United States
Environmental Protection
Agency

Information Compendium for Contaminants for the Final Unregulated Contaminant Monitoring Rule (UCMR 5)

Office of Water (4607M)
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Disclaimer

This document provides additional technical detail to support UCMR 5 but is not a regulation. It does not change or substitute for any legal requirements. In the event of a conflict between the content of this document and any statute or regulation, this document is not controlling.

Contents

Abbreviations and Acronyms

µg/L	Micrograms per Liter
11Cl-PF3OUdS	11-chloroeicosafluoro-3-oxaundecane-1-sulfonic Acid
4:2 FTS	1H,1H,2H,2H-perfluorohexane Sulfonic Acid
6:2 FTS	1H,1H,2H,2H-perfluorooctane Sulfonic Acid
8:2 FTS	1H,1H,2H,2H-perfluorodecane Sulfonic Acid
9Cl-PF3ONS	9-chlorohexadecafluoro-3-oxanone-1-sulfonic Acid
ADONA	4,8-dioxa-3H-perfluorononanoic Acid, parent acid of the ammonium salt
ASTM	ASTM International
ATSDR	Agency for Toxic Substances and Disease Registry
AWIA	America's Water Infrastructure Act of 2018
CASRN	Chemical Abstracts Service Registry Number
CCL	Contaminant Candidate List
CDR	Chemical Data Reporting
CWS	Community Water System
EPA	United States Environmental Protection Agency
FR	Federal Register
FY	Fiscal Year
HA	Health Advisory
HESD	Health Effects Support Document
HFPO-DA	Hexafluoropropylene Oxide Dimer Acid
HSDB	Hazardous Substances Data Bank
IARC	International Agency for Research on Cancer
ICP-AES	Inductively Coupled Plasma-Atomic Emission Spectrometry
IRIS	Integrated Risk Information System
ITRC	Interstate Technology Regulatory Council
IUR	Inventory Update Rule
L/kg	Liters per Kilogram
lbs/yr	Pounds per Year
K_H	Henry's Law Constant
K_{oc}	Organic Carbon Partitioning Coefficient
LC/MS/MS	Liquid Chromatography/Tandem Mass Spectrometry
log K_{ow}	Logarithm of the Octanol-Water Partitioning Coefficient
MAC	Maximum Acceptable Concentration
MCL	Maximum Contaminant Level
mg/kg	Milligrams per Kilogram
mg/kg-day	Milligrams per Kilogram per Day
mg/L	Milligram per Liter

mol/L	Moles per Liter
MRL	(1) EPA Minimum Reporting Level or (2) ATSDR Minimal Risk Level, as noted
NAWQA	National Water Quality Assessment
NDAA	National Defense Authorization Act for Fiscal Year 2020
NEtFOSAA	N-ethyl Perfluorooctanesulfonamidoacetic Acid
NFDHA	Nonafluoro-3,6-dioxaheptanoic Acid
NIRS	National Inorganics and Radionuclides Survey
NMeFOSAA	N-methyl Perfluorooctanesulfonamidoacetic Acid
NPDWR	National Primary Drinking Water Regulation
NPL	National Priorities List
OW	EPA Office of Water
ORD	EPA Office of Research and Development
PCCL	Preliminary Contaminant Candidate List
PFAS	Per- and Polyfluoroalkyl Substances
PFBA	Perfluorobutanoic Acid
PFBS	Perfluorobutanesulfonic Acid
PFDA	Perfluorodecanoic Acid
PFDoA	Perfluorododecanoic Acid
PFEESA	Perfluoro (2-ethoxyethane) Sulfonic Acid
PFHpA	Perfluoroheptanoic Acid
PFHpS	Perfluoroheptanesulfonic Acid
PFHxA	Perfluorohexanoic Acid
PFHxS	Perfluorohexanesulfonic Acid
PFMBA	Perfluoro-4-methoxybutanoic Acid
PFMPA	Perfluoro-3-methoxypropanoic Acid
PFNA	Perfluorononanoic Acid
PFOA	Perfluorooctanoic Acid
PFOS	Perfluorooctanesulfonic Acid
PFPeA	Perfluoropentanoic Acid
PFPeS	Perfluoropentanesulfonic Acid
PFTA	Perfluorotetradecanoic Acid
PFTrDA	Perfluorotridecanoic Acid
PFUnA	Perfluoroundecanoic Acid
PPRTV	Provisional Peer-Reviewed Toxicity Value
p-RFD	Provisional Reference Dose
PST	Pre-Screen Testing
PWS	Public Water System

RfD	Reference Dose
SDWA	Safe Drinking Water Act
SM	Standard Methods
SPE	Solid Phase Extraction
SWTR	Surface Water Treatment Rule
UCMR	Unregulated Contaminant Monitoring Rule
USEPA	United States Environmental Protection Agency
USGS	United States Geological Survey
WHO	World Health Organization

Introduction

As part of its responsibilities under the Safe Drinking Water Act (SDWA), the U.S. Environmental Protection Agency (EPA) implements Section 1445(a)(2), Monitoring Program for Unregulated Contaminants. This section, as amended in 1996, requires that once every five years, EPA identify unregulated contaminants in drinking water to be monitored by public water systems (PWSs). These contaminants may be present in drinking water but are not yet subject to EPA's drinking water standards set under SDWA. The Unregulated Contaminant Monitoring Rule (UCMR) generates nationally representative drinking water occurrence data to support EPA's regulatory determinations and, as appropriate, assists in the development of standards for drinking water contaminants that may be of public health concern. Each UCMR revision establishes a new list of contaminants for monitoring, provides information on which PWSs are required to monitor, identifies the sampling locations, and defines the analytical methods to be used. The "UCMR 5" final rule addresses the terms for the fifth cycle of monitoring under the program.

Section 2021 of America's Water Infrastructure Act of 2018 (AWIA) (Public Law 115-270) amended Section 1445 of SDWA by expanding the number of PWSs required to monitor, subject to the availability of appropriations for such purpose and sufficient laboratory capacity. SDWA now specifies that EPA must require PWSs serving 3,300 or more people, as well as a nationally representative sample of PWSs serving fewer than 3,300 people, to conduct monitoring. Section 7311 of the National Defense Authorization Act for Fiscal Year 2020 (NDAA) (Public Law 116-92) amended Section 1445 of SDWA and specifies that the Administrator shall include each PFAS in UCMR 5 for which a drinking water method has been validated by the Administrator and that are not subject to National Primary Drinking Water Regulations (NPDWRs).

In establishing the contaminant list for UCMR 5, EPA evaluated unregulated contaminants in accordance with SDWA as amended by AWIA and the NDAA, and in consideration of "EPA's Per- and Polyfluoroalkyl Substances (PFAS) Action Plan" (USEPA, 2019a). EPA considered the current (fourth) Contaminant Candidate List (CCL 4) (81 FR 81099, November 17, 2016; USEPA, 2016a), which includes 97 chemicals or chemical groups and 12 microbes. EPA evaluated contaminants nominated by the public for potential inclusion in CCL 5 (83 FR 50364, October 5, 2018; USEPA, 2018), as well as other priority contaminants.

EPA evaluated candidate UCMR 5 contaminants using a stepwise prioritization process (see Appendix A). The process started with a universe of 457 contaminants which included all the CCL 4 contaminants, plus the non-CCL contaminants that fell within the scope of analytical methods under consideration for the CCL 4 contaminants. Considering non-CCL contaminants for UCMR provides an opportunity to collect occurrence data at little-to-no additional expense (i.e., collection takes place concurrently with CCL contaminants) and reduces the likelihood of needing to include them (at a higher expense) in a future UCMR should they subsequently become higher priorities.

The first step included identifying contaminants that: (1) were not monitored under prior UCMR cycles (with the exception of six PFAS), (2) may occur in drinking water, and (3) are expected to have a completed, validated drinking water method in time for rule proposal. This step identified 208 contaminants.

The next step was to retain contaminants with one or more of the following: (1) an available health assessment to facilitate regulatory determinations[1], (2) high public interest (e.g., PFAS), (3) critical health endpoints (e.g., likely or suggestive carcinogen), and (4) active use (e.g., pesticides that are registered for application). This step identified 69 contaminants with 13 methods.

During the final step, EPA considered stakeholder input; looked at cost-effectiveness of the potential monitoring approaches; considered implementation factors (e.g., laboratory capacity); and further evaluated health effects (e.g., children), occurrence, and persistence/mobility data to identify the list of UCMR 5 contaminants. Please refer to Appendix B for further information on the priority rationale for a subset of the contaminants described in the stepwise approach.

During the public comment period following publication of the proposed UCMR 5 in March 2021 (86 FR 13846; USEPA, 2021a), EPA received 75 sets of comments from organizations and individuals. The commenters were generally supportive of the stepwise prioritization process and the 30 proposed contaminants. Commenters expressed mixed opinion on the inclusion of additional contaminants (*Legionella pneumophila*, 1,2,3-trichloropropane, and four haloacetonitriles) that were considered by EPA but not proposed for monitoring. After considering the public comments, EPA elected to finalize the contaminant list as proposed (USEPA, 2021b). For more information on EPA's rationale, please see "Response to Comments on the Fifth Unregulated Contaminant Monitoring Rule (UCMR 5) Proposal" (USEPA, 2021c).

This Information Compendium provides supporting information for the 30 contaminants included in the UCMR 5 final rule (see Exhibit 1).

The individual information sheets were compiled to help EPA consider and compare health effects and occurrence information, as well as provide information to interested stakeholders. The primary source for this information is the CCL program (i.e., CCL 4). Other publicly available data sources were reviewed (as described in Appendix C) to complete the information sheets.

The information sheet for each of the UCMR 5 contaminants generally includes the following five sections:

1. **Background & Use,** which may include contaminant use, chemical class, and synonym information.

   The PFAS acronyms match those used in EPA Methods 533 and 537.1. Additional names listed for each PFAS include one or two synonyms selected from EPA's

[1] SDWA directs EPA to select five or more contaminants from the current CCL and determine whether or not to regulate those contaminants with a National Primary Drinking Water Regulation (NPDWR) (*https://www.epa.gov/ccl/basic-information-ccl-and-regulatory-determination*).

CompTox Chemicals Dashboard (USEPA, 2020a), or are included because they are synonyms commonly used in the literature (e.g., F-53B major and F-53B minor).

2. **Health Effects,** which may include: Reference Dose (RfD), ATSDR Minimal Risk Level, cancer slope factor, and cancer class data. Also presented, as available, are health-based values and Health Advisories (HA), which are derived based on critical health endpoints (see Appendix D). For additional information, the Interstate Technology Regulatory Council (ITRC) provides a regularly updated summary of additional federal, State, and international PFAS standards and guidance values not included in this document for ground water, drinking water, and surface water/wastewater (ITRC, 2021).
3. **Occurrence in Water,** which may include occurrence data for raw water, finished drinking water, and ambient water.

   EPA is aware of PFAS monitoring efforts by States and local communities to better understand PFAS occurrence in drinking water, including both statewide drinking water monitoring efforts and targeted sampling at locations that have potentially been impacted by releases or where PFAS-containing materials are known to have been used. While these efforts are not detailed in this compendium, results are generally publicly available through State websites. The "Final Regulatory Determination 4 Support Document" (USEPA, 2021d) presents a sample-level summary of State results for PFOA and PFOS individually and includes discussion on State monitoring efforts as well as uncertainties in occurrence data. The ITRC has further details on how federal and State regulatory programs differ in their PFAS guidance documents (ITRC, 2020a).
4. **Production, Release, & Usage,** which may include information from the Chemical Data Reporting Rule (CDR).
5. **Persistence & Mobility,** which may include estimated biodegradation half-life data, water solubility, organic carbon partitioning coefficient (K_{oc}), logarithm of the octanol-water partitioning coefficient (log K_{ow}), and Henry's law constant (K_H). Please refer to Appendix E for information on interpreting the physiochemical properties presented for the contaminants.

   The included PFAS exist in aqueous solution primarily as anions at typical environmental pH values. Physical and chemical property data for various PFAS often correspond to the protonated acid form of the compound in contrast to the deprotonated anion (ITRC, 2020b). Thus, the available physical and chemical property data for PFOA, for example, may not be representative of how PFOA partitions in the environment. In particular, values for K_H may be misleading. If these values are for the protonated acid form of the compound and not for the corresponding anion, the degree of volatility may be over-estimated since anions do not volatilize from water (ATSDR, 2021). For each persistence and mobility data element, the form of the compound is denoted, if known.

   Selected physicochemical properties from EPA's CompTox Chemicals Dashboard (USEPA, 2020a) are presented as the average or reported ranges of experimentally determined or predicted values. The K_{oc} is provided using reported values from the CompTox Chemicals Dashboard or those reported by the Interstate Technology

Regulatory Council (ITRC, 2020c). The K_{oc} values were converted from the log K_{oc} values in "Log K_{oc} Values for Select PFAS" (ITRC, 2020c).

Exhibit 1: UCMR 5 Analytes

Assessment Monitoring

Twenty-five PFAS using EPA Method 533[1]	
11-chloroeicosafluoro-3-oxaundecane-1-sulfonic acid (11Cl-PF3OUdS)	Perfluoroundecanoic acid (PFUnA)
4,8-dioxa-3H-perfluorononanoic acid (ADONA)[2]	1H, 1H, 2H, 2H-perfluorodecane sulfonic acid (8:2 FTS)
9-chlorohexadecafluoro-3-oxanone-1-sulfonic acid (9Cl-PF3ONS)	1H, 1H, 2H, 2H-perfluorohexane sulfonic acid (4:2 FTS)
Hexafluoropropylene oxide dimer acid (HFPO-DA) (GenX)	1H, 1H, 2H, 2H-perfluorooctane sulfonic acid (6:2 FTS)
Perfluorobutanesulfonic acid (PFBS)	Nonafluoro-3,6-dioxaheptanoic acid (NFDHA)
Perfluorodecanoic acid (PFDA)	Perfluoro (2-ethoxyethane) sulfonic acid
Perfluorododecanoic acid (PFDoA)	Perfluoro-3-methoxypropanoic acid (PFMPA)
Perfluoroheptanoic acid (PFHpA)	Perfluoro-4-methoxybutanoic acid (PFMBA)
Perfluorohexanesulfonic acid (PFHxS)	Perfluorobutanoic acid (PFBA)
Perfluorohexanoic acid (PFHxA)	Perfluoroheptanesulfonic acid (PFHpS)
Perfluorononanoic acid (PFNA)	Perfluoropentanesulfonic acid (PFPeS)
Perfluorooctanesulfonic acid (PFOS)	Perfluoropentanoic acid (PFPeA)
Perfluorooctanoic acid (PFOA)	
Four PFAS using EPA Method 537.1[3]	
N-ethyl perfluorooctanesulfonamidoacetic acid (NEtFOSAA)	Perfluorotetradecanoic acid (PFTA)
N-methyl perfluorooctanesulfonamidoacetic acid (NMeFOSAA)	Perfluorotridecanoic acid (PFTrDA)
One Metal/Pharmaceutical using EPA Method 200.7[4] or alternate SM[5] or ASTM[6]	
Lithium	

[1] EPA Method 533 (Solid phase extraction (SPE) liquid chromatography/tandem mass spectrometry (LC/MS/MS)) (USEPA, 2019b).
[2] Although the abbreviation used is ADONA, indicating the ammonium salt, 4,8-dioxa-3H-perfluorononanoic acid is the parent acid.
[3] EPA Method 537.1 Version 2.0 (Solid phase extraction (SPE) liquid chromatography/tandem mass spectrometry (LC/MS/MS)) (USEPA, 2020b).
[4] EPA Method 200.7 (Inductively coupled plasma-atomic emission spectrometry (ICP-AES)) (USEPA, 1994).
[5] Standard Methods (SM) 3120 B (SM, 2017) or SM 3120 B-99 (SM Online, 1999).
[6] ASTM International (ASTM) D1976-20 (ASTM, 2020).

11-chloroeicosafluoro-3-oxaundecane-1-sulfonic acid (11Cl-PF3OUdS)

CASRN: 763051-92-9

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: C10 Cl-PFESA; F-53B minor
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 8.31x10^4 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 3.13 (predicted value for acid form; USEPA, 2020a)
- K_H: 3.30x10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 4.68x10^{-6} mol/L (predicted value for acid form; USEPA, 2020a) converts to 2.96 mg/L

4,8-dioxa-3H-perfluorononanoic acid (ADONA*)

CASRN: 919005-14-4

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: *4,8-dioxa-3H-perfluorononanoic acid is the parent acid form of the ammonium salt, ADONA; DONA
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 967 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 1.89 (predicted value for acid form; USEPA, 2020a)
- K_H: 1.90×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 5.45×10^{-4} mol/L (predicted value for acid form; USEPA, 2020a) converts to 206 mg/L

9-chlorohexadecafluoro-3-oxanone-1-sulfonic acid (9Cl-PF3ONS)

CASRN: 756426-58-1

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: C8 Cl-PFESA; F-53B major
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 329 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 3.39 (predicted value for acid form; USEPA, 2020a)
- K_H: 1.81×10^{-11} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 1.31×10^{-5} mol/L (predicted value for acid form; USEPA, 2020a) converts to 6.97 mg/L

Hexafluoropropylene oxide dimer acid (HFPO-DA)

CASRN: 13252-13-6

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: GenX non-salted; GenX parent acid
- View Structure

Health Effects

- EPA Health Assessment: Human Health Toxicity Values for Hexafluoropropylene Oxide (HFPO) Dimer Acid and Its Ammonium Salt (CASRN 13252-13-6 and CASRN 62037-80-3) (USEPA, 2021e)
  - Chronic Reference Dose (RfD) = 0.000003 mg/kg-day
  - Subchronic RfD = 0.00003 mg/kg-day
  - Cancer Classification: Suggestive evidence of carcinogenic potential

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 409 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 1.98 (predicted value for acid form; USEPA, 2020a)
- K_H: 2.37×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 5.31×10^{-4} mol/L (predicted value for acid form; USEPA, 2020a) converts to 175 mg/L

N-ethyl perfluorooctanesulfonamidoacetic acid (NEtFOSAA)

CASRN: 2991-50-6

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: NEtPFOSA-AcOH
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021). NEtFOSAA is a precursor that can degrade to more stable terminal carboxylic or sulfonic acids.
- K_{oc}: 1,698-3,090 L/kg (experimentally determined range for acid form; ITRC, 2020c)
- log K_{ow}: 3.40-9.34 (predicted range for acid form; USEPA, 2020a)
- K_H: 3.13×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 1.24×10^{-10}-4.18×10^{-4} mol/L (predicted range for acid form; USEPA, 2020a) converts to 7.26×10^{-5}-2.45×10^{2} mg/L

N-methyl perfluorooctanesulfonamidoacetic acid (NMeFOSAA)

CASRN: 2355-31-9

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: NMePFOSA-AcOH
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021). NMeFOSAA is a precursor that can degrade to more persistent terminal carboxylic or sulfonic acids.
- K_{oc}: 1,288-2,239 L/kg (experimentally determined range for acid form; ITRC, 2020c)
- log K_{ow}: 3.35-8.81 (predicted range for acid form; USEPA, 2020a)
- K_H: 3.15×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 1.21×10^{-6}-2.58×10^{-4}mol/L (predicted range for acid form; USEPA, 2020a) converts to 6.91×10^{-1}-1.47×10^{2} mg/L

Perfluorobutanesulfonic acid (PFBS)

CASRN: 375-73-5

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: 1-Perfluorobutanesulfonic acid
- View Structure

Health Effects

- EPA Health Assessment: Human Health Toxicity Values for Perfluorobutane Sulfonic Acid (CASRN 375-73-5) and Related Compound Potassium Perfluorobutane Sulfonate (CASRN 29420-49-3) (USEPA, 2021f)
    - Chronic RfD = 0.0003 mg/kg-day (thyroid)
    - Subchronic RfD = 0.001 mg/kg-day (thyroid)
  - Cancer Classification: Inadequate information to assess carcinogenic potential

Occurrence in Water

- Finished Water:
  - UCMR 3: Detected in 0.16% of public water systems (PWSs) at concentrations greater than or equal to 0.09 µg/L (Minimum Reporting Level [MRL]) (USEPA, 2017)
  - Detected in 96% of partially treated samples from 25 PWSs; median concentration detected 0.00117 µg/L (Boone et al., 2019)
- Ambient Water:
  - Detected in 96% of samples from 25 PWSs; median concentration detected 0.00112 µg/L (Boone et al., 2019)

Production, Release, & Usage

- No production data available in the sources reviewed
- No release data available in the sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 15.85-61.66 L/kg (experimentally determined range for sulfonate form; ITRC, 2020c)
- log K_{ow}: $7.32x10^{-1}$-3.68 (predicted range for acid form; USEPA, 2020a)
- K_H: $3.04x10^{-10}$ atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: $1.70x10^{-3}$ mol/L (experimentally determined value for acid form; USEPA, 2020a) converts to 510 mg/L

Perfluorodecanoic acid (PFDA)

CASRN: 335-76-2

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: EC 206-400-3
- View Structure

Health Effects

- EPA Health Assessment: Not available
- Additional Health Information:
    - Integrated Risk Information System (IRIS) assessment in process (public comment anticipated Fiscal Year [FY] 22; external peer-review FY 22) (USEPA, 2021g)

Occurrence in Water

- Finished Water:
    - Detected in 52% of partially treated samples from 25 public water systems (PWSs); median concentration detected 0.00033 µg/L (Boone et al., 2019)
    - U.S. PWS and Related Waters Study: The mean concentration detected in 2 of 7 PWSs with varying degrees of wastewater impact 0.0015 to 0.0033 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)
- Ambient Water:
    - Detected in 60% of samples from 25 PWSs; median concentration detected 0.00043 µg/L (Boone et al., 2019)
    - U.S. PWS and Related Waters Study: The mean concentration detected in 6 of 6 sites heavily impacted by treated wastewater 0.0033 to 0.015 µg/L; the mean concentration detected in 3 of 7 PWSs with varying degrees of wastewater impact 0.0016 to 0.0033 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{OC}: 575-912 L/kg (experimentally determined range for carboxylate form; ITRC, 2020c)
- log K_{OW}: 3.14-9.53 (predicted range for acid form; USEPA, 2020a)
- K_H: 3.55×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)

- Water solubility: $2.62x10^{-10}$-$8.81x10^{-3}$ mol/L (predicted range for acid form; USEPA, 2020a) converts to $1.35x10^{-4}$-$4.53x10^{3}$ mg/L

Perfluorododecanoic acid (PFDoA)

CASRN: 307-55-1

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: PFDoDA; PFDDA; PFDOA
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- Finished Water:
  - Detected in 4% of partially treated samples from 25 public water systems (PWSs); median concentration detected 0.00009 µg/L (Boone et al., 2019)
- Ambient Water:
  - Detected in 8% of samples from 25 PWSs; median concentration detected 0.00021 µg/L (Boone et al., 2019)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 8.55×10^4 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 5.03-11.3 (predicted range for acid form; USEPA, 2020a)
- K_H: 3.62×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 1.10×10^{-12}-6.38×10^{-5} (predicted range for acid form; USEPA, 2020a) converts to 6.76×10^{-7}-39.2 mg/L

Perfluoroheptanoic acid (PFHpA)

CASRN: 375-85-9

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: EC 206-798-9
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- Finished Water:
  - UCMR 3: Detected in 1.75% of public water systems (PWSs) at concentrations greater than or equal to 0.01 µg/L (Minimum Reporting Level [MRL]) (USEPA, 2017)
  - Detected in 92% of partially treated samples from 25 PWSs; median concentration detected 0.00079 µg/L (Boone et al., 2019)
- Ambient Water:
  - Detected in 96% of samples from 25 PWSs; median concentration detected 0.00113 µg/L (Boone et al., 2019)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 42.66 L/kg (experimentally determined value for carboxylate form; ITRC, 2020c)
- log K_{ow}: 1.37-6.86 (predicted range for acid form; USEPA, 2020a)
- K_H: 2.22×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 0.324 mol/L (experimentally determined value for acid form; USEPA, 2020a) converts to 117,956 mg/L

Perfluorohexanesulfonic acid (PFHxS)

CASRN: 355-46-4

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: EC 206-587-1; PFHS
- View Structure

Health Effects

- EPA Health Assessment: Not available
- Additional Health Information:
    - Integrated Risk Information System (IRIS) assessment in process (public comment anticipated Fiscal Year [FY] 22; external peer-review FY 22) (USEPA, 2021g)
    - Agency for Toxic Substances and Disease Registry (ATSDR): Minimal Risk Level = 0.00002 mg/kg-day (intermediate duration); thyroid and kidney endpoints; drinking water concentrations = 0.517 µg/L (adult) and 0.140 µg/L (child) (ATSDR, 2021).

Occurrence in Water

- Finished Water:
    - UCMR 3: Detected in 1.12% of public water systems (PWSs) at concentrations greater than or equal to 0.03 µg/L (Minimum Reporting Level [MRL]) (USEPA, 2017)
    - Detected in 80% of partially treated samples from 25 PWSs; median concentration detected 0.00079 µg/L (Boone et al., 2019)
    - U.S. PWS and Related Waters Study: The mean concentration detected in 4 of 7 PWSs with varying degrees of wastewater impact 0.0014 to 0.012 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)
- Ambient Water:
    - Detected in 92% of samples from 25 PWSs; median concentration detected 0.00086 µg/L (Boone et al., 2019)
    - U.S. PWS and Related Waters Study: The mean concentration detected in 6 of 6 sites heavily impacted by treated wastewater 0.0042 to 0.01 µg/L; the mean concentration detected in 5 of 7 PWSs with varying degrees of wastewater impact 0.0021 to 0.012 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 251-1,259 L/kg (experimentally determined range for carboxylate form; ITRC, 2020c)
- log K_{ow}: 2.20 (experimentally determined value for acid form; USEPA, 2020a)
- K_H: 1.96×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 6.08×10^{-4} mol/L (experimentally determined value for acid form; USEPA, 2020a) converts to 243 mg/L

Perfluorohexanoic acid (PFHxA)

CASRN: 307-24-4

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: Perfluoro-n-hexanoic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available
- Additional Health Information:
  - Integrated Risk Information System (IRIS) assessment in process (public comment anticipated Fiscal Year [FY] 22; external peer-review FY 22) (USEPA, 2021g)

Occurrence in Water

- Finished Water:
  - Detected in 100% of partially treated samples from 25 public water systems (PWSs); median concentration detected 0.00143 µg/L (Boone et al., 2019)
  - U.S. PWS and Related Waters Study: The mean concentration detected in 5 of 7 PWSs with varying degrees of wastewater impact 0.0011 to 0.023 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)
- Ambient Water:
  - Detected in 96% of samples from 25 PWSs; median concentration detected 0.00202 µg/L (Boone et al., 2019)
  - U.S. PWS and Related Waters Study: The mean concentration detected in 6 of 6 sites heavily impacted by treated wastewater 0.012 to 0.079 µg/L; the mean concentration detected in 6 of 7 PWSs with varying degrees of wastewater impact 0.0011 to 0.029 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 20.42 L/kg (experimentally determined value for carboxylate form; ITRC, 2020c)
- log K_{ow}: 2.51 (experimentally determined value for acid form; USEPA, 2020a)
- K_H: 2.51×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)

- Water solubility: 9.39×10^{-5} mol/L (experimentally determined value for acid form; USEPA, 2020a) converts to 29.49 mg/L

Perfluorononanoic acid (PFNA)

CASRN: 375-95-1

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: C 1800
- View Structure

Health Effects

- EPA Health Assessment: Not available
- Additional Health Information:
  - Agency for Toxic Substances and Disease Registry (ATSDR): Minimal Risk Level = 0.000003 mg/kg-day (intermediate duration); body weight and developmental endpoints; drinking water concentrations = 0.078 µg/L (adult) and 0.021 µg/L (child) (ATSDR, 2021)
  - Integrated Risk Information System (IRIS) assessment in process (public comment anticipated Fiscal Year [FY] 22; external peer-review FY 22) (USEPA, 2021g)

Occurrence in Water

- Finished Water:
  - UCMR 3: Detected in 0.28% of public water systems (PWSs) at concentrations greater than or equal to 0.02 µg/L (Minimum Reporting Level [MRL]) (USEPA, 2017)
  - Detected in 88% of partially treated samples from 25 PWSs; median concentration detected 0.00074 µg/L (Boone et al., 2019)
  - U.S. PWS and Related Waters Study: The mean concentration detected in 4 of 7 PWSs 0.001 to 0.0097 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)
- Ambient Water:
  - Detected in 96% of samples from 25 PWSs; median concentration detected 0.00086 µg/L (Boone et al., 2019)
  - U.S. PWS and Related Waters Study: The mean concentration detected in 6 of 6 sites heavily impacted by treated wastewater 0.0057 to 0.021 µg/L; the mean concentration detected in 4 of 7 PWSs with varying degrees of wastewater impact 0.0013 to 0.01 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 229-4,898 L/kg (experimentally determined range for carboxylate form; ITRC, 2020c)
- log K_{ow}: 2.84-8.64 (predicted range for acid form; USEPA, 2020a)
- K_H: 1.64×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 4.06×10^{-9}-3.97×10^{-3} mol/L (predicted range for acid form; USEPA, 2020a) converts to 1.88×10^{-3}-1.84×10^{3} mg/L

Perfluorooctanesulfonic acid (PFOS)

CASRN: 1763-23-1

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: EF 101
- Listed on the Fourth Contaminant Candidate List (CCL 4)
- View Structure

Health Effects

- EPA Health Assessment: Office of Water (OW) Health Effects Support Document (HESD), 2016 (USEPA, 2016b); Drinking Water Health Advisory (HA) (USEPA, 2016c)
  - Non-Cancer Health Value = 0.07 µg/L (Chronic)
  - Reference Dose (RfD) = 0.00002 mg/kg-day (subject to change based on current EPA reevaluation of toxicity information for PFOS)
  - Critical Effect: Reduced pup body weight in the two-generation study in rats
- Additional Health Information:
  - Health Canada Maximum Acceptable Concentration (MAC) = 0.6 µg/L (Health Canada, 2018a)
  - Agency for Toxic Substances and Disease Registry (ATSDR): Minimal Risk Level = 0.000002 mg/kg-day (intermediate duration); kidney, immune, and developmental endpoints; drinking water concentrations = 0.052 µg/L (adult) and 0.014 µg/L (child) (ATSDR, 2021)
  - Cancer Classification: Suggestive evidence of carcinogenic potential

Occurrence in Water

- Finished Water:
  - UCMR 3: Detected in 1.93% of public water systems (PWSs) at concentrations greater than or equal to 0.04 µg/L (Minimum Reporting Level [MRL]) (USEPA, 2017)
  - Detected in 80% of partially treated samples from 25 PWSs; median concentration detected 0.00162 µg/L (Boone et al., 2019)
  - U.S. PWS and Related Waters Study: The mean concentration detected in 5 of 7 PWSs with varying degrees of wastewater impact 0.0014 to 0.057 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)
  - State-specific PFOS data from community water systems (USEPA, 2021d) and private wells
- Ambient Water:
  - Detected in 88% of samples from 25 PWSs; median concentration detected 0.00228 µg/L (Boone et al., 2019)
  - U.S. PWS and Related Waters Study: The mean concentration detected in 6 of 6 sites heavily impacted by treated wastewater 0.0037 to 0.024 µg/L; the mean concentration

detected in 6 of 7 PWSs with varying degrees of wastewater impact 0.0014 to 0.041 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)
  - Targeted PFOS data from specific ambient water locations

Production, Release, & Usage

- EPA's Chemical Data Reporting (CDR) Rule (USEPA, 2020c): Production Volume
  - 10K to 500K lbs/yr (2002)
  - 0 lbs/yr (2003 (EPA est.))

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 251-5,012 L/kg (experimentally determined range for carboxylate form; ITRC, 2020c)
- log K_{ow}: -5.69×10^{-1}-7.03 (predicted range for acid form; USEPA, 2020a)
- K_H: 1.85×10^{-11} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 6.25×10^{-9}-1.07×10^{-3}(predicted range for acid form; USEPA, 2020a) converts to 3.13×10^{-3}-5.35×10^{2} mg/L

Perfluorooctanoic acid (PFOA)

CASRN: 335-67-1

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: Pentadecafluorooctanoic acid
- Listed on the Fourth Contaminant Candidate List (CCL 4)
- View Structure

Health Effects

- EPA Health Assessment: Office of Water (OW) Health Effects Support Document (HESD), 2016 (USEPA, 2016d); Drinking Water Health Advisory (HA) (USEPA, 2016e)
  - Non-Cancer Health Value = 0.07 µg/L (Chronic)
  - Reference Dose (RfD) = 0.00002 mg/kg-day (subject to change based on current EPA reevaluation of toxicity information for PFOA)
  - Critical Effect: Pup reduced ossification and accelerated male puberty, decreased antibody protection, and increased adult kidney weight with decreased body weight
- Additional Health Information:
  - EPA HESD, 2016: Cancer Risk 10^{-4} = 50 µg/L (USEPA, 2016d)
  - Agency for Toxic Substances and Disease Registry (ATSDR): Minimal Risk Level = 0.000003 mg/kg-day (intermediate duration); kidney, immune, and developmental endpoints; drinking water concentrations = 0.078 µg/L (adult) and 0.021 µg/L (child) (ATSDR, 2021)
  - Health Canada Maximum Acceptable Concentration (MAC) = 0.2 µg/L (Health Canada, 2018b)
  - Cancer Classification: Suggestive evidence of carcinogenic potential
  - International Agency for Research on Cancer (IARC) Cancer Classification: Possibly carcinogenic to humans (Group 2B) (WHO, 2017)

Occurrence in Water

- Finished Water:
  - UCMR 3: Detected in 2.38% of public water systems (PWSs) at concentrations greater than or equal to 0.02 µg/L (Minimum Reporting Level [MRL]) (USEPA, 2017)
  - Detected in 76% of partially treated samples from 25 PWSs; median concentration detected 0.00415 µg/L (Boone et al., 2019)
  - U.S. PWS and Related Waters Study: The mean concentration detected in 4 of 7 PWSs 0.011 to 0.030 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.005 µg/L) (Quiñones and Snyder, 2009)
  - State-specific PFOA data from community water systems (USEPA, 2021d) and private wells
- Ambient Water:

  - Detected in 76% of samples from 25 PWSs; median concentration detected 0.00632 µg/L (Boone et al., 2019)
  - U.S. PWS and Related Waters Study: The mean concentration detected in 6 of 6 sites heavily impacted by treated wastewater 0.026 to 0.12 µg/L; the mean concentration detected in 6 of 7 PWSs with varying degrees of wastewater impact 0.0056 to 0.031 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.005 µg/L) (Quiñones and Snyder, 2009)
  - Targeted PFOA data from specific ambient water locations

Production, Release, & Usage

- Chemical Data Reporting (CDR) Rule (USEPA, 2020c): Production Volume
  - 10K to 500K lbs/yr in 2002
  - < 500K lbs/yr in 2006

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{OC}: 78-427 L/kg (experimentally determined range for carboxylate form; ITRC, 2020c)
- log K_{OW}: 3.60 (experimentally determined value for acid form; USEPA, 2020a)
- K_H: 2.02×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 8.21×10^{-3}-2.29×10^{-2} mol/L (experimentally determined range; USEPA, 2020a) converts to 3.40×10^3-9.48×10^3 mg/L

Perfluorotetradecanoic acid (PFTA)

CASRN: 376-06-7

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: PFTeDA
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- Finished Water:
  - Detected in 0% of partially treated samples from 25 public water systems (PWSs) (Boone et al., 2019)
- Ambient Water:
  - Detected in 0% of samples from 25 PWSs (Boone et al., 2019)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: $2.33x10^{5}$ L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 5.12-13.1 (predicted range for acid form; USEPA, 2020a)
- K_H: $3.72x10^{-10}$ atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: $4.60x10^{-15}$-$2.85x10^{-5}$ (predicted range for acid form; USEPA, 2020a) converts to $3.28x10^{-9}$-20.4 mg/L

Perfluorotridecanoic acid (PFTrDA)

CASRN: 72629-94-8

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: EINECS 276-745-2
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- Finished Water:
  - Detected in 0% of partially treated samples from 25 public water systems (PWSs) (Boone et al., 2019)
- Ambient Water:
  - Detected in 0% of samples from 25 PWSs (Boone et al., 2019)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: $1.84x10^5$ L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 5.19-12.2 (predicted range for acid form; USEPA, 2020a)
- K_H: $3.67x10^{-10}$ atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: $4.46x10^{-7}$-$3.67x10^{-5}$ mol/L (predicted range for acid form; USEPA, 2020a) converts to 2.96x10-1-24.4 mg/L

Perfluoroundecanoic acid (PFUnA)

CASRN: 2058-94-8

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: PFUnDA; PFUdA
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- Finished Water:
    - Detected in 16% of partially treated samples from 25 public water systems (PWSs); median concentration detected 0.00054 µg/L (Boone et al., 2019)
    - U.S. PWS and Related Waters Study: The mean concentration detected in 1 of 7 PWSs with varying degrees of wastewater impact 0.0019 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)
- Ambient Water:
    - Detected in 32% of samples from 25 PWSs; median concentration detected 0.00014 µg/L (Boone et al., 2019)
    - U.S. PWS and Related Waters Study: The mean concentration detected in 1 of 7 PWSs with varying degrees of wastewater impact 0.0014 µg/L (Detects are concentrations greater than or equal to a method reporting limit of 0.001 µg/L) (Quiñones and Snyder, 2009)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 1,995-3,631 L/kg (experimentally determined range for carboxylate form; ITRC, 2020c)
- log K_{ow}: 4.11-10.4 (predicted range for acid form; USEPA, 2020a)
- K_H: 3.58×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 1.70×10^{-11}-6.71×10^{-3} mol/L (predicted range for acid form; USEPA, 2020a) converts to 9.59×10^{-6}-3.79×10^{3} mg/L

1H,1H,2H,2H-Perfluorodecane sulfonic acid (8:2 FTS)

CASRN: 39108-34-4

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: 8:2 Fluorotelomer sulfonic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021). 8:2 FTS is a precursor that can degrade to more persistent terminal carboxylic or sulfonic acids.
- K_{oc}: 1.69×10^{3} kg/L (predicted value for acid form; USEPA. 2020a)
- log K_{ow}: 2.10-5.78 (predicted range for acid form; USEPA, 2020a)
- K_{H}: 1.84×10^{-11} atm-m^{3}/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 1.04×10^{-8}-3.45×10^{-4} mol/L (predicted range for acid form; USEPA, 2020a) converts to 5.49×10^{-3}-1.82×10^{2} mg/L

1H,1H,2H,2H-Perfluorohexane sulfonic acid (4:2 FTS)

CASRN: 757124-72-4

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: 4:2 Fluorotelomer sulfonic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021). 4:2 FTS is a precursor that can degrade to more persistent terminal carboxylic or sulfonic acids.
- K_{OC}: 495 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{OW}: 3.06 (predicted value for acid form; USEPA, 2020a)
- K_H: 2.45×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 5.10×10^{-3} mol/L (predicted value for acid form; USEPA, 2020a) converts to 1,674 mg/L

1H,1H,2H,2H-Perfluorooctane sulfonic acid (6:2 FTS)

CASRN: 27619-97-2

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: 6:2 Fluorotelomer sulfonic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021). 6:2 FTS is a precursor that can degrade to more persistent terminal carboxylic or sulfonic acids.
- K_{oc}: 948 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 1.36-3.88(predicted range for acid form; USEPA, 2020a)
- K_H: $1.85x10^{-10}$ atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: $2.48x10^{-6}$-$3.17x10^{-3}$ mol/L (predicted range for acid form; USEPA, 2020a) converts to 1.06-$1.36x10^3$ mg/L

Nonafluoro-3,6-dioxaheptanoic acid (NFDHA)

CASRN: 151772-58-6

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: Perfluoro-3,6-dioxaheptanoic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 51.02 kg/L (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 1.64-7.69(predicted range for acid form; USEPA, 2020a)
- K_H: 1.14×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 9.33×10^{-4}-1.18×10^{-2} mol/L (predicted range for acid form; USEPA, 2020a) converts to 2.76×10^{2}-3.49×10^{3} mg/L

Perfluoro (2-ethoxyethane) sulfonic acid (PFEESA)

CASRN: 113507-82-7

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: 1,1,2,2-Tetrafluoro-2-(perfluoroethoxy)ethanesulfonic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 353 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 9.83×10^{-1}-5.09 (predicted range for acid form; USEPA, 2020a)
- K_H: 2.23×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 1.04x10-3-2.78x10-2 mol/L (predicted range for acid form; USEPA, 2020a) converts to 3,479 3.29×10^2-8.79×10^3 mg/L

Perfluoro-3-methoxypropanoic acid (PFMPA)

CASRN: 377-73-1

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: PFPE-2; perfluoromethoxypropionic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 64.3 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 1.79-5.41 (predicted range for acid form; USEPA, 2020a)
- K_H: 3.26×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 1.34×10^{-3}-8.14×10^{-2} mol/L (predicted range for acid form; USEPA, 2020a) converts to 3.08×10^{2}-1.87×10^{4} mg/L

Perfluoro-4-methoxybutanoic acid (PFMBA)

CASRN: 863090-89-5

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: PFPE-7; PFMOBA
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 57.3 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 1.59-6.42 (predicted range for acid form; USEPA, 2020a)
- K_H: 5.95×10^{-5} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 5.40×10^{-4}-4.67×10^{-3} mol/L (predicted value for acid form; USEPA, 2020a) converts to 1.51×10^{2}-1.31×10^{3} mg/L

Perfluorobutanoic acid (PFBA)

CASRN: 375-22-4

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: Fluorad FC 23; Perfluoro-n-butanoic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available
- Additional Health Information:
  - Integrated Risk Information System (IRIS) assessment in process (public comment closed fiscal year [FY] 22 (1st quarter; 86 FR 47100; USEPA, 2021h); external peer-review anticipated FY 22) (USEPA, 2021g)

Occurrence in Water

- Finished Water:
  - Detected in 88% of partially treated samples from 25 public water systems (PWSs); median concentration detected 0.00362 µg/L (Boone et al., 2019)
- Ambient Water:
  - Detected in 92% of samples from 25 PWSs; median concentration detected 0.00305 µg/L (Boone et al., 2019)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 75.86 L/kg (experimentally determined value for carboxylate form; ITRC, 2020c)
- log K_{ow}: 1.43 (experimentally determined value for acid form; USEPA, 2020a)
- K_H: 4.99×10^{-5} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 2.09×10^{-3} mol/L (experimentally determined value for acid form; USEPA, 2020a) converts to 447 mg/L

Perfluoroheptanesulfonic acid (PFHpS)

CASRN: 375-92-8

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: Pentadecafluoro-1-heptanesulfonic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 1.23×10^{3} L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 2.55-6.14 (predicted range for acid form; USEPA, 2020a)
- K_H: 2.34×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 9.66×10^{-8}-1.25×10^{-3} mol/L (predicted range for acid form; USEPA, 2020a) converts to 4.35×10^{-2}-5.63×10^{2} mg/L

Perfluoropentanesulfonic acid (PFPeS)

CASRN: 2706-91-4

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: EINECS 220-301-2; EC 220-301-2
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- No occurrence data available in the data sources reviewed

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 1,049.54 L/kg (predicted value for acid form; USEPA, 2020a)
- log K_{ow}: 1.82-4.37 (predicted range for acid form; USEPA, 2020a)
- K_H: 2.18×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 2.31×10^{-5}-4.91×10^{-3} mol/L (predicted range for acid form; USEPA, 2020a) converts to 666 mg/L

Perfluoropentanoic acid (PFPeA)

CASRN: 2706-90-3

Background & Use

- Per- and Polyfluoroalkyl Substances (PFAS); PFAS are used in non-stick cookware, water-repellent clothing, stain resistant fabrics and carpets, some cosmetics, some firefighting foams, and products that resist grease, water, and oil (ATSDR, 2018).
- Names & Synonyms: EC 220-300-7; Perfluoro-n-pentanoic acid
- View Structure

Health Effects

- EPA Health Assessment: Not available

Occurrence in Water

- Finished Water:
  - Detected in 96% of partially treated samples from 25 public water systems (PWSs); median concentration detected 0.00178 µg/L (Boone et al., 2019)
- Ambient Water:
  - Detected in 92% of samples from 25 PWSs; median concentration detected 0.00195 µg/L (Boone et al., 2019)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- PFAS terminal carboxylic and sulfonic acids are of high environmental stability and are resistant to biodegradation, photooxidation, direct photolysis, and hydrolysis (ATSDR, 2021)
- K_{oc}: 23.44 L/kg (experimentally determined value for carboxylate form; ITRC, 2020c)
- log K_{ow}: 1.98 (experimentally determined value for acid form; USEPA, 2020a)
- K_H: 3.22×10^{-10} atm-m^3/mol (predicted value for acid form; USEPA, 2020a)
- Water solubility: 4.54×10^{-4} mol/L (experimentally determined value for acid form; USEPA, 2020a) converts to 120 mg/L

Lithium

CASRN: 7439-93-2

Background & Use

- Metal; lithium salts used as pharmaceuticals. Used as an anode in electrochemical cells and batteries; as chemical intermediate in organic syntheses (HSDB, 2015).
- Lithium is a naturally occurring metal that may be concentrated in brine waters.

Health Effects

- EPA Health Assessment: Provisional Peer-Reviewed Toxicity Values (PPRTV), 2008 (USEPA, 2008)
  - Provisional Reference Dose (p-RFD) = 0.002 mg/kg-day (Chronic and Subchronic)
  - Critical Effect: Adverse effects in several organs and systems (e.g., kidney effects); lower bound of the therapeutic serum concentration range selected as basis
- Additional Health Information:
  - Cancer Classification: Inadequate information to assess carcinogenic potential

Occurrence in Water

- Finished Water:
  - National Inorganics and Radionuclides Survey (NIRS), 1984-1986: Detected in 551 of 988 (55.8%) public water systems (PWSs); detection range 5 to 7,929 µg/L; median concentration 15 µg/L (USEPA, 2021i)
  - Detected in 56% of partially treated samples from 25 PWSs (mostly surface water systems); median concentration detected 10.8 µg/L (Glassmeyer et al., 2017)
- Ambient Water:
  - Detected in 56% of samples from 25 PWSs; median concentration detected 10.7 µg/L (Glassmeyer et al., 2017)
  - National Water Quality Assessment (NAWQA), 1991-2004: Detected in 558 of 649 (86%) domestic ground water wells; median concentration 5.87 µg/L (DeSimone, 2009)
  - NAWQA, 1993-2007: Detected in 448 of 458 (98%) public-supply wells; detection range <1 to 650 µg/L; median concentration 4.8 µg/L (Toccalino et al., 2010)
  - Concentrations in untreated ground water across 33 principal U.S. aquifers ranged from <1 to 396 µg/L (median of 8.1) for 1,464 public-supply wells and <1 to 1700 µg/L (median of 6 µg/L) for 1,676 private-supply wells (Lindsey et al., 2021)

Production, Release, & Usage

- No production data available in the data sources reviewed
- No release data available in the data sources reviewed

Persistence & Mobility

- Lithium is considered to be persistent with minimal or no removal observed during drinking water treatment (Glassmeyer et al., 2017)

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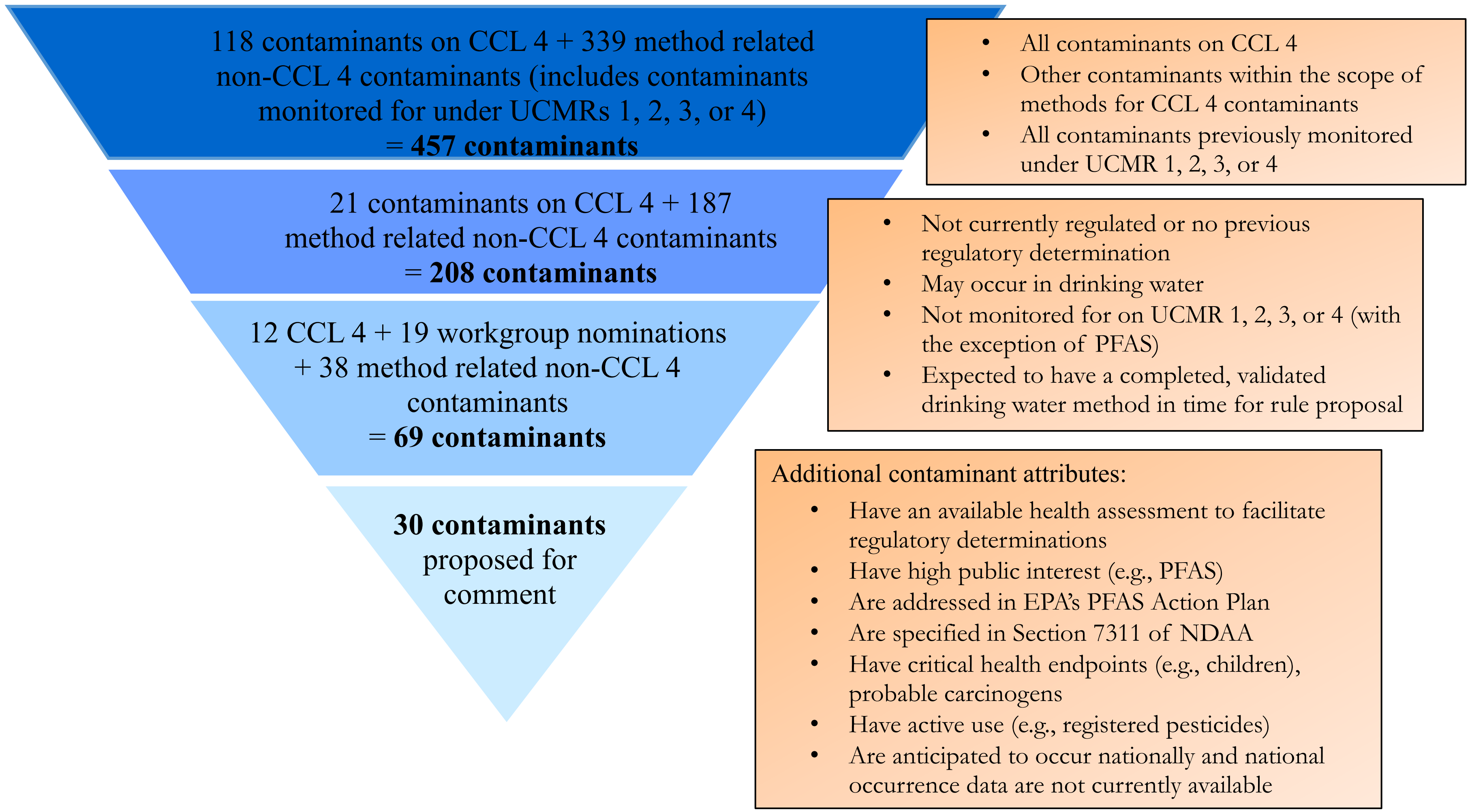
Appendix A: UCMR 5 Prioritization Process

UCMR 5 Prioritization Process



Appendix B: CCL 4, Method-Related, and Nominated Contaminants Considered for Inclusion on UCMR 5

The following appendix describes a subset of the 457 contaminants considered for UCMR 5

CASRN	Name	CCL 4[1]	UCMR 1[2,6,7]	UCMR 2[3]	UCMR 3[4]	UCMR 4[5]	UCMR 5	Priority Rationale[8]
630-20-6	1,1,1,2-Tetrachloroethane	x						A
75-34-3	1,1-Dichloroethane	x			x			E
96-18-4	1,2,3-Trichloropropane	x			x			E
106-99-0	1,3-Butadiene	x			x			E
123-91-1	1,4-Dioxane	x			x			E
763051-92-9	11-chloroeicosafluoro-3-oxaundecane-1-sulfonic acid (11Cl-PF3OUdS)						x	
57-91-0	17-α-Estradiol	x						B
71-36-3	1-Butanol	x				x		F
39108-34-4	1H, 1H, 2H, 2H-perfluorodecane sulfonic acid (8:2 FTS)						x	
757124-72-4	1H, 1H, 2H, 2H-perfluorohexane sulfonic acid (4:2 FTS)						x	
27619-97-2	1H, 1H, 2H, 2H-perfluorooctane sulfonic acid (6:2 FTS)						x	
109-86-4	2-Methoxyethanol	x				x		F
107-18-6	2-Propen-1-ol	x				x		F
16655-82-6	3-Hydroxycarbofuran	x						A
101-77-9	4,4'-Methylenedianiline	x						B
919005-14-4	4,8-dioxa-3H-perfluorononanoic acid (ADONA)						x	
756426-58-1	9-chlorohexadecafluoro-3-oxanone-1-sulfonic acid (9Cl-PF3ONS)						x	
30560-19-1	Acephate	x						A
75-07-0	Acetaldehyde	x						A
60-35-5	Acetamide	x						B

CASRN	Name	CCL 4[1]	UCMR 1[2,6,7]	UCMR 2[3]	UCMR 3[4]	UCMR 4[5]	UCMR 5	Priority Rationale[8]
34256-82-1	Acetochlor	x	x	x				C, D
187022-11-3	Acetochlor ethanesulfonic acid (ESA)	x		x				D
194992-44-4	Acetochlor oxanilic acid (OA)	x		x				D
107-02-8	Acrolein	x						B
142363-53-9	Alachlor ethanesulfonic acid (ESA)	x		x				D
171262-17-2	Alachlor oxanilic acid (OA)	x		x				D
319-84-6	alpha-Hexachlorocyclohexane	x				x		F
64285-06-9	Anatoxin-a	x				x		F
62-53-3	Aniline	x						B
741-58-2	Bensulide	x						A
100-44-7	Benzyl chloride	x						B
82657-04-3	Bifenthrin							A
83463-62-1	Bromochloroacetonitrile (BCAN)							G
74-97-5	Bromochloromethane (Halon 1011)	x			x			E
74-83-9	Bromomethane (Methyl bromide)	x			x			E
25013-16-5	Butylated hydroxyanisole	x				x		F
133-06-2	Captan	x						B
298-46-4	Carbamazepine							A
63-25-2	Carbaryl							A
14866-68-3	Chlorate	x			x			E
75-45-6	Chlorodifluoromethane (Freon 22) (HCFC-22)	x			x			E
74-87-3	Chloromethane (Methyl chloride)	x			x			E
1897-45-6	Chlorothalonil							A
110429-62-4	Clethodim	x						B

CASRN	Name	CCL 4[1]	UCMR 1[2,6,7]	UCMR 2[3]	UCMR 3[4]	UCMR 4[5]	UCMR 5	Priority Rationale[8]
7440-48-4	Cobalt	x			x			E
80-15-9	Cumene hydroperoxide	x						B
143545-90-8	Cylindrospermopsin	x				x		F
439-14-5	Diazepam							A
3252-43-5	Dibromoacetonitrile (DBAN)							G
3018-12-0	Dichloroacetonitrile (DCAN)							G
15307-86-5	Diclofenac							A
141-66-2	Dicrotophos	x						A
55290-64-7	Dimethipin	x				x		F
330-54-1	Diuron	x	x					C
75847-73-3	Enalapril							A
517-09-9	Equilenin	x						B
474-86-2	Equilin	x			x			E
114-07-8	Erythromycin	x						A
66230-04-4	Esfenvalerate							A
50-28-2	Estradiol (17-beta estradiol)	x			x			E
50-27-1	Estriol	x			x			E
53-16-7	Estrone	x			x			E
57-63-6	Ethinyl Estradiol (17-alpha ethynyl estradiol)	x			x			E
13194-48-4	Ethoprop	x				x		F
107-21-1	Ethylene glycol	x						B
75-21-8	Ethylene Oxide	x						B
96-45-7	Ethylene thiourea	x						B
54910-89-3	Fluoxetine							A
50-00-0	Formaldehyde	x						A
25812-30-0	Gemfibrozil							A
7440-56-4	Germanium	x				x		F

CASRN	Name	CCL 4[1]	UCMR 1[2,6,7]	UCMR 2[3]	UCMR 3[4]	UCMR 4[5]	UCMR 5	Priority Rationale[8]
13252-13-6	Hexafluoropropylene oxide dimer acid (HFPO-DA)						x	
110-54-3	Hexane	x						B
51235-04-2	Hexazinone							A
302-01-2	Hydrazine	x						B
7439-93-2	Lithium						x	
121-75-5	Malathion							A
7439-96-5	Manganese	x				x		F
72-33-3	Mestranol	x						B
10265-92-6	Methamidophos	x						A
67-56-1	Methanol	x						B
16752-77-5	Methomyl							A
1634-04-4	Methyl tert-butyl ether	x	x					C
51218-45-2	Metolachlor	x		x				D
171118-09-5	Metolachlor ethanesulfonic acid (ESA)	x		x				D
152019-73-3	Metolachlor oxanilic acid (OA)	x		x				D
21087-64-9	Metribuzin							A
-	Microcystin-LA	x				x		F
-	Microcystin-LF	x				x		F
101043-37-2	Microcystin-LR	x				x		F
-	Microcystin-LY	x				x		F
111755-37-4	Microcystin-RR	x				x		F
101064-48-6	Microcystin-YR	x				x		F
7439-98-7	Molybdenum	x			x			E
1529-99-7	Napropamide							A

CASRN	Name	CCL 4[1]	UCMR 1[2,6,7]	UCMR 2[3]	UCMR 3[4]	UCMR 4[5]	UCMR 5	Priority Rationale[8]
22204-53-1	Naproxen							A
2991-50-6	N-ethyl perfluorooctanesulfonamidoacetic acid (NEtFOSAA)						x	
98-95-3	Nitrobenzene	x	x (AM and SS)					C
55-63-0	Nitroglycerin	x						B
2355-31-9	N-methyl perfluorooctanesulfonamidoacetic acid (NMeFOSAA)						x	
872-50-4	N-Methyl-2-pyrrolidone	x						A
55-18-5	N-Nitrosodiethylamine (NDEA)	x		x				D
62-75-9	N-Nitrosodimethylamine (NDMA)	x		x				D
621-64-7	N-Nitroso-di-n-propylamine (NDPA)	x		x				D
86-30-6	N-Nitrosodiphenylamine (NDPhA)	x						B
930-55-2	N-Nitrosopyrrolidine (NPYR)	x		x				D
151772-58-6	Nonafluoro-3,6-dioxaheptanoic acid (NFDHA)						x	
25154-52-3	Nonylphenol	x						A
68-22-4	Norethindrone	x						B
27314-13-2	Norflurazon							A
103-65-1	n-Propylbenzene	x						A
29-94-3	Octylphenol							A
95-53-4	o-Toluidine	x				x		F
75-56-9	Oxirane, methyl-	x						B
301-12-2	Oxydemeton-methyl	x						A
42874-03-3	Oxyfluorfen	x				x		F
113507-82-7	Perfluoro (2-ethoxyethane) sulfonic acid (PFEESA)						x	
377-73-1	Perfluoro-3-methoxypropanoic acid (PFMPA)						x	
863090-89-5	Perfluoro-4-methoxybutanoic acid (PFMBA)						x	

CASRN	Name	CCL 4[1]	UCMR 1[2,6,7]	UCMR 2[3]	UCMR 3[4]	UCMR 4[5]	UCMR 5	Priority Rationale[8]
375-73-5	Perfluorobutanesulfonic acid (PFBS)				x		x	
375-22-4	Perfluorobutanoic acid (PFBA)						x	
335-76-2	Perfluorodecanoic acid (PFDA)						x	
307-55-1	Perfluorododecanoic acid (PFDoA)						x	
375-92-8	Perfluoroheptanesulfonic acid (PFHpS)						x	
375-85-9	Perfluoroheptanoic acid (PFHpA)				x		x	
355-46-4	Perfluorohexanesulfonic acid (PFHxS)				x		x	
307-24-4	Perfluorohexanoic acid (PFHxA)						x	
375-95-1	Perfluorononanoic acid (PFNA)				x		x	
1763-23-1	Perfluorooctanesulfonic acid (PFOS)	x			x		x	
335-67-1	Perfluorooctanoic acid (PFOA)	x			x		x	
2706-91-4	Perfluoropentanesulfonic acid (PFPeS)						x	
2706-90-3	Perfluoropentanoic acid (PFPeA)						x	
376-06-7	Perfluorotetradecanoic acid (PFTA)						x	
72629-94-8	Perfluorotridecanoic acid (PFTrDA)						x	
2058-94-8	Perfluoroundecanoic Acid (PFUnA)						x	
52645-53-1	Total permethrin (cis- & trans-)	x				x		F
57-41-0	Phenytoin							A
298-02-2	Phorate							A
41198-08-7	Profenofos	x				x		F
7287-19-6	Prometryn							A
91-22-5	Quinoline	x				x		F
121-82-4	RDX	x		x				D
135-98-8	sec-Butylbenzene	x						A
723-46-6	Sulfamethoxazole							A
107534-96-3	Tebuconazole	x				x		F

CASRN	Name	CCL 4[1]	UCMR 1[2,6,7]	UCMR 2[3]	UCMR 3[4]	UCMR 4[5]	UCMR 5	Priority Rationale[8]
112410-23-8	Tebufenozide	x						A
13494-80-9	Tellurium	x						B
59669-26-0	Thiodicarb	x						B
23564-05-8	Thiophanate-methyl	x						B
26471-62-5	Toluene diisocyanate	x						B
n/a-n/a	Total Microcystins and Nodularins	x				x		F
78-48-8	Tribufos	x				x		F
545-06-2	Trichloroacetonitrile (TCAN)							G
338-34-5	Triclosan							A
121-44-8	Triethylamine	x						B
1582-09-8	Trifluralin							A
738-70-5	Trimethoprim							A
76-87-9	Triphenyltin hydroxide (TPTH)	x						B
51-79-6	Urethane	x						A
7440-62-2	Vanadium	x			x			E
50471-44-8	Vinclozolin	x						A
137-30-4	Ziram	x						B

[1] USEPA. 2016. Drinking Water Contaminant Candidate List 4; Notice. *Federal Register*. November 17, 2016. Vol. 81, No. 222, p. 81099.
[2] USEPA. 1999. Revisions to the Unregulated Contaminant Monitoring Regulation for Public Water Systems; Final Rule. *Federal Register*. September 17, 1999. Vol. 64, No. 180, p. 50556.
[3] USEPA. 2007. Unregulated Contaminant Monitoring Regulation (UCMR) for Public Water Systems Revisions. *Federal Register*. January 4, 2007. Vol. 72, No. 2, p. 367.
[4] USEPA. 2012. Revisions to the Unregulated Contaminant Monitoring Regulation (UCMR 3) for Public Water Systems; Final Rule. *Federal Register*. May 2, 2012. Vol. 77, No. 85, p. 26072.
[5] USEPA. 2016. Revisions to the Unregulated Contaminant Monitoring Rule (UCMR 4) for Public Water Systems and Announcement of Public Meeting; Final Rule. *Federal Register.* December 20, 2016. Vol. 81, No. 244, p. 92666.
[6] Screening Survey (List 2); includes contaminants measured using specialized analytical method technologies not commonly used by drinking water laboratories
[7] Assessment Monitoring (List 1); includes contaminants measured with common analytical method technologies used by drinking water laboratories
[8] A = Lower priority
B = No validated drinking water method available in time for rulemaking

C= Listed on UCMR 1
D = Listed on UCMR 2
E = Listed on UCMR 3
F = Listed on UCMR 4
G = Took public comment (please see "Response to Comments on the Fifth Unregulated Contaminant Monitoring Rule (UCMR 5) Proposal," EPA 815-R-21-008, December 2021)

Microbe	CCL 4[1]	UCMR 3[2] (PST)[3]	Existing Rules[4]	Priority rationale
Adenovirus	x		Surface Water Treatment Rules	Method not ready for UCMR 5
Campylobacter jejuni	x			Very low occurrence expected
Enterovirus	x	x	Surface Water Treatment Rules	On UCMR 3
***Escherichia coli* (O157)**	x			Very low occurrence expected
Helicobacter pylori	x			Method not ready for UCMR 5
Hepatitis A virus	x		Surface Water Treatment Rules	No recent outbreaks, vaccines are available, not expected to be a drinking water public health concern
Legionella pneumophila	x		Surface Water Treatment Rules	Conditions for its proliferation have been reported to a higher degree in building water systems. The degree to which its proliferation in municipal supplies occurs is unknown. Regulated via SWTR treatment technique; EPA has identified SWTR for potential regulatory revision because of the opportunity to further reduce residual risk from pathogens, including opportunistic pathogens such as *Legionella.* Took public comment
Mycobacterium avium	x			Method not ready for UCMR 5
Naegleria fowleri	x			Regional/localized occurrence, method not ready for UCMR 5
Norovirus (listed as Caliciviruses on CCL)	x	x	Surface Water Treatment Rules	On UCMR 3

Microbe	CCL 4[1]	UCMR 3[2] (PST)[3]	Existing Rules[4]	Priority rationale
Salmonella enterica	x			Very low occurrence expected
Shigella sonnei	x			Very low occurrence expected

[1] USEPA. 2016. Drinking Water Contaminant Candidate List 4; Notice. *Federal Register*. Vol. 81 No. 222, p 81099, November 17, 2016.
[2] USEPA. 2012. Revisions to the Unregulated Contaminant Monitoring Regulation (UCMR 3) for Public Water Systems. *Federal Register*. Vol. 77, No. 85, p. 26072, May 2, 2012.
[3] PST = Pre-Screen Testing (List 3).
[4] USEPA. 1989. National Primary Drinking Water Regulations; Filtration, Disinfection; Turbidity, Giardia Lamblia, Viruses, *Legionella*, and Heterotrophic Bacteria; Final Rule. Part II. *Federal Register*. Vol. 54, No. 124. p. 27486, June 29, 1989.
USEPA. 1998. Interim Enhanced Surface Water Treatment; Final Rule. *Federal Register*. Vol. 63, No 241. p. 69478, December 16, 1998.
USEPA. 2002. Long Term 1 Enhanced Surface Water Treatment Rule (LT1ESWTR); Final Rule. *Federal Register*. Vol. 67, No. 9. p. 1813. January 14, 2002.
USEPA. 2006. Long Term 2 Enhanced Surface Water Treatment Rule (LT2ESWTR); Final Rule. *Federal Register*. Vol. 71, No. 3. p. 654, January 5, 2006.
USEPA. 2001. National Primary Drinking Water Regulations: Filter Backwash Recycling Rule (FBRR). *Federal Register*. Vol. 66, No. 111 p. 31086, June 8, 2001.

Appendix C: Data Sources Reviewed

The following descriptions are from the respective websites.

I. Health Effects Data Sources

1. EPA's Office of Water (OW)

https://www.epa.gov/dwstandardsregulations/drinking-water-contaminant-human-health-effects-information

The Office of Water provides information on EPA's drinking water regulations and health advisories to provide technical guidance to State agencies, and other public health officials on health effects, analytical methodologies, and treatment technologies for drinking water contaminants. The information contains drinking water standards in the form of non-enforceable concentrations of drinking water contaminants, or Maximum Contaminant Level Goals, as well as enforceable Maximum Contaminant Levels (MCLs). MCLs are the maximum permissible level of a contaminant in water delivered to users of a public water system (PWS). The Office of Water also publishes Health Advisories (HAs) to provide information on unregulated contaminants that can cause human health effects and are known or anticipated to occur in drinking water. EPA's HAs are non-enforceable. HAs may be developed for cancer and/or non-cancer health effects. Health Effects Support Documents (HESD) or Regulatory Support Documents are developed to support the Regulatory Determination process.

2. EPA's Integrated Risk Information System (IRIS)

https://www.epa.gov/iris

EPA's Integrated Risk Information System (IRIS) Program is a human health assessment program that identifies and characterizes the health hazards of chemicals found in the environment. Each IRIS assessment can cover a chemical, a group of related chemicals, or a complex mixture. IRIS assessments are the preferred source of toxicity information used by EPA and are an important source of toxicity information used by State and local health agencies, other federal agencies, and international health organizations. The IRIS Program is located within EPA's Center for Public Health and Environmental Assessment in the Office of Research and Development (ORD). The placement of the IRIS Program in ORD is intentional. It ensures that IRIS can develop impartial toxicity information independent of its use by EPA's program and regional offices to set national standards and clean up hazardous sites.

3. EPA's Provisional Peer-Reviewed Toxicity Values (PPRTV) for Superfund

https://www.epa.gov/pprtv

The Provisional Peer-Reviewed Toxicity Values (PPRTVs) currently represent the second tier of human health toxicity values for EPA Superfund and Resource Conservation and Recovery Act hazardous waste programs. A PPRTV is a toxicity value derived for use in the Superfund Program when such value is not available in EPA's Integrated Risk Information System (IRIS). PPRTVs are derived after a review of the relevant scientific literature using the methods, sources of data, and guidance for value derivation used by EPA's IRIS Program. All provisional peer-reviewed toxicity values receive internal review by EPA scientists and external peer review by independent scientific experts. PPRTVs differ from IRIS values in that PPRTVs do not undergo a multi-program internal agency review, inter-agency review, or public comment. Additionally, IRIS values are generally intended to be used in all EPA programs, while PPRTVs are developed specifically for the Superfund Program.

4. Agency for Toxic Substances and Disease Registry (ATSDR)

https://www.atsdr.cdc.gov/az/a.html

By Congressional mandate, the Agency for Toxic Substances and Disease Registry (ATSDR) produces peer-reviewed "toxicological profiles" for hazardous substances found at National Priorities List (NPL) sites. These hazardous substances are ranked based on frequency of occurrence at NPL sites, toxicity, and potential for human exposure. Toxicological profiles are developed from a priority list of substances. ATSDR also prepares toxicological profiles for the U.S. Department of Defense and the U.S. Department of Energy on substances related to federal sites. In addition to using ATSDR as a general resource, their Toxicological Profile for PFAS (ATSDR, 2021) was utilized for describing the environmental persistence of PFAS.

5. Health Canada

https://www.canada.ca/en/health-canada/services/environmental-workplace-health/water-quality/drinking-water/canadian-drinking-water-guidelines.html

Health Canada has developed over 100 Guidelines for Canadian Drinking Water Quality including treatment goals, indicator organisms, maximum acceptable concentrations (MAC), operational guidance values, or aesthetic objectives for microbiological, physical/chemical, and radiological contaminants that are associated with drinking water and are known, or suspected to be, harmful.

Health Canada has published Guidelines for Canadian Drinking Water Quality since 1968. The guidelines are prepared by the Federal-Provincial-Territorial Committee on Drinking Water. This Committee is composed of representatives from each province and territory, as well as from Health Canada. The guidelines contain authoritative information on exposure, health effects, analytical methods, and treatment for drinking water contaminants. Coverage of the documents includes microbiological, chemical (both organic and inorganic), physical, and radiological issues. Each contaminant or issue is covered in a separate guideline document, which addresses the derivation of MACs for each substance or water quality parameter.

6. International Agency for Research on Cancer (IARC) - Summaries and Evaluations

https://monographs.iarc.fr/

In 1969, the International Agency for Research on Cancer (IARC) initiated a program on the evaluation of the carcinogenic risk of chemicals to humans involving the production of critically evaluated monographs on individual chemicals. In 1980 and 1986, the program was expanded to include evaluations of carcinogenic risks associated with exposures to complex mixtures and other agents. The objective of the program is to elaborate and publish in the form of monographs critical reviews of data on carcinogenicity for agents to which humans are known to be exposed and on specific exposure situations; to evaluate these data in terms of human risk with the help of international working groups of experts in chemical carcinogenesis and related fields; and to indicate where additional research efforts are needed.

II. Occurrence Data and Information Sources

1. Finished Water Data for Chemicals

A. Unregulated Contaminant Monitoring Rule (UCMR)

https://www.epa.gov/dwucmr

EPA uses the Unregulated Contaminant Monitoring Rule (UCMR) to collect data for contaminants suspected to be present in drinking water, but that do not have regulatory standards set under the Safe Drinking Water Act (SDWA). The monitoring provides EPA and other interested parties with nationally representative data on the occurrence of priority contaminants in drinking water, the number of people potentially being exposed, and an estimate of the levels of that exposure. These data can support future regulatory determinations and other actions to protect public health. The Compendium only cites UCMR 3 data. Please refer to the website if you would like more information about past and current UCMRs.

Assessment Monitoring

Designed to provide nationally representative contaminant occurrence data. Conducted by all PWSs serving more than 10,000 people (a "census") and a statistically designed national sample of 800 PWSs serving 10,000 or fewer people. Includes all 50 States, five Territories, and one Tribal land. For UCMR 3, monitoring was conducted during a continuous 12-month period at each participating PWS for seven volatile organic compounds, one synthetic organic compound, six metals, one oxyhalide anion, and six PFAS.

Screening Survey

In UCMR 3, a census of all systems serving more than 100,000 (approximately 400 PWSs and the largest portion of the national population served by PWSs), a statistically selected national sample of 320 PWSs serving 10,001 to 100,000 people, and 480 PWSs serving 10,000 or fewer people were required to monitor for seven contaminants during a continuous 12-month period.

Pre-Screen Testing

In UCMR 3, a representative sample of 800 non-disinfecting ground water systems serving 1,000 or fewer retail customers, including community water systems (CWSs), non-transient non-community water systems, and transient systems, were required to monitor for two viruses during a continuous 12-month period.

B. National Inorganics and Radionuclides Survey (NIRS) (1984 – 1986)

Summary of these data are provided in tabular form at *https://www.regulations.gov*, Docket ID EPA-HQ-OW-2007-1189 (data in raw form are provided in Docket ID EPA-HQ-OW-2019-0583; USEPA, 2021i). The NIRS was designed and conducted by EPA specifically to provide data on the occurrence in ground water of a set of 42 radionuclides and inorganic chemicals being considered for National Primary Drinking Water Regulations (NPDWRs). NIRS provides contaminant occurrence data from a statistical sample comprised of 989 nationally representative CWSs (located in 49 States and Puerto Rico) that treat ground water for distribution. Samples were collected from the distribution system subsequent to treatment. Each of these randomly selected PWSs was sampled a single time between 1984 and 1986.

2. Supplemental Drinking Water and Ambient Water Data for Chemicals

A. National Water Quality Assessment Program (NAWQA)

https://water.usgs.gov/nawqa/

The NAWQA database, maintained by the United States Geological Survey (USGS), describes the status and trends in the quality of the nation's ground water and surface water resources. USGS began its NAWQA program in 1991, systematically collecting chemical, biological, and physical water quality data from 51 study units (basins) across the nation. This database may be useful for examining nationally representative pesticide and volatile organic compound occurrence in ambient water and drinking water sources; however, the composition and presentation of the data vary widely from region to region. NAWQA provides high-quality, nationally representative data reviewed by the National Academies of Science, Engineering, and Medicine.

3. Production, Release, Usage, and Other Data for Chemicals

A. EPA's Chemical Data Reporting (CDR)

https://www.epa.gov/chemical-data-reporting

The CDR database contains both non-confidential and confidential data reported by industry (approximately 2,200 companies in the 2016 submission) as a partial update of the Toxic Substances Control Act. The CDR rule requires manufacturers (including importers) to provide EPA with information on the manufacturing, processing, and use of commercial chemical substances in large quantities. This allows EPA to collect and publish current information on production volumes, manufacturing sites, and how the substances are used. Before August 2011, the CDR Rule was called the Inventory Update Reporting Rule, also known as the Inventory Update Rule (IUR). Inventory data reported under the IUR were stored in the Chemical Update System database. This database contains comprehensive use on the most widely used chemicals in the United States. Under the IUR, manufacturers and importers were required to report company information (e.g., plant site name, address, and Data Universal Numbering System number) and chemical information (e.g., Chemical Abstracts Service Registry Number (CASRN), Premanufacture Notification number/Bonafide/Test Marketing Exemption Application or Confidential Chemicals Identification System Accession Number, and production volume) for chemicals they manufactured or imported in excess of 25,000 pounds (up from 10,000 pounds in 2002) in the previous fiscal year. EPA released the 2006 IUR information on more than 6,200 chemicals in commerce. Due to changes in production volume reporting requirements, categorical binning of national production volumes changed between 2002 and 2006. EPA had previously compiled the 1998 and 2002 IUR data for CCL 3. EPA downloaded the 2006 IUR data in August 2010 for use in CCL 4.

B. Interstate Technology Regulatory Council (ITRC)

https://pfas-1.itrcweb.org/fact-sheets/

ITRC is a State-led coalition with members in both the private and public sector from all 50 States and the District of Columbia. Managed by the Environmental Research Institute of the States, the ITRC produces documents and training that broaden and deepen technical knowledge and expedite quality regulatory decision making. ITRC developed several technical fact sheets and datasets relevant to PFAS. These include naming conventions and physical and chemical properties; regulations, guidance, and advisories; history and use; environmental fate and transport, including tabulated values for K_{oc}; site characterization considerations, sampling precautions, and laboratory analytical methods; remediation technologies and methods; and aqueous film forming foam.

C. EPA's CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard

EPA's CompTox Chemicals Dashboard contains experimentally determined and predicted chemical property data for over 875,000 substances. The CompTox Chemicals Dashboard is a part of a suite of databases and web applications that support EPA's computational toxicology research efforts to develop innovative methods to change how chemicals are currently evaluated for potential health risks. EPA researchers integrate advances in biology, biotechnology, chemistry, and computer science to identify important biological processes that may be disrupted by the chemicals. The combined information helps prioritize chemicals based on potential health risks. Using computational toxicology research methods, thousands of chemicals can be evaluated for potential risk at small cost in a very short amount of time. This resource is a compilation of information sourced from many sites, databases, and sources including U.S. federal and State sources and international bodies that saves the user time by providing information in one location. The data are not reviewed by EPA – the user must apply judgment in use of the information.

D. Hazardous Substances Data Bank (HSDB)

https://pubchem.ncbi.nlm.nih.gov/source/11933

HSDB is a toxicology data file on the National Library of Medicine's Toxicology Data Network (TOXNET®). It focuses on the toxicology of potentially hazardous chemicals. It is enhanced with information on human exposure, industrial hygiene, emergency handling procedures, environmental fate, regulatory requirements, and related areas. All data are referenced and derived from a core set of books, government documents, technical reports, and selected primary journal literature. HSDB is peer-reviewed by the Scientific Review Panel, a committee of experts in the major subject areas within the data bank's scope. HSDB is organized into individual chemical records and contains over 4,500 such records.

Appendix D: Health Effects Definitions

10^{-4} Cancer Risk: The concentration of a chemical in drinking water corresponding to an excess estimated lifetime cancer risk of 1 in 10,000.

Cancer Classification: A descriptive weight-of-evidence judgment as to the likelihood that an agent is a human carcinogen and the conditions under which the carcinogenic effects may be expressed. Under the 2005 EPA Guidelines for Carcinogen Risk Assessment, Cancer Descriptors replace the earlier alpha numeric Cancer Group designations (USEPA 1986 guidelines). The Cancer Descriptors in the 2005 EPA Guidelines for Carcinogen Risk Assessment are as follows:

- Carcinogenic to humans (H)
- Likely to be carcinogenic to humans (L)
- Likely to be carcinogenic above a specified dose but not likely to be carcinogenic below that dose because a key event in tumor formation does not occur below that dose (L/N)
- Suggestive evidence of carcinogenic potential (S)
- Inadequate information to assess carcinogenic potential (I)
- Not likely to be carcinogenic to humans (N)

Cancer Group: A qualitative weight-of-evidence judgment as to the likelihood that a chemical may be a carcinogen for humans. Each chemical was placed into one of the following six categories (USEPA 1986 guidelines).

Group	**Category**
A	Human carcinogen
B	Probable human carcinogen:
	B1 Indicates limited human evidence
	B2 Indicates sufficient evidence in animals and inadequate or no evidence in humans
C	Possible human carcinogen
D	Not classifiable as to human carcinogenicity
E	Evidence of non-carcinogenicity for humans

Group 1	Carcinogenic to humans
Group 2A	Probably carcinogenic to humans
Group 2B	Possibly carcinogenic to humans
Group 3	Not classifiable as to its carcinogenicity to humans 500 agents

Health Advisory (HA): An estimate of acceptable drinking water levels for a chemical substance based on health effects information for a specific exposure duration (e.g., one-day, ten-day, lifetime); a HA is not a federal regulatory standard, but serves as technical guidance to assist federal, State, and local officials.

Maximum Acceptable Concentration (MAC): Health Canada level of a contaminant that is allowed in drinking water.

Minimal Risk Level: An Agency for Toxic Substances and Disease Registry (ATSDR) estimate of daily human exposure to a hazardous substance at or below which that substance is unlikely to pose a measurable risk of harmful (adverse), non-cancerous effects. Minimal Risk Levels are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic).

Reference Dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime.

Adapted from the following references:

ATSDR. 2010. *Glossary of Terms*. Available at: https://www.atsdr.cdc.gov/glossary.html. Accessed September 1, 2021.

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Appendix E: Persistence and Mobility

A contaminant's persistence and mobility in the environment can be estimated using experimental or estimated physicochemical properties. The properties that are most relevant for predicting fate and transport in environmental waters are summarized in Table 1. The properties listed in the table are arranged in hierarchical order, with the most relevant at the top. The scales used to categorize persistence and mobility were recommended by the National Drinking Water Advisory Committee Contaminant Candidate List 3 (CCL 3) workgroup.

Table 1a. Mobility Scales for Environmental Fate Data[1]

Mobility Parameters	Units	Low Likelihood of Partitioning to Water	Moderate Likelihood of Partitioning to Water	High Likelihood of Partitioning to Water
Organic Carbon Partitioning Coefficient (K_{oc})	mL/g	>1,000	100-1,000	<100
Octanol-Water Partitioning Coefficient (log K_{ow})	Dimensionless	>4	1-4	<1
Henry's Law Coefficient (K_H)[2]	atm-m^3/mol	>10^{-3}	10^{-7}-10^{-3}	<10^{-7}
Water Solubility[3]	mg/L	<1	1-1,000	>1,000

[1] Table 1 was modified from Exhibit A.8 in *Final Contaminant Candidate List 3 Chemicals: Classification of the PCCL to CCL* (EPA 815–R–09–008, August 2009).
[2] The mobility parameters indicate the degree to which a contaminant will tend to partition to water relative to other environmental media (i.e., soil, sediment, and air). K_H represents the ratio of the concentration of a contaminant that partitions to air relative to the concentration of a contaminant that partitions to water in an air-water system. Larger values of K_H indicate that the contaminant tends to partition to air more than to water. Thus, larger values of K_H (i.e., >10^{-3} atm-m^3/mol) categorize a contaminant as "not very mobile" because the contaminant will tend to partition to air rather than to water.
[3] Some water solubilities are provided in moles per liter (mol/L). To convert these values to mg/L use the following equation: mg/L = (mol/L) x (molecular weight in g/mol) x 1,000 mg/g.

Table 1b. Persistence Scales for Environmental Fate Data[1]

Persistence Parameters	Units	Not Persistent	Moderately Persistent	Persistent
Half-Life ($t_{1/2}$)	Days	<1-14	>14-59	60 and greater
Modeled Degradation Rate	N/A	Biodegrades Fast; Biodegrades Fast with Acclimation	Biodegrades Slowly; Biodegrades Slowly with Acclimation	Biodegrades Sometimes/Persistent

[1] Table 1 was modified from Exhibit A.8 in *Final Contaminant Candidate List 3 Chemicals: Classification of the PCCL to CCL* (EPA 815–R–09–008, August 2009).