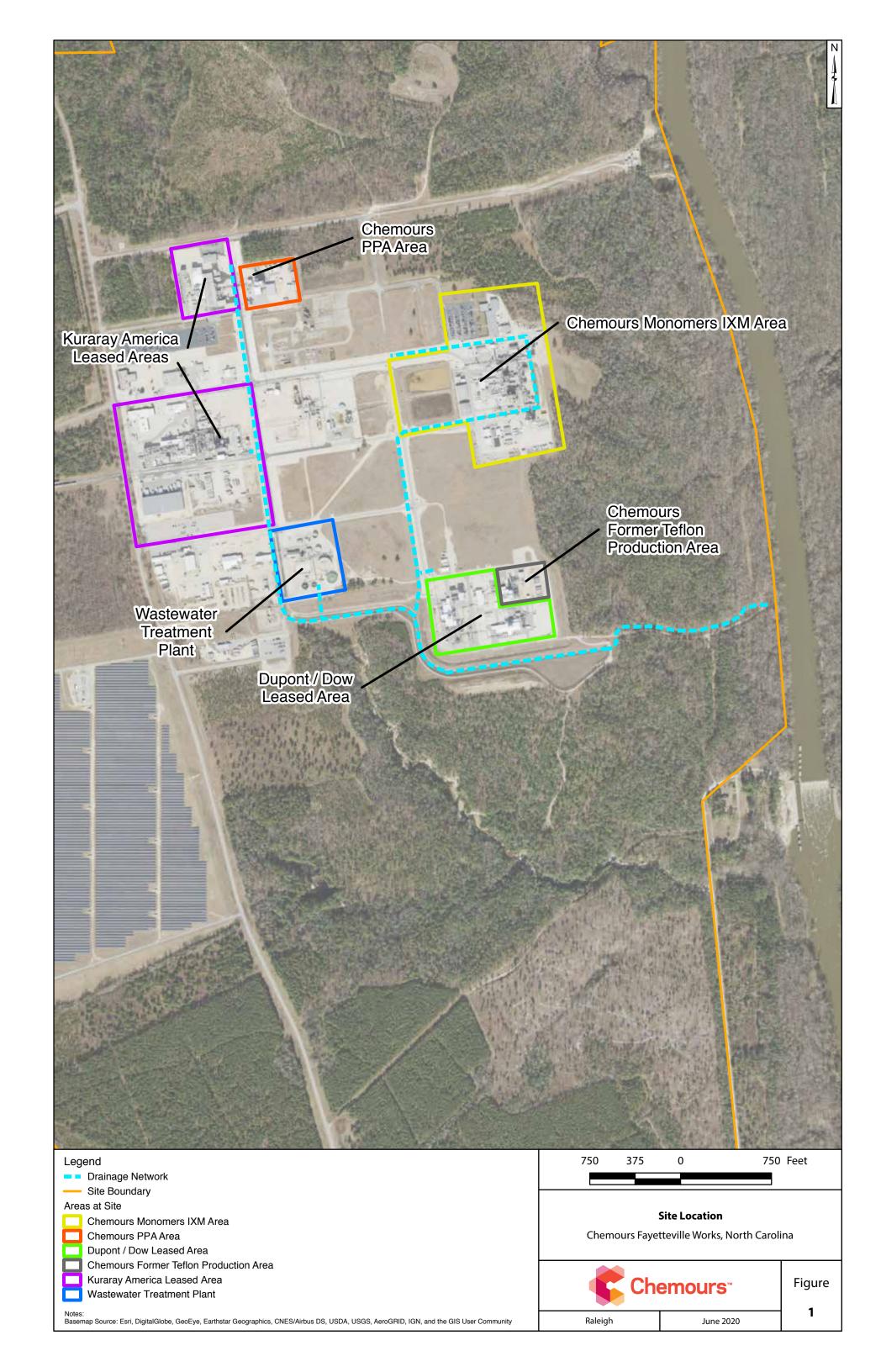
O - oxygen

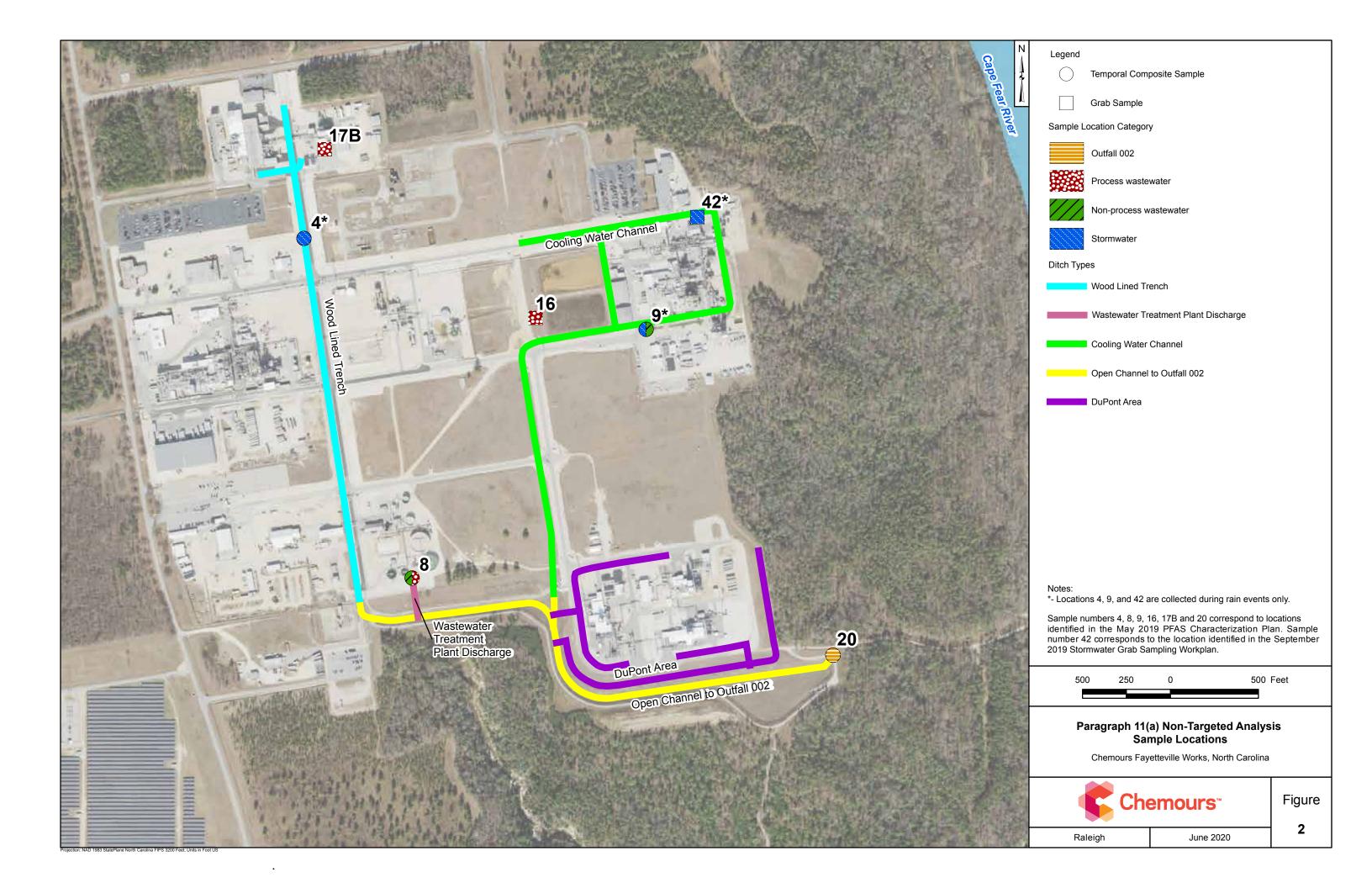
PFAS - per- and polyfluoroalkyl substances

S - sulfur

TFA - trifluoroacetic acid

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Desired Milesters (Delices ble				2019									20	20									2021			
Project Milestone/Deliverable	06	07	08	09	10	11	12	01	02	03	04	05	06	07	08	09	10	11	12	01	02	03	04	05	06	07
Sampling Event	•		•		•		\boxtimes	¥			¥															
Sample Preparation	0	0	0	0	0	0	0	0	0	0	0															
Instrumental Analysis																										
Initial Data Assessment				•	•	♦	♦	•	•	•	•	•	•	•	•											
Enhanced Assessment					‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	‡	
Test Method Development								•																		
Report Submission													×						×							××

•	Completed collection at sample locations 8, 16, 17B and 20.
X	Completed collection at sample locations 4, 9, 16, and 42.
A	Completed collection at sample location 16.
0	Sample preparation by filtration and direct injection.
	Instrumental analysis of samples by liquid chromatography coupled to Q-TOF-MS.
♦	Initial assessment to determine the empirical formulas and tentative structural information for unknown analytes.
‡	Enhanced assessment to confirm structural identity of select analytes following preparation of authentic standards.
	Test method development for additional PFAS identified by non-targeted analyses.
×	Interim report submission.
××	Final report submission.

Abbreviations

PFAS - per- and polyfluoroalkyl substances Q-TOF-MS - quadrupole time of flight mass spectrometry

Revised Non-Targeted Analysis Schedule Chemours Fayetteville Works

North Carolina



Figure 3