

PFAS

Purpose:

This document describes the process for obtaining the US Environmental Protection Agency's (EPA) Per- and polyfluoroalkyl substances (PFAS) Library. The Library is a collection of 430 PFAS (list of PFAS available here: https://comptox.epa.gov/dashboard/chemical_lists/epapfasinv) quantities of which can be ordered from EPA to facilitate independent research and testing. The information within this document describes the EPA PFAS Library, primary contacts for obtaining the library, and the process to request shipment of the library.

Availability for Federal & State Partners

Background:

Per- and polyfluoroalkyl substances (PFAS) are a large group of man-made fluorinated substances of interest to researchers, regulators, and the public due to their presence in the environment. Some PFAS have extensive amounts of human epidemiological, exposure, and experimental animal toxicity data (e.g., perfluorooctanoic acid (PFOA)). However, some PFAS have little toxicity and exposure information available.

The US EPA's Office of Research and Development (ORD) and the National Toxicology Program (NTP), headquartered at the National Institute of Environmental Health Sciences (NIEHS), are collaborating to develop a risk-based approach for testing PFAS using new approach methods (NAMs), including *in vitro* high-throughput screening (HTS) (Patlewicz et al., 2019, <https://ehp.niehs.nih.gov/doi/10.1289/EHP4555>¹).

¹ Patlewicz et. al., A Chemical Category-based Prioritization Approach for Selecting 75 Per- and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing. *Environmental Health Perspectives*, <https://ehp.niehs.nih.gov/doi/10.1289/EHP4555>

Using NAMs to develop a risk-based approach for testing PFAS is one part of the US EPA's research strategy to identify solutions to address PFAS in the environment. More information about EPA's research strategy is available here: <https://www.epa.gov/pfas/epa-pfas-research>.

To aid with testing PFAS using NAMs, EPA researchers assembled the EPA PFAS Library. The EPA PFAS Library or subsets of the library can be shipped to Federal and State partners for hazard testing, development of analytical methods, exposure monitoring, or other testing that would benefit environmental decision-making. PFAS, depending on the specific compound, can be difficult to obtain. EPA's consolidated PFAS Library established a consistent and reliable source of available compounds will help facilitate research and testing needs.

PFAS Library Details:

EPA purchased the 430 PFAS Chemical Library (list of PFAS chemicals available here: https://comptox.epa.gov/dashboard/chemical_lists/epapfasinv) from a wide range of commercial suppliers and have solubilized chemicals primarily in DMSO. EPA can ship

chemicals in neat (i.e., powder or pure) or solution form in a variety of vial or plating formats (e.g., 96 or 384 well plates).

EPA curated several publicly available PFAS lists to exclude most high (>500) and low (<50) molecular weight compounds, aromatic compounds, metal-containing compounds, and chemicals with a low ratio of fluorine to carbon. There are three PFAS lists, which encompass EPA's entire PFAS Chemical Library.

These lists are published on EPA's Computational Toxicology Chemicals Dashboard, along with their chemical IDs (name, CAS) and structures. Federal and State partners can request the entire EPA PFAS library, any of the sub-libraries below and/or specific PFAS within the library. Before submitting requests, the lists below should be reviewed to determine which PFAS to request.

- I. EPAPFASINV, https://comptox.epa.gov/dashboard/chemical_lists/epapfasinv

List contains the entire 430 PFAS chemicals in the current inventory found to be soluble in DMSO. All 430 have DMSO solution available at 20-30mM DMSO concentration. A subset of these will also have available neat sample.

2. EPAPFAS75SI, https://comptox.epa.gov/dashboard/chemical_lists/epapfas75s1

A subset of the 430 PFAS Library, the list contains 74 unique chemicals (75 samples) prioritized for testing by EPA and National Toxicology Program researchers to generate data to inform read-across approaches.

3. EPAPFASINSOL, https://comptox.epa.gov/dashboard/chemical_lists/epapfasinsol

List of 43 chemicals procured but found to be insoluble in DMSO above 5mM. All or some subset of these 43 chemicals may be available in neat form.

Guidelines for Quantities and Format of Request:

EPA typically purchases small quantities (100-200mg) of neat samples to test chemicals using NAMs, with half that amount solubilized in DMSO to create stock solutions and the remainder stored as neat. In the case of the PFAS library, 200mg neat samples were purchased and a portion (75-100mg) was solubilized in DMSO to create 20-30mM stock solutions. DMSO solutions are available for all chemicals in the EPAPFASINV list but neat samples may not be available for all compounds in the PFAS Library (https://comptox.epa.gov/dashboard/chemical_lists/epapfasinv).

Typical DMSO solution quantities for plating orders are 50-200ul (20-30mM), provided in 96 (or 384) well plating formats, where the latter can be customized to leave specified columns or rows blank. Alternatively, individual solution vials can be provided upon request. All samples are barcoded and a plate map (blinded or unblinded) is provided with the shipment and linked to DSSTox IDs (<https://comptox.epa.gov/dashboard>).

Neat samples typically are on the order of 5-20mg, and based on sample availability and condition (i.e., weighable), *however EPA will consider all requests.*

Chemicals are stored frozen and shipped overnight on dry ice by FedEx. It is recommended that the chemicals be stored frozen (-20 degrees C) when not in use, and exposure to air and moisture be limited.

Requesting Chemicals from the PFAS Library:

To request the PFAS Library, a Materials Transfer Agreement (<https://www.epa.gov/ftta/materials-transfer-agreement-template-fillable-form>) should be completed and submitted to Monica Linnenbrink (Linnenbrink.Monica@epa.gov). If you have questions regarding the PFAS Library, please contact Monica via email or at 919-541-1522.