Most frequently detected PFAS in North Carolina~							
			Physical Characteristics				
PFAS Type	PFAS Group	PFAS Compound	Fluorinated Carbons	Total Chain Length	Molecular Formula	Molecular Weight (g/mol)	Water Solublity [38] (20-25C (g/L))
Legacy Compounds	Sulfonic Acids	PFBS	4	5	$C_4HF_9O_3S$	300.1	56.6
		PFHxS	6	7	$C_6HF_{13}O_3S$	400.12	2.3
		PFOS	8	9	$C_8HF_{17}O_3S$	500.13	1.57
	Carboxylic Acids	PFBA	3	4	$C_7H_5FO_2$	140.11	0.4
		PFPeA	4	5	C_5HF_9O	264.05	112.6
		PFHxA	5	6	C_6HF_{11}	314.05	21.7
		PFOA	8	8	$C_8HF_{15}O_2$	414.07	9.5
		PFNA	8	9	$C_9HF_{17}O_2$	464.08	9.5
		PFDA	9	10	$C_{10}HF_{19}O_2$	514.08	5.1
Consent Order Compounds		PFHpA	6	7	$C_7HF_{13}O_2$	364.06	4.2
		PFMOPrA#	3	5	$C_4HF_7O_3$	230.04	
		PFMOBA#	4	6	$C_5HF_9O_3$	280.04	
	Ether Carboxylic Acids	PFMOAA	2	4	$C_3HF_5O_3$	180.03	
		PMPA#	3	5	$C_4HF_7O_3$	230.04	13.4 [39]
		PFO2HxA	3	6	$C_4HF_7O_4$	246.04	
		PEPA#	4	6	$C_5HF_9O_3$	280.04	
		PFO3OA	4	8	$C_5HF_9O_5$	312.04	
		HFPO-DA (GenX)	5	7	$C_6HF_{11}O_3$	330.05	300 [37]
		PFO4DA	5	10	$C_6HF_{11}O_6$	378.05	
		PFO5DA	6	12	$C_7HF_{13}O_7$	444.06	
		HydroEVE	6	10	$C_8H_2F_{14}O_4$	428.08	
	Ether Sulfonic Acids	Nafion By-prod1	7	10	$C_7HF_{13}O_5S$	444.12	
		Nafion by-prod2	7	10	$C_7H_2F_{14}O_5S$	464.13	

 # isomer pairs

~ based on SSAB presentations Dec 2020

Most frequently detected PFAS in North Carolina~

PFAS Type	PFAS Group	PFAS Compound	Toxicity Data: Nuclear Receptor Activity (mean fold inducton realtive to control)[9]				
			PPARα[9]	PPARγ[9]	RXRβ[9]	ERα[9]	Other Active Sites[10]
Legacy Compounds	Sulfonic Acids	PFBS	1 - 5``	1.5 - 11	1 - 1.5	0.5 - 5	CYP3A4, CYP2D6, CNG, ALDH1A1, NPSR, HTTQ103, VP16,RORγ, G9a, JMJD2A, Nrf2, ELG1, Smad3, Gsgap, DNA re-replication, GLP-1, ATXN, HT-1080-NT, DT40-hTDP1, Plk PBD
		PFHxS					
		PFOS					
	Carboxylic Acids	PFBA	1 - 12``` PFOA =15	1 - 21 PFOA = 22	1 - 18 PFOA = 13	1 - 9 PFOA = 7	
		PFPeA					
		PFHxA					
		PFOA					
		PFNA					
		PFDA					
Consent Order Compounds		PFHpA					
		PFMOPrA#					
		PFMOBA#					
	Ether Carboxylic Acids	PFMOAA	3 - 7`````	5.5 - 9	1.5 - 11	1 - 2	CYP2D6, HTTQ103, G9a, JMJD2A, ATXN, HT-1080-NT, DT40-hTDP1
		PMPA#					
		PFO2HxA					
		PEPA#					
		PFO3OA					
		HFPO-DA (GenX)					
		PFO4DA					
		PFO5DA					
		HydroEVE					
	Ether Sulfonic Acids	Nafion By-prod1					
		Nafion by-prod2					

 # isomer pairs

~ based on SSAB pı

`` COMBINED scores of toxprint groups 1 & 2

``toxprint grpoup 7 scores; PFOA singulart score from group 9

````` based on GenX and Pfmopra isomer- group 5

Most frequently detected PFAS in North Carolina~					
PFAS Type	PFAS Group	PFAS Compound	Toxicity Data		
			Non- Mammalian	Mammalian	Relative Potency in Rat (as compared to PFOA)
Legacy Compounds	Sulfonic Acids	PFBS	Zebrafish, Medaka, Trout[11-13]	Rat[26]	0.001 [36]
		PFHxS	Zebrafish[14,15]	Mouse[21]	0.6 [36]
		PFOS	Zebrafish, Daphnia, Mysid Shrimp, Trout[14-16]	Rat[26,27]	2 [36]
	Carboxylic Acids	PFBA	Daphnia, Zebrafish, Trout[17-19]	Rat[26]	0.05 [36]
		PFPeA	Daphnia, Trout[17-18]	Rat, Mouse[26,28]	0.01<RPF<0.05[36]
		PFHxA	Zebrafish, Daphnia, Trout[15,17-19]	Rat, Mouse[26,28]	0.01 [36]
		PFOA	Zebrafish, Minnow, Daphnia[14-18]	Rat, Mouse[26,28,29]	***1*** [36]
		PFNA	Daphnia [20,21]	Mouse[34]	10 [36]
		PFDA	Daphnia, Trout[21]	Rat[26]	0.01<RPF<10[36]
Consent Order Compounds		PFHpA	Zebrafish, Daphnia[14,21]	Mouse[28]	0.01<RPF<1[36]
		PFMOPrA#		Mouse[30]	
		PFMOBA#	Zebrafish[22]	Mouse[30]	
	Ether Carboxylic Acids	PFMOAA	Zebrafish[22]	Mouse[30,31]	~1[22,35]
		PMPA#	Zebrafish[22]		~1[22,35]
		PFO2HxA	Zebrafish[22]		~1[22,35]
		PEPA#	Zebrafish[22]		~1[22,35]
		PFO3OA	Zebrafish[22,23]		~1[22,35]
		HFPO-DA (GenX)	Zebrafish[22,24,25]*	Rat, Mouse[26,29,32]	~1[22,35]
		PFO4DA	Zebrafish[22,23]	*[24,25]	~1[22,35]
		PFO5DA	Zebrafish[22,24,25]*	*[24,25]	~1[22,35]
		HydroEVE	Zebrafish[22,24,25]*	*[24,25]	~1[22,35]
	Ether Sulfonic Acids	Nafion By-prod1			
		Nafion by-prod2	*[24,25]	Mouse[33]	

 # isomer pairs

~ based on SSAB presentations Dec 2020

Most frequently detected PFAS in North Carolina~

PFAS Type	PFAS Group	PFAS Compound	Environmental Data: DAQ Total Atmospheric Deposition 2018-2021	
			Chemours Area (n = 42)	Regional Sites (n = 19)
Legacy Compounds	Sulfonic Acids	PFBS		
		PFHxS	5.9	
		PFOS	4.2 - 9.7	4.1 - 37
	Carboxylic Acids	PFBA	2.0 - 40	4.0 - 8.0
		PFPeA	4.3 - 14	
		PFHxA		
		PFOA	5.4 - 120	5.2 - 7.9
		PFNA		
		PFDA		
Consent Order Compounds		PFHpA	4.6	
		PFMOPrA#		
		PFMOBA#		
	Ether Carboxylic Acids	PFMOAA		
		PMPA#		
		PFO2HxA		
		PEPA#		
		PFO3OA		
		HFPO-DA (GenX)		
		PFO4DA		
		PFO5DA		
		HydroEVE		
	Ether Sulfonic Acids	Nafion By-prod1		
		Nafion by-prod2		

 # isomer pairs

~ based on SSAB presentations Dec 2020

Most frequently detected PFAS in North Carolina~						
PFAS Type	PFAS Group	PFAS Compound	Environmental Data Concentration in water (median (range)) ng/L ppt Surface water			
			DWR Chemours Outfall 002 (n = 213+)	Cape Fear, Lock & Dam [1] (mean)	Chemours area (mean)[2] (n=100)	DWR Lake data (n = 140)
Legacy Compounds	Sulfonic Acids	PFBS	36 (2 - 82)	<10	1.3	40 (37 - -42)
		PFHxS	37 (2 - 82)	27	0.7	40 (20 - 70)
		PFOS	37 (2 - 82)	29	2.1	40 (17 - 590)
	Carboxylic Acids	PFBA	40 (3 - 160)	31	8.6	40 (17 - 160)
		PFPeA	35 (5 - 310)	35	6.3	40 (17 - 260)
		PFHxA	40 (3 - 98)	33	2	40 (31-350)
		PFOA	40 (4 - 130)	21	1	40 (26 - 90)
		PFNA	40 (1 - 82)	<10	0.4	40 (16 - 160)
		PFDA	40 (1 - 200)		3.7	40 (20 - 160)
Consent Order Compounds		PFHpA	37 (2 - 82)	25	1.3	40 (13 - 280)
		PFMOPrA#		@		
		PFMOBA#		@		
	Ether Carboxylic Acids	PFMOAA		95000	76	
		PMPA#		740	696.6	
		PFO2HxA		8200	296.6	
		PEPA#		280		
		PFO3OA		7000	37.2	
		HFPO-DA (GenX)	110 (21 - 39000)+	790	475.2	40 (16 - 42)
		PFO4DA		330	5.9	
		PFO5DA		153	0.2	
		HydroEVE		<10		
	Ether Sulfonic Acids	Nafion By-prod1				
		Nafion by-prod2		<10	18.8	

 # isomer pairs *+ n=234* *@ isomers combined in this dataset*

~ based on SSAB presentations Dec 2020

Most frequently detected PFAS in North Carolina~				
PFAS Type	PFAS Group	PFAS Compound	Environmental Data Concentration in water ng/L ppt Drinking Water Wells/ Groundwater	
			DEQ Chemours area (n=3406)	% Detection (n)
Legacy Compounds	Sulfonic Acids	PFBS	2.9 (0.9 - 21)	1.8% (63)
		PFHxS	3.5 (1.9 - 11)	1% (37)
		PFOS	6.9 (2.2 - 39)	1.4% (49)
	Carboxylic Acids	PFBA	7.5 (2.2 - 300)	3.2% (109)
		PFPeA	6.8 (2 - 53)	3.2% (109)
		PFHxA	3.4 (1.9 - 29)	2.5% (85)
		PFOA	4.5 (1.1 -61)	2.6% (89)
		PFNA	3.5 (2.3 - 7.5)	0.2% (8)
		PFDA	3.2 (3 - 7.5)	0.1% (3)
Consent Order Compounds		PFHpA	3 (0.9 - 43)	22% (740)
		PFMOPrA#	@	@
		PFMOBA#	@	@
	Ether Carboxylic Acids	PFMOAA	13 (2 - 3500)	66% (2241)
		PMPA#	63 (2 - 8800)	92% (3117)
		PFO2HxA	13 (1.5 - 2800)	73% (2495)
		PEPA#	33 (2 - 2100)	23% (792)
		PFO3OA	4.6 (1.3 - 490)	21% (704)
		HFPO-DA (GenX)	15 (2 - 3200)	69% (2355)
		PFO4DA	3.5 (1.1 - 230)	6% (216)
		PFO5DA	5.1 (2.1 - 460)	1% (34)
		HydroEVE		
	Ether Sulfonic Acids	Nafion By-prod1	4.6 (1.5 - 20)	0.4% (14)
		Nafion by-prod2	5.5 (1.1 - 110)	51% (1748)

 # isomer pairs *@ isomers combined in this dataset*

~ based on SSAB presentations Dec 2020

Most frequently detected PFAS in North Carolina~						
PFAS Type	PFAS Group	PFAS Compound	Biological Data Blood Serum Data NC Striped Bass Serum[4] [mean (range)] ng/L ppt			
			Pamlico Field Lab (n = 29)	% Detection (n)	Cape Fear River (n= 58)	% Detection (n)
Legacy Compounds	Sulfonic Acids	PFBS	10 (10 - 200)	45% (13)	150 (10 - 1350)	24% (14)
		PFHxS	590	3.4% (1)	800 (200 - 1000)	98.3% (57)
		PFOS	9410 (4620 - 16500)	100% (29)	490000 (122000 - 977000)	100% (58)
	Carboxylic Acids	PFBA	<108 (LOD)	0% (0)	100 (100 - 200)	14% (8)
		PFPeA				
		PFHxA				
		PFOA	160 (160 - 1140)	14% (4)	570 (160 - 4290)	15% (9)
		PFNA	480 (340 - 820)	96% (28)	4500 (800 - 11600)	100% (58)
		PFDA	2500 (1680 - 4600)	96% (28)	68000 (10200 - 146000)	100% (58)
Consent Order Compounds		PFHpA				
		PFMOPrA#				
		PFMOBA#				
	Ether Carboxylic Acids	PFMOAA				
		PMPA#	120 (120 -140)	10% (3)	120 (120 - 190)	14% (8)
		PFO2HxA				
		PEPA#				
		PFO3OA				
		HFPO-DA (GenX)	1640 (240 - 2300)	10.3% (3)	1910 (310 - 5850)	48% (28)
		PFO4DA				
		PFO5DA	<5 (LOD)	0% (0)	490 (10 - 1350)	22% (13)
		HydroEVE				
	Ether Sulfonic Acids	Nafion By-prod1				
		Nafion by-prod2	<248 (LOD)	0% (0)	300 (250-1030)	77.6% (45)

 # isomer pairs

~ based on SSAB presentations Dec 2020

Most frequently detected PFAS in North Carolina~						
PFAS Type	PFAS Group	PFAS Compound	Biological Data			
			Blood Serum Data [median (range)] ng/L ppt			
			Wilmington NC[5]			
			Adults (n=289)	% Detection (n)	Children (n=55)	% Detection (n)
Legacy Compounds	Sulfonic Acids	PFBS				
		PFHxS	3500 (1200 - 8600)	98% (282)	1900 (1.2-4.7)	98% (54)
		PFOS	9400 (3800-28200)	99% (287)	5100 (2800-11500)	100% (55)
	Carboxylic Acids	PFBA				
		PFPeA				
		PFHxA				
		PFOA	4800 (1700 - 11300)	99.7% (288)	3000 (1900 - 6500)	100% (*55)
		PFNA	1300 (600 - 3600)	97% (280)	800 (400 - 1500)	82% (45)
		PFDA				
Consent Order Compounds		PFHpA	200 (100 - 1400)	59% (170)	400 (200 - 1000)	98% (54)
		PFMOPrA#				
		PFMOBA#				
	Ether Carboxylic Acids	PFMOAA				
		PMPA#				
		PFO2HxA				
		PEPA#				
		PFO3OA				
		HFPO-DA (GenX)	<2000 (LOD)	0%	<2000 (LOD)	0%
		PFO4DA	2300 (400 - 13700)	98% (284)	2600 (700 - 8900)	100% (55)
		PFO5DA	300 (100 - 1000)	89% (256)	200 (100 - 400)	84% (46)
		HydroEVE				
	Ether Sulfonic Acids	Nafion By-prod1				
		Nafion by-prod2	3200 (1000 - 8500)	99% (286)	1600 (600 - 3800)	100% (55)

 # isomer pairs

~ based on SSAB presentations Dec 2020

Most frequently detected PFAS in North Carolina~

PFAS Type	PFAS Group	PFAS Compound	Biological Data		
			Blood Serum Data [median (range)] ng/L ppt		
			Pittsboro NC[6]	Fayetville Works adjacent, NC[7]	NHANES Data US Population[8] [geo mean (95%CI)] (n=1929)
			Adults (n=49)	Aduts (n=30)	
Legacy Compounds	Sulfonic Acids	PFBS			
		PFHxS	3000 (20 - 12500)	2100 (700 - 6700)	1080 (990 - 1180)
		PFOS	11600 (3200 - 31800)	5500 (1400 - 34600)	4250 (3900 - 4620)
	Carboxylic Acids	PFBA			
		PFPeA			
		PFHxA	1500 (300 - 4000)		<100 (LOD)
		PFOA	6400 (2100 - 42400)	1800 (400 - 7300)	1420 (1330 - 1520)
		PFNA	1500 (300 - 9500)	600 (<100 - 2100)	411 (360 - 460)
		PFDA	600 (400 - 2400)	200 (<100 - 1300)	200 (180 - 210)
Consent Order Compounds		PFHpA		100 (<100 - 600)	
		PFMOPrA#			
		PFMOBA#			
	Ether Carboxylic Acids	PFMOAA			
		PMPA#			
		PFO2HxA			
		PEPA#			
		PFO3OA			
		HFPO-DA (GenX)	<100 (LOD)	<100 (LOD)	<100 (LOD)
		PFO4DA			
		PFO5DA			
		HydroEVE			
	Ether Sulfonic Acids	Nafion By-prod1			
		Nafion by-prod2			

 # isomer pairs

~ based on SSAB presentations Dec 2020

Most frequently detected PFAS in North Carolina~			
PFAS Type	PFAS Group	PFAS Compound	States with Regulation or Guidance
Legacy Compounds	Sulfonic Acids	PFBS	MI, MN
		PFHxS	VT, RI, MA, NH, MN,CT, AK, CO, DE, ME, MI, NM [3]
		PFOS	MN, NH, RI, CA, NJ, NY[3]
	Carboxylic Acids	PFBA	MN
		PFPeA	None
		PFHxA	MI
		PFOA	CA, RI, MA, NH, NY, CT, ME, AK, CO, DE, NM [3]
		PFNA	MA, CT, NJ, NH, RI,
		PFDA	MA
Consent Order Compounds		PFHpA	VT, CT , MA, RI
		PFMOPrA#	None
		PFMOBA#	None
	Ether Carboxylic Acids	PFMOAA	None
		PMPA#	None
		PFO2HxA	None
		PEPA#	None
		PFO3OA	None
		HFPO-DA (GenX)	NC, MI, OH
		PFO4DA	None
		PFO5DA	None
		HydroEVE	None
	Ether Sulfonic Acids	Nafion By-prod1	None
		Nafion by-prod2	None

 # isomer pairs

~ based on SSAB presentations Dec 2020

abridged from Cheng & Ng 2019

Target Class	Target	Description
G protein-coupled receptors (GPCRs)	NPSR	The neuropeptide S receptor (NPSR), which is highly expressed in brain areas involving modulation of arousal, stress and anxiety, could be a novel drug target for sleep and anxiety disorders. This assay is conducted to identify NPSR antagonists. the treatment of
	GLP-1	The overall aim of this assay is to discover ligands for class B1 GPCRs. Specifically, this assay focused on class B1 receptor for glucagon-like peptide-1 (GLP-1), which is a potential therapeutic target for diabetes and neurodegenerative disease.
ion channel	CNG	The cyclic nucleotide gated (CNG) ion channel was used as a biosensor for cAMP induction in this assay. The rationale is that cAMP stimulation will cause the CNG ion channel to open and subsequent membrane depolarization to occur.
miscellaneous	DNA re-replication	This assay is used to screen small molecules that induce DNA re-replication, which can cause the DNA damage response, arrest cell proliferation, and trigger apoptosis.
other enzymes	CYP2C9 , CYP3A4, CYP2D6	Cytochromes P450 (CYP) are a group of heme-thiolate monooxygenases that oxidize a variety of substances including steroids, fatty acids, and xenobiotics. In these assays, three different CYPs (CYP2C99, CYP3A410, and CYP2D611) were used to screen inhibitors and substrates for those CYP enzymes.
	ALDH1A1	Aldehyde dehydrogenase 1 (ALDH1A1) is an enzyme that oxidizes a variety of endogenous and exogenous aldehydes to the corresponding carboxylic acids and is the critical step for retinoic acid metabolism. In this assay, inhibitors of ALDH1A1 were identified.
	G9a	G9a is a histone methyltransferase that is responsible for histone H3 lysine 9 (H3K9) mono- and di-methylation. It has been recognized as a potential drug target for several human diseases, including cancer. The goal of this assay is to identify inhibitors of G9a.
promoter	ELG1	As the major subunit of a Replication Factor C-like complex, ELG1 is critical to ensure genomic stability during DNA replication14. This assay identifies small molecules that block ELG1 function.
	ATXN	Ataxin-2 protein (ATXN2) is encoded by the ATXN2 gene. The mutation in ATXN2 could cause Spinocerebellar ataxia type 2 (SCA2) disease. The objective of this assay is toidentify compounds that inhibit the expression of ATXN2.
protein kinase	Plk1 PBD	Polo-like kinase 1 (Plk1) is a member of a conserved subfamily of serine / threonine protein kinases and plays a central role in cell proliferation. Plk1 is a potential target for anti-cancer therapy. This assay aimed to identify inhibitors that target the Plk1 polo-box domain (PBD).
protein-protein interaction	K18	In this assay, a recombinantly expressed fragment of tau, K18 was used to identify inhibitors of tau (which is an abundant protein in the axons of neurons that stabilizesmicrotubules) aggregation.
	HTTQ103	When exon 1 of HTTQ103 (Huntingtin protein containing 103 polyglutamines expansion) is expressed, it causes cell death and GFP aggregates. This assay screens for small molecules that reduce aggregate formation.
	JMJD2A	JMJD2A is a jumonji-domain-containing lysine demethylase. In this assay, the inhibitors of JMJD2A-tudor domain interactions (which is helpful in probing the regulatory pathways of selective demethylation of a given methyllysine locus) were identified20. signaling pathway Gsgsp The objective of this assay is to identify molecules with inhibitory activity at gsp mutations, which are responsible for McCune-Albright syndrome.
transcription factor	RORγ	The goal of this assay is to identify small molecules that inhibit ROR (retinoic acid-related orphan receptor) gamma activity.
	VP16	The goal of this assay is to identify small molecules that inhibit components common to both ROR gamma and VP16 transcription factor.
	Nrf2	Nrf2 is a transcription factor that maintains cellular redox homeostasis and protects cells from xenobiotics. This assay is used to screen inhibitors of Nrf2 function, which could be potential therapeutic targets for improvement in cancer treatment.
	Smad3	TGF-b signaling pathway plays important roles in cellular and development pathways. Smad3 is the primary transducer of TGF-b's signals and regulates many functions related to TGF-b signaling. The goal of this assay is to identify Smad3-small molecule antagonists.
viability	HT-1080-NT	In this assay, a synthetic lethal screen was conducted for chemical probes specific for 2HG-producing tumor cells using HT-1080-NT fibrosarcoma cell line.
	DT40-hTDP1	Human tyrosyl-DNA phosphodiesterase 1 (HTDP1) is a novel repair gene and can be used as a new target for anti-cancer drug development. In this assay, after exposure to small molecules in the absence of camptothecin, the growth kinetics of DT40-hTDP1 cells were evaluated to determine whether the molecules can inhibit the TDP1-mediated repair pathway.
	DT40-hTDP1	In this assay, after exposure to small molecules in the presence of camptothecin, the growth kinetics of DT40-hTDP1 cells were evaluated to determine whether the molecules can inhibit the TDP1-mediated repair pathway.

code	ToxPrint Group Name	Casrn	Chemical name in Houck et al 2021	abbrv	Notes
1	Perfluoroalkane sulfonate	3871-99-6	Potassium perfluorohexanesulfonate	PfHxS	salt form
		29420-49-3	Potassium perfluorobutanesulfonate	PFBS	salt form
		2795-39-3	Potassium perfluorooctanesulfonate	PFOS	salt form
		2806-15-7	Sodium perfluorodecanesulfonate	PFDS	not in NC table; salt form
2	Perfluorakyl (linear) sulfonates	1763-23-1	Perfluorooctanesulfonic acid	PFOS	
		355-46-4	Perfluorohexanesulfonic acid	PFHxS	
		375-92-8	Perfluoroheptanesulfonic acid	PFHpS	not in NC table
		375-73-5	Perfluorobutanesulfonic acid	PFBS	
5	Perfluoroalkyl ether carboxylates	62037-80-3	Ammonium perfluoro-2-methyl-3-oxahexanoate	Gen X	salt form
		55621-21-1	Perfluoro-3,6-dioxaoctane-1,8-dioic acid	PFDoDa	
		377-73-1	Perfluoro-3-methoxypropanoic acid	PFMOPra	
		801212-59-9	Perfluoro-4-isopropoxybutanoic acid	PFPE-1	not in NC table
		13252-13-6	Perfluoro-2-methyl-3-oxahexanoic acid	GenX	
7	Perfluoroalkyl (linear) Carboxylic Acids	422-64-0	Perfluoropropanoic acid		
		2706-90-3	Perfluoropentanoic acid	PFPeA	
		335-67-1	Perfluorooctanoic acid	PFOA	
		375-95-1	Perfluorononanoic acid	PFNA	
		307-24-4	Perfluorohexanoic acid	PFHxA	
		375-22-4	Perfluorobutanoic acid	PFBA	
		335-76-2	Perfluorodecanoic acid	PFDA	
		375-85-9	Perfluoroheptanoic acid	PFHpA	
9	Perfluoroaklyl carboxylic acids (PFCAs) their salts and esters	865-79-2	Chloro-perfluorononanoic acid	PFOA	salt form

References

1 Zhang, C., Hopkins, Z. R., McCord, J., Strynar, M. J. & Knappe, D. R. Fate of per-and polyfluoroalkyl ether acids in the total oxidizable precursor assay and implications for the analysis of impacted water. *Environ. Sci. Technol. Lett.* **6**, 662–668 (2019).

2 Petre, M.-A. *et al.* Per- and Polyfluoroalkyl Substance (PFAS) Transport from Groundwater to Streams near a PFAS Manufacturing Facility in North Carolina, USA. *Environ. Sci. Technol.* **55**,

3 Kindschuh, J. & Lee, T. State-by-State Regulation of PFAS Substances in Drinking Water. *Bryan Cave Leighton Paisner* https://www.bclplaw.com/en-US/insights/state-by-state-regulation-of-pfas-

4 Guillette, T. C. *et al.* Elevated levels of per- and polyfluoroalkyl substances in Cape Fear River Striped Bass (Morone saxatilis) are associated with biomarkers of altered immune and liver function.

5 Kotlarz, N. *et al.* Measurement of novel, drinking water-associated PFAS in blood from adults and children in Wilmington, North Carolina. *Environ. Health Perspect.* **128**, 077005 (2020).

6 Stapleton, H. M. PFAS Exposure Study – Duke's Research in the NC Piedmont. https://sites.nicholas.duke.edu/pfas/.

7 Pritchett, J. R. *et al.* Notes from the Field: Targeted Biomonitoring for GenX and Other Per- and Polyfluoroalkyl Substances Following Detection of Drinking Water Contamination — North Carolina, 2018. *MMWR Morb. Mortal. Wkly. Rep.* **68**, 647–648 (2019).

8 Calafat, A. M., Wong, L.-Y., Kuklenyik, Z., Reidy, J. A. & Needham, L. L. Polyfluoroalkyl chemicals in the US population: data from the National Health and Nutrition Examination Survey (NHANES) 2003–2004 and comparisons with NHANES 1999–2000. *Environ. Health Perspect.* **115**, 1596–1602 (2007).

9 Houck, K. A. *et al.* Bioactivity Profiling of Per-and Polyfluoroalkyl Substances (PFAS) Identifies Potential Toxicity Pathways Related to Molecular Structure. *Toxicology* 152789 (2021).

10 Cheng, W. & Ng, C. A. Using machine learning to classify bioactivity for 3486 per-and polyfluoroalkyl substances (PFASs) from the OECD list. *Environ. Sci. Technol.* **53**, 13970–13980 (2019).

11 Foguth, R., Sepúlveda, M. S. & Cannon, J. Per-and Polyfluoroalkyl Substances (PFAS) Neurotoxicity in Sentinel and Non-Traditional Laboratory Model Systems: Potential Utility in Predicting Adverse

12 Chen, L. *et al.* Accumulation of perfluorobutane sulfonate (PFBS) and impairment of visual function in the eyes of marine medaka after a life-cycle exposure. *Aquat. Toxicol.* **201**, 1–10 (2018).

13 Ulhaq, M., Örn, S., Carlsson, G., Morrison, D. A. & Norrgren, L. Locomotor behavior in zebrafish (Danio rerio) larvae exposed to perfluoroalkyl acids. *Aquat. Toxicol.* **144**, 332–340 (2013).

14 Menger, F., Pohl, J., Ahrens, L., Carlsson, G. & Örn, S. Behavioural effects and bioconcentration of per-and polyfluoroalkyl substances (PFASs) in zebrafish (Danio rerio) embryos. *Chemosphere* **245**,

15 Gaballah, S. *et al.* Evaluation of developmental toxicity, developmental neurotoxicity, and tissue dose in zebrafish exposed to GenX and other PFAS. *Environ. Health Perspect.* **128**, 047005 (2020).

16 Hekster, F. M., Laane, R. W. & De Voogt, P. Environmental and toxicity effects of perfluoroalkylated substances. *Rev. Environ. Contam. Toxicol.* 99–121 (2003).

17 Hoke, R. A., Bouchelle, L. D., Ferrell, B. D. & Buck, R. C. Comparative acute freshwater hazard assessment and preliminary PNEC development for eight fluorinated acids. *Chemosphere* **87**,

18 Valsecchi, S. *et al.* Deriving environmental quality standards for perfluorooctanoic acid (PFOA) and related short chain perfluorinated alkyl acids. *J. Hazard. Mater.* **323**, 84–98 (2017).

19 Mahapatra, C. T. *et al.* Comparative in vitro toxicity assessment of perfluorinated carboxylic acids. *J. Appl. Toxicol.* **37**, 699–708 (2017).

20 Lu, G.-H., Liu, J.-C., Sun, L.-S. & Yuan, L.-J. Toxicity of perfluorononanoic acid and perfluorooctane sulfonate to Daphnia magna. *Water Sci. Eng.* **8**, 40–48 (2015).

21 Viberg, H., Lee, I. & Eriksson, P. Adult dose-dependent behavioral and cognitive disturbances after a single neonatal PFHxS dose. *Toxicology* **304**, 185–191 (2013).

22 Gebreab, K. Y. *et al.* Comparative toxicometabolomics of perfluorooctanoic acid (PFOA) and next-generation perfluoroalkyl substances. *Environ. Pollut.* **265**, 114928 (2020).

23 Wang, J. *et al.* Perfluoropolyether carboxylic acids (novel alternatives to PFOA) impair zebrafish posterior swim bladder development via thyroid hormone disruption. *Environ. Int.* **134**, 105317

24 Pelch, K. E., Reade, A., Wolffe, T. A. & Kwiatkowski, C. F. PFAS health effects database: Protocol for a systematic evidence map. *Environ. Int.* **130**, 104851 (2019).

25 Vendl, C. *et al.* Profiling Research on PFAS in Wildlife: Protocol of a Systematic Evidence Map and Bibliometric Analysis. (2021).

26 Bil, W. *et al.* Risk assessment of per-and polyfluoroalkyl substance mixtures: a relative potency factor approach. *Environ. Toxicol. Chem.* **40**, 859–870 (2021).

27 Pedersen, K. E. *et al.* Brain region-specific perfluoroalkylated sulfonate (PFSA) and carboxylic acid (PFCA) accumulation and neurochemical biomarker responses in east Greenland polar bears

28 Han, J.-S. *et al.* Subacute dermal toxicity of perfluoroalkyl carboxylic acids: comparison with different carbon-chain lengths in human skin equivalents and systemic effects of perfluoroheptanoic acid in Sprague Dawley rats. *Arch. Toxicol.* **94**, 523–539 (2020).

29 Blake, B. E. *et al.* Evaluation of Maternal, Embryo, and Placental Effects in CD-1 Mice following Gestational Exposure to Perfluorooctanoic Acid (PFOA) or Hexafluoropropylene Oxide Dimer Acid (HFPO-DA or GenX). *Environ. Health Perspect.* **128**, 027006 (2020).

30 Woodlief, T., Vance, S., Hu, Q. & DeWitt, J. Immunotoxicity of Per-and Polyfluoroalkyl Substances: Insights into Short-Chain PFAS Exposure. *Toxics* **9**, 100 (2021).

31 Vance, S. 30-Day Immunotoxicity Study of PFMOAA in C57BL/6 Mice. (2019).

32 Conley, J. M. *et al.* Adverse maternal, fetal, and postnatal effects of hexafluoropropylene oxide dimer acid (GenX) from oral gestational exposure in Sprague-Dawley rats. *Environ. Health Perspect.*

33 Lang, J. R. *et al.* Toxicity of Balb-c mice exposed to recently identified 1, 1, 2, 2-tetrafluoro-2-[1, 1, 1, 2, 3, 3-hexafluoro-3-(1, 1, 2, 2-tetrafluoroethoxy) propan-2-yl] oxyethane-1-sulfonic acid

34 Wolf, C. J., Zehr, R. D., Schmid, J. E., Lau, C. & Abbott, B. D. Developmental Effects of Perfluorononanoic Acid in the Mouse Are Dependent on Peroxisome Proliferator-Activated Receptor-Alpha.

35 Gomis, M. I., Vestergren, R., Borg, D. & Cousins, I. T. Comparing the toxic potency in vivo of long-chain perfluoroalkyl acids and fluorinated alternatives. *Environ. Int.* **113**, 1–9 (2018).

36 Zeilmaker, M. J., Fragki, S., Verbruggen, E. M. J., Bokkers, B. G. H. & Lijzen, J. P. A. Mixture exposure to PFAS: A relative potency factor approach. (2018).

37 Augspurger, T. North Carolina Department of Environmental Quality and North Carolina Department of Health and Human Services Secretaries' Science Advisory Board Review of the North Carolina Drinking Water Provisional Health Goal for GenX. (2018).

38 SGS. *Physical and Chemical Properties of PFAS compounds*. https://www.sgs-ehsusa.com/wp-content/uploads/2018/09/Physical-and-Chemical-Properties-of-PFAS-compounds_vKFMH.pdf (2018).

39 NIH. *PubChem* . https://pubchem.ncbi.nlm.nih.gov/compound/464205#section=Solubility (2021).