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Supplementary Material

Linking Analysis to Atmospheric PFAS: An Integrated Framework for Exposure Assessment, Health Risks, and Future Management Strategies

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Table S1. PFAS abbreviations, full names, and chemical formulas

abbreviation	Full name	Chemical formula
10:2 FTOH	10:2 Fluorotelomer Alcohol	$C_{12}H_5F_{21}O$
4:2 FTOH	4:2 Fluorotelomer Alcohol	$C_6H_5F_9O$
6:2 Cl-PFESA	Chlorinated Perfluoroether Sulfonic Acid	$C_8HF_{15}ClO_4S$
6:2 diPAP	6:2 Polyfluoroalkyl Phosphate Triester	$C_{16}H_8F_{25}O_8P_2$
6:2 FTOH	6:2 Fluorotelomer Alcohol	$C_8H_5F_{13}O$
6:2 PAP	6:2 Polyfluoroalkyl Phosphate Diester	$C_8H_4F_{13}O_4P$
8:2 diPAP	8:2 Polyfluoroalkyl Phosphate Triester	$C_{20}H_8F_{33}O_8P_2$
8:2 FTOH	8:2 Fluorotelomer Alcohol	$C_{10}H_5F_{17}O$
8:2 PAP	8:2 Polyfluoroalkyl Phosphate Diester	$C_{10}H_4F_{17}O_4P$
ADONA	Ammonium 4,8-Dioxa-3H-Perfluorononanoate	$C_9H_5F_{13}NO_4$
Et-PFOSA-AcOH	Ethyl Perfluorooctane Sulfonamide Acetic Acid	$C_{10}H_5F_{17}NO_3S$
EtFOSA	Ethylperfluorooctane Sulfonamide	$C_{10}H_5F_{17}NO_2S$
EtFOSE	Ethylperfluorooctane Sulfonamidoethanol	$C_{12}H_7F_{17}NO_3S$
F53B	Fluorinated Electrochemical Substance B	Variable
FTCA	Fluorotelomer Carboxylic Acid	Variable
FTIs	Fluorotelomer Iodides	$C_nF_{2n+1}CH_2CH_2I$
FTUCA	Fluorotelomer Unsaturated Carboxylic Acid	Variable
HFPO-DA	Hexafluoropropylene Oxide Dimer Acid	$C_6HF_{11}O_3$
Me-PFOSA-AcOH	Methyl Perfluorooctane Sulfonamide Acetic Acid	$C_9H_3F_{17}NO_3S$
MeFOSA	Methylperfluorooctane Sulfonamide	$C_9H_3F_{17}NO_2S$
MeFOSE	Methylperfluorooctane Sulfonamidoethanol	$C_{11}H_5F_{17}NO_3S$
N-Et-FOSA	N-Ethylperfluorooctane Sulfonamide	$C_{10}H_5F_{17}NO_2S$
N-Et-FOSE	N-Ethylperfluorooctane Sulfonamidoethanol	$C_{12}H_7F_{17}NO_3S$
N-Me-FOSA	N-Methylperfluorooctane Sulfonamide	$C_9H3F_{17}NO_2S$
N-Me-FOSE	N-Methylperfluorooctane Sulfonamidoethanol	$C_{11}H_5F_{17}NO_3S$
PASF	Perfluoroalkyl Sulfonyl Fluoride	$C_nF_{2n+1}SO_2F$
PFBA	Perfluorobutanoic Acid	$C_3HF_7O_2$
PFBS	Perfluorobutane Sulfonic Acid	$C_4HF_9SO_3$
PFDA	Perfluorodecanoic Acid	$C_9HF_{19}O_2$
PFDoDA	Perfluorododecanoic Acid	$C_{11}HF_{23}O_2$
PFDPA	Perfluorodecanophosphonic Acid	$C_{10}HF_{21}O_3P$
PFDS	Perfluorodecane Sulfonic Acid	$C_{10}HF_{21}SO_3$
PFECAs	Perfluoroether Carboxylic Acids	$C_nF_{2n+1}O(CF_2)_mCOOH$
PFESAs	Perfluoroether Sulfonic Acids	$C_nF_{2n+1}O(CF_2)_mSO_3H$
PFHpA	Perfluoroheptanoic Acid	$C_6HF_{13}O_2$
PFHpS	Perfluoroheptane Sulfonic Acid	$C_7HF_{15}SO_3$
PFHxA	Perfluorohexanoic Acid	$C_5HF_{11}O_2$
PFHxDA	Perfluorohexadecanoic Acid	$C_{16}HF_{31}O_2$
PFHxPA	Perfluorohexanophosphonic Acid	$C_6HF_{13}O_3P$
PFHxS	Perfluorohexane Sulfonic Acid	$C_6HF_{13}SO_3$
PFNA	Perfluorononanoic Acid	$C_8HF_{17}O_2$
PFNS	Perfluorononane Sulfonic Acid	$C_9HF_{19}SO_3$
PFOA	Perfluorooctanoic Acid	$C_7HF_{15}O_2$
PFOPA	Perfluorooctanophosphonic Acid	$C_8HF_{17}O_3P$
PFOS	Perfluorooctane Sulfonic Acid	$C_8HF_{17}SO_3$
PFOSA	Perfluorooctane Sulfonamide	$C_8H_2F_{17}NO_2S$
PFPAs	Perfluorophosphonic Acids	$C_nF_{2n+1}P(O)(OH)_2$
PFPeA	Perfluoropentanoic Acid	$C_4HF_9O_2$
PFPEs	Perfluoropolyethers	$F–(CF(CF_3)–CF_2–O)_n–CF_2CF_3$
PFPIA	Perfluoroalkyl Iodides	$C_nF_{2n+1}I$
PFTeDA	Perfluorotetradecanoic Acid	$C_{13}HF_{27}O_2$
PFTrDA	Perfluorotridecanoic Acid	$C_{12}HF_{25}O_2$
PFUnDA	Perfluoroundecanoic Acid	$C_{10}HF_{21}O_2$
SAPAP	Sulfonamide Alcohol Phosphate Acrylate Polymer	Variable

Table S2. Classes, Compounds, Human and Environmental Effects, and Sources of Per- and Polyfluoroalkyl Substances (PFAS).

Class	Compounds	Human and Environmental Effects	Sources	References
perfluoroalkyl acid (PFAAs)	PFCAs	Bioaccumulation, liver toxicity, potential carcinogen	Fluoropolymers, coatings, water repellents	[1,2]
	PFBA	Lower toxicity, persistent in environment	Textile coatings, water repellents	[3]
	PFPeA	Kidney and liver effects, persistent	Anti-corrosion agents	[4]
	PFHxA	Immune suppression, neurotoxicity	Semiconductor cleaners, fire-fighting foams	[1]
	PFHpA	Bioaccumulation, environmental toxicity	Food packaging, textile coatings	[2]
	PFOA	Carcinogenic potential, liver damage, fetal effects	Non-stick coatings (Teflon), water repellents	[5]
	PFNA	Reproductive toxicity, immune system effects	Cleaning agents, polishes, electronics	[6]
	PFDA	Hormonal disruption, reproductive toxicity	Waterproof textiles, electronics	[4]
	PFUnDA	Environmental persistence, ecosystem disruption	Industrial coatings	[2]
	PFDoDA	Bioaccumulation, ecological toxicity	Electrical components, coatings	[1]
	PFTrDA	Ecotoxicity, long-term environmental impacts	Automotive components, specialty coatings	[3]
	PFTA, PFTeDA	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	PFSAs	Persistent, bioaccumulative	Fire-fighting foams, repellents	[5]
	PFBS	Low toxicity, short-term accumulation	Coatings, cleaning agents	[2]
	PFPeS	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	PFHxS	Immune system, kidney effects	Firefighting foams, repellents	[4]
	PFHpS, PFDS, PFNS	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	PFOS	Carcinogenic potential, hormonal disruption	Fire-fighting foams, water repellents	[5]
	PFPAs	Ecotoxicity, bioaccumulation risk	Industrial chemicals	[3]
	PFPIAs	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	C4/C4, C8/C8 PFPIA	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	C6/C6 PFPIA	Persistent, ecological toxicity	Specialty chemical additives	[4]

Table S2 (continued). Classes, Compounds, Human and Environmental Effects, and Sources of Per- and Polyfluoroalkyl Substances (PFAS).

Class	Compounds	Human and Environmental Effects	Sources	References
perfluoroalkyl acid (PFAAs)	PFECAs & PFESAs	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	ADONA	Lower bioaccumulation, relatively lower toxicity	Teflon alternatives	[1]
	GenX	Carcinogenic potential, liver toxicity	Teflon alternatives, coatings	[2]
	EEA	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	F53B	Ecotoxicity, environmental risks	Metal surface treatments	[4]
PFAA precursors	PASF-based substances	Bioaccumulation risks, environmental toxicity	Fire-fighting foams, cleaners	[3]
	MeFBSA	Lower toxicity, accumulation risk	Water and oil repellents	[2]
	MeFOSA	Bioaccumulative, hormonal disruption	Coatings, specialty products	[5]
	EtFBSA, EtFOSA, MeFBSE, MeFOSE, EtFOSE, FOSA, SAPAP	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	Fluorotelomer-base-dsubstances	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	4:2 FTOH	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	6:2 FTOH	Ecotoxicity, bioaccumulation risk	Coatings, water-repellent textiles	[3]
	8:2 FTOH	Reproductive toxicity, environmental persistence	Firefighter gear, water repellents	[4]
	10:2 FTOH, 12:2 FTOH, 6:2 diPAP, 8:2 diPAP	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
Others	Fluoropoly-mers	Persistent, lower toxicity	Teflon, piping, insulation	[1]
	PTFE	Relatively safe, non-biodegradable	Non-stick coatings, insulation	[2]
	PVDF	Long-term environmental effects	Electrical wiring, electronics	[4]
	FEP, PFA	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	
	PFPEs	Limited research; potential for bioaccumulation	Experimental use, industrial coatings	

Table S3. Standard Methods for the Analysis of PFAS in Various Environmental Matrices.

Standard Method	Matrix	Compounds Analyzed	Number of Analytes	Quantification Scheme	Analytical Method	Detection Limit
(US) EPA 537 (EPA, 2008) [7]	Drinking water	PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFTeDA, PFBS, PFHxS, PFOS	14	Internal standard	LC-MS/MS (MRM)	2.9–14 ng/L (water)
(US) EPA 533 (EPA, 2019) [8]	Drinking water	PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFTeDA, PFBS, PFHxS, PFOS	25	Isotope dilution standard	LC-MS/MS (MRM)	1.4–16 ng/L (water)
(US) EPA 537.1 (EPA, 2020) [9]	Drinking water	PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFTeDA, PFBS, PFHxS, PFOS	18	Internal standard	LC-MS/MS (MRM)	0.53–6.3 ng/L (water)
(US) EPA SW-846 Method 8327 (EPA, 2019) [10]	Surface water, groundwater, and wastewater	PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFTeDA, PFBS, PFHxS, PFOS, PFDS	24	External standard	LC-MS/MS (MRM)	10–50 ng/L (water)
ISO 21675:2019 (ISO, 2019) [11]	Unfiltered drinking water, groundwater, surface water, and wastewater	PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFTeDA, PFHxDA, PFHpS, PFOS	30	External or internal standard	LC-MS/MS (MRM)	LOQ > 0.2 ng/L (water)
ISO 25101:2009 (ISO, 2009) [12]	Filtered drinking water, groundwater, and surface water	PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFTeDA, PFHxS, PFOS	2	Isotope dilution standard	LC-MS/MS (MRM)	Reporting Limit: 2.0 PFOS, 10 PFOA
ASTM D7979-20 (ASTM, 2020) [13]	Water (sludge, influent, effluent), wastewater with solids (1–2 g/L)	PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFTeDA, PFBS, PFHxS, PFOS	21	Internal standard	LC-MS/MS (MRM)	0.7–106.8 ng/L (water)
ASTM D7968-17a (ASTM, 2017) [14]	Soil	PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTrDA, PFTeDA, PFBS, PFHxS, PFOS	21	Internal standard	LC-MS/MS (MRM)	2.41–258.37 ng/kg (soil)

Table S4. Extraction Methods for PFAS Analysis: Description, Common Matrices, Solvents, Advantages, and References.

Extraction Method	Description	Common Matrices	Solvent	Advantages	References
SPE (Solid-Phase Extraction)	PFAS are selectively extracted by binding to a solid phase	Water, serum, marine samples, sediments	Methanol, Acetonitrile	Excellent purification process; high reproducibility	[15,16]
SLE (Solvent Liquid Extraction)	PFAS are extracted using solvents	Soil, sludge, food samples	Methanol, Ethyl Acetate	Relatively simple; allows use of various solvents	[17,18]
PLE (Pressurized Liquid Extraction)	Efficient extraction of PFAS using high pressure and temperature	Sediments, food packaging	Methanol, Acetone, Hexane	Time-saving and efficient extraction	[19,20]
LLE (Liquid-Liquid Extraction)	PFAS are separated using immiscible solvents	Human blood, soil, water	Acetonitrile, Hexane	Simple and widely used method	[21,22]
Automated SPE	Automated solid-phase extraction ensuring high precision	River water, drinking water, serum	Methanol, Acetonitrile	Suitable for large sample processing; high reproducibility	[23,24]
FUSLE (Focused Ultrasonic Extraction)	Rapid PFAS extraction using ultrasonic energy	Fish, plants, soil	Methanol, Acetone	Fast extraction speed and high recovery rate	[25,26]
Soxhlet Extraction	Repeated solvent circulation to extract PFAS from solid samples	Sediments, food packaging, indoor dust	Methanol, Toluene, Acetone	Complete extraction achievable but time-consuming	[27,28]
Micro-LLE (Micro-Liquid Extraction)	Efficient extraction of PFAS using small amounts of solvent	Groundwater, soil	Methanol, Acetonitrile	Eco-friendly; minimizes solvent usage	[29,30]
Turbulent Flow Chromatography	Online PFAS purification and extraction by adjusting flow conditions	River water	Methanol, Acetonitrile	Simultaneous sample preparation and analysis	[31]
SPME (Solid Phase Microextraction)	PFAS are adsorbed onto a solid phase in small amounts for extraction	Surface water, river water, packaging	Methanol, Acetonitrile	Simple sample preparation with high precision	[32]

Table S5. Regulatory Guidelines for PFAS Levels in Drinking Water Across Regions.

Region	Country/State	Authority/Organization	Guideline Value	Water Type	Compounds Included	References
North America	United States	U.S. Environmental Protection Agency (EPA)	PFOA: 4 ng/L, PFOS: 4 ng/L	Drinking water	PFOA, PFOS	[33]
North America	United States	New York State Department of Environmental Conservation (NYSDEC)	PFOA: 10 ng/L, PFOS: 10 ng/L	Drinking water	PFOA, PFOS	[34]
North America	United States	Massachusetts Department of Environmental Protection (MassDEP)	Total: 20 ng/L	Drinking water	PFOA, PFOS, PFHxS, PFNA, PFHpA, PFDA	[35]
Europe	European Union	European Drinking Water Directive	Total PFAS: 0.5 µg/L, Individual PFAS: 0.1 µg/L	Drinking water	20 individual PFAS	[36]
Europe	Germany	German Federal Environment Agency (UBA)	Total PFAS: 100 ng/L	Drinking water	20 individual PFAS	[37]
Oceania	Australia	National Health and Medical Research Council (NHMRC)	PFOS: 4 ng/L, PFHxS: 30 ng/L, PFOA: 200 ng/L	Drinking water	PFOS, PFHxS, PFOA	[38]
Asia	Japan	Ministry of the Environment (MOE Japan)	PFOA: 50 ng/L, PFOS: 50 ng/L	Drinking water	PFOA, PFOS	[39]
Asia	China	National Health Commission of China (NHC)	PFOA: 85 ng/L, PFOS: 47 ng/L	Drinking water	PFOA, PFOS	[40]
Africa	South Africa	Department of Water and Sanitation (DWS RSA)	PFOA: 100 ng/L, PFOS: 100 ng/L	Drinking water	PFOA, PFOS	[41]
South America	Brazil	Brazilian Institute of Environment and Renewable Natural Resources (IBAMA)	PFOA: 70 ng/L, PFOS: 70 ng/L	Drinking water	PFOA, PFOS	[42]

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