

Structure-based categorization of Per- & Polyfluoroalkyl substances in the DSSTox database and EPA's ToxCast inventory using Markush representations

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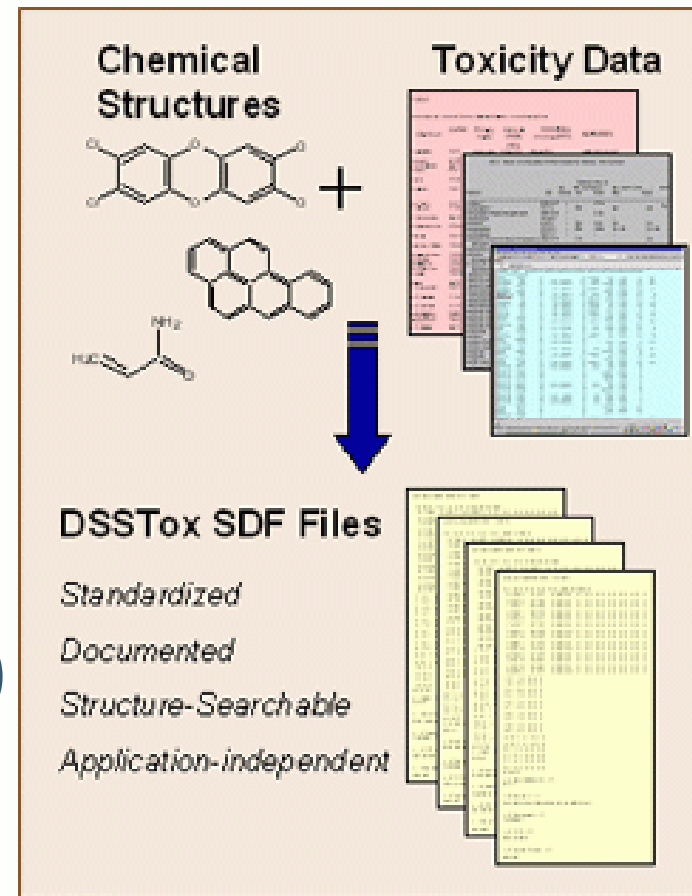
American Chemical Society Meeting, Spring 2019

2 April 2019, Orlando FL

DSSTox Background

Goal: Linking data to chemical structures enabling SAR

- First release of data files in 2004
- Focused on high impact sets of data
 - Carcinogenic Potency Database
 - Drinking water disinfection by-products
 - EPA's Integrated Risk Information System
 - FDA's Maximum Daily Dose dataset
 - EPA's Fat Head Minnow Toxicity dataset
 - ToxCast and Tox21 chemicals
- Currently contains: 876K records (32K manually curated)
- Check it out: <https://comptox.epa.gov/dashboard>



Non-Targeted Analysis PFAS Suspect Lists (Early 2017)



- Several PFAS chemicals have been reported in environmental media and biota
 - Houde *et al.* [2011](#)
 - Post *et al.* [2012](#)
 - Long *et al.* [2013](#)
 - Lang *et al.* [2017](#)
 - Scher *et al.* [2018](#)
 - Etc...
- NORMAN Network surfaces lists of “Suspects” to support NTA and suspect screening (<https://www.norman-network.com/?q=node/236>)

- PFASTRIER

https://comptox.epa.gov/dashboard/chemical_lists/pfastrier

- Supplied by: Xenia Trier et al
- Release date: November 2015
- Substance Count: 597
- Category Count: 119

- PFASKEMI

https://comptox.epa.gov/dashboard/chemical_lists/pfaskemi

- Supplied by: Swedish Chemicals Agency
- Release date: July 2015
- Substance Count: 2397
- Category Count: 31

PFAS: EPA Cross-Agency Research List (Late 2017)

https://comptox.epa.gov/dashboard/chemical_lists/epapfasrl

490 Total Source-PFAS
chemicals listed

19 EPA PFAS
Source Lists

Lists from EPA research labs
& program offices

Curation

- ✓ Correct misspelled names
- ✓ Correct CASRN
- ✓ Fix errors in mappings of anions, salts, parents
- ✓ Create unique acronym
- ✓ Map to unique DTXSID

EPAPFASRL

19 lists collapsed to
single list of 194 unique
DTXSID substances



DTXSID	Substance_Name	Substance_CASRN	Source_Name (incorrect or ambiguous)	Source_CASRN (incorrect or invalid)	Source_Acronym (incorrect or ambiguous)	Unique_Acronym
DTXSID20874028	2H,2H,3H,3H-Perfluorooctanoic acid	914637-49-3	5:3 Polyfluorinated acid	914637-49-3	5:3 acid	5:3 PFOA
DTXSID7027831	N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide	24448-09-7	N-Methyl perfluorooctanesulfonamideeoethanol		NMeFOSE, MeFOSE	NMeFOSE
DTXSID10892352	Perfluoro-2-[[perfluoro-3-(perfluoroethoxy)-2-propanyl]oxy]ethanesulfonic acid	749836-20-2	Ethanesulfonic acid, 2-[1-[difluoro(1,2,2,2-tetrafluoroethoxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoro	749836-20-2	PFESA Byproduct 2	PFESA Byproduct 2
DTXSID70892479	Perfluoropentanesulfonate	175905-36-9	Perfluoropentansulfonate	2706-91-4	PFPeS	PFPeS_ion
DTXSID8071354	Ammonium perfluoropentanesulfonate	68259-09-6	Ammonium perfluoropentansulfonate	68259-09-6		APFPeS
DTXSID40881350	4,8-Dioxa-3H-perfluorononanoic acid	919005-14-4	2,2,3-Trifluoro-3-(1,1,2,2,3,3-hexafluoro-3-(trifluoromethoxy)propoxy)propanoic acid	919005-14-4	ADONA	ADONA parent acid
DTXSID00874026	Ammonium 4,8-dioxa-3H-perfluorononanoate	958445-44-8	Ammonium 4,8-dioxa-3H-perfluorononanoate	958445-44-8	ADONA	ADONA
DTXSID3037707	Potassium perfluorobutanesulfonate	29420-49-3	Potassium perfluoro-1-butanesulfonate		PFBS	PFBS-K
DTXSID5030030	Perfluorobutanesulfonic acid	375-73-5	Perfluorobutanesulfonic acid	375-73-5	PFBS	PFBS
DTXSID60873015	Perfluorobutanesulfonate	45187-15-3	Perfluorobutanesulfonate	375-73-5	PFBS	PFBS_ion
DTXSID3040148	Perfluorodecanesulfonic acid	335-77-3	Perfluorodecanesulfonic acid		PEDS	PEDS

PFAS Library and Chemical Selection

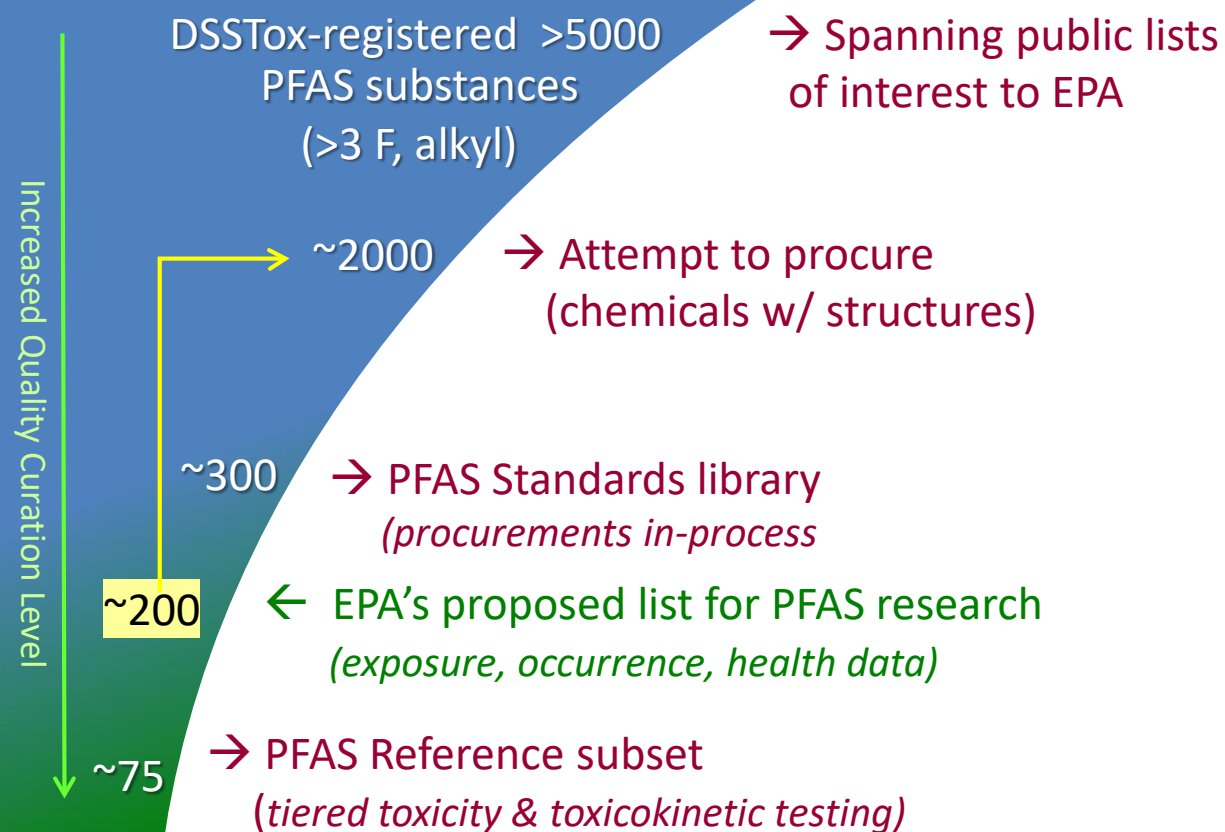
<https://comptox.epa.gov/dashboard>

EPA DSSTox Database: > 758K chemicals



- Chemical structures, downloadable files
- Predicted phys-chem properties
- External links & list overlaps

PFAS Chemical Landscape:



Per(poly)-fluorinated substances (PFAS)

- PFAS chemical names, acronyms, synonyms
- PFAS chemical structure categories

PFOS
1763-23-1 | DTXSID3031864

Searched by Approved Name: Found 1 result for PFOS.

Wikipedia
Perfluorooctanesulfonic acid (conjugate base perfluorooctanesulfonate) (PFOS)
Read more

Intrinsic Properties

Structural Identifiers

Related Compounds

Presence in Lists

Record Information

Chemical

Similar M

Abso

Potassium perfluorobutanesulfo...
29420-49-3

Ammonium perfluorooctanoate
3825-26-1

Potassium perfluorohexanesulfo...
3871-99-6

10:2 Fluorotelomer acrylate
17741-60-5

6:2 Fluorotelomer acrylate
17527-29-6

Perfluorooctanesulfonamide
754-91-6

Perfluorodecanesulfonic acid
335-77-3

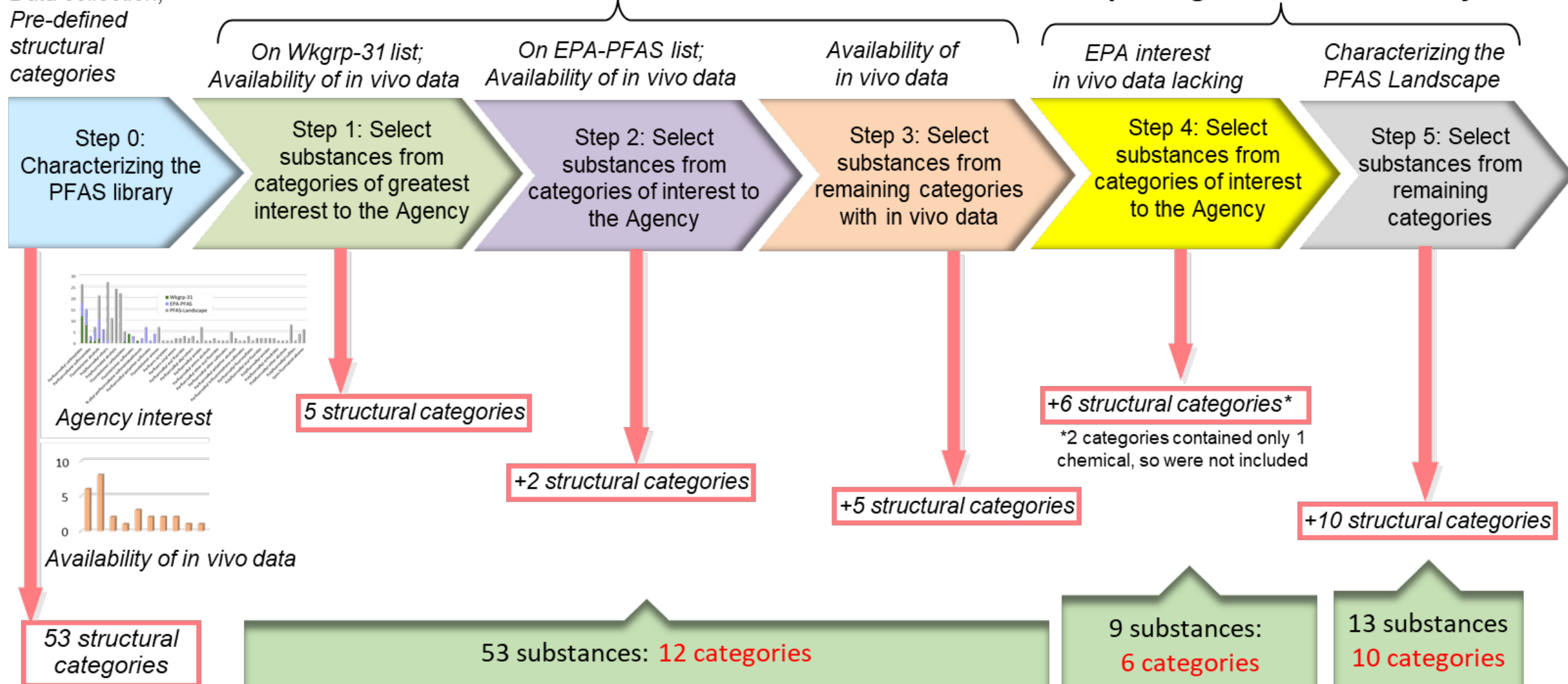
Pentafluoroiodoethane
354-64-3

Designing our library

Data collection;
Pre-defined
structural
categories

Maximizing Read-across

Capturing Structural Diversity



OECD PFAS List (Early 2018)

- Released May 2018
- Substance Count: 4729
- Category Count: 173



Portal on Per and Poly Fluorinated Chemicals

HOME

ABOUT
PFAS

RISK
REDUCTION

ALTERNATI

Contribute to the development of risk reduction

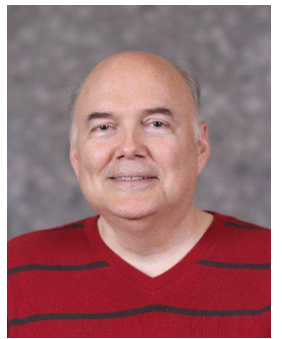
Why this Portal?

This Portal serves to facilitate the exchange of information on per and poly-fluorinated specifically on per- and polyfluoroalkyl substances (PFASs). In order to support a glob alternatives, the Portal provides information on the following areas:

- › What are PFASs?
- › Alternatives
- › In
- › Risk reduction approaches
- › Production and emissions

Information provided in this portal comes principally from the work done within the for

Follow us

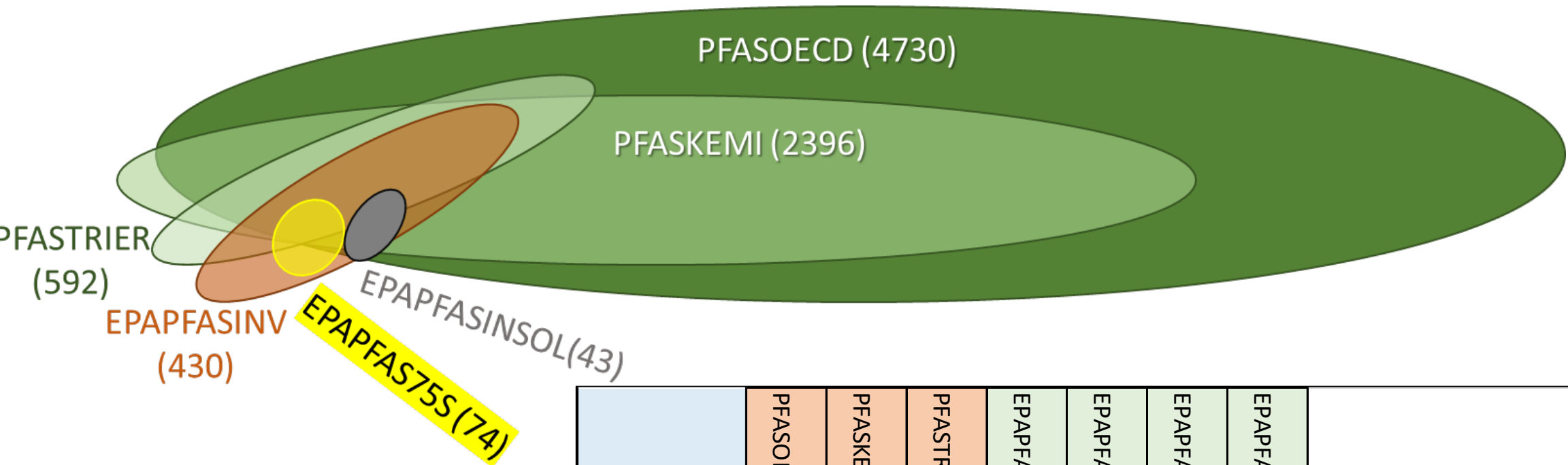


Toward a new comprehensive Global Database of Per- And Polyfluoroalkyl Substances (PFASs) —



Read the [New Comprehensive Global Database of PFASs](#) and the [methodology report](#).

PFAS List Overlap

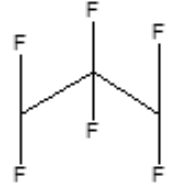


PFASMASTER LISTS	PFASOECD	PFASKEMI	PFASTRIER	EPAPFASRL	EPAPFASINV	EPAPFASINSOL	EPAPFAS75S1	
PFASOECD	4730							OECD PFAS List
PFASKEMI	2206	2396						KEMI (Swedish Chem Agency) PFAS List
PFASTRIER	493	578	592					Community PFAS List (2015)
EPAPFASRL	132	116	71	199				EPA PFAS Research List
EPAPFASINV	309	324	226	61	430			EPA PFAS Inventory (DMSO Soluble)
EPAPFASINSOL	43	42	24	12	0	43		EPA PFAS Inventory (DMSO Insoluble)
EPAPFAS75S1	51	47	38	25	74	0	74	EPA PFAS 75 Test Sample (Set 1)

PFAS “Categories”: Per & Poly-fluorinated alkyl substances

- **Expert**-assigned PFAS categories – manual, subjective
 - Buck et al. (DuPont), based on chemical & series informed by synthetic pathways (e.g., fluorotelomers)
 - data-gathering, occurrence reports, ecotox
 - OECD PFAS listing (>4500 chemicals) – manually assigned groupings

Poly- and Perfluorochemicals



Acyclic - Pure

Atoms: N, P, O, S, Si, Cl, Br, I = **NOT**

AND # of Cycles = 0

Cyclic - Pure

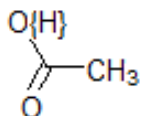
Atoms: N, P, O, S, Si, Cl, Br, I = **NOT**

AND # of Cycles ≥ 1

Carboxylic Acids

Atoms: N, P, S, Si, Cl, Br, I = **NOT**

AND



Expert category		
Fluorotelomer acrylates		
Fluorotelomer alcohols		
Polyfluorinated alcohols		
Fluorotelomer sulfonates		
N-alkyl perfluoroalkyl sulfonamidoacetic acids		
N-alkyl perfluoroalkyl sulfonamidoethanols		
Perfluoroalkyl aldehydes		
Perfluoroalkyl amides		
Perfluoroalkyl carboxylates		
Perfluoroalkyl acyl fluorides		
Perfluoro vinyl esters		
Perfluoroalkyl ketones		
Semi-fluorinated alkenes		
Perfluoroalkyl vinyl ethers		
Perfluoroalkyl alkyl ethers		
Fluorotelomer amines		
Perfluoroalkyl sulfonamides		
Class	Category_Name1	Category_Name2
Alcohol	Fluorotelomer alcohols	Fluorotelomer (linear) n:2 alcohols
Sulfonic Acid	Perfluoroalkyl sulfonic acids	Perfluoroalkyl (linear C4-C10) sulfonic acids
		Polyfluoroalkyl carboxylates
		Perfluoroalkyl ethers
		Fluorotelomer phosphates

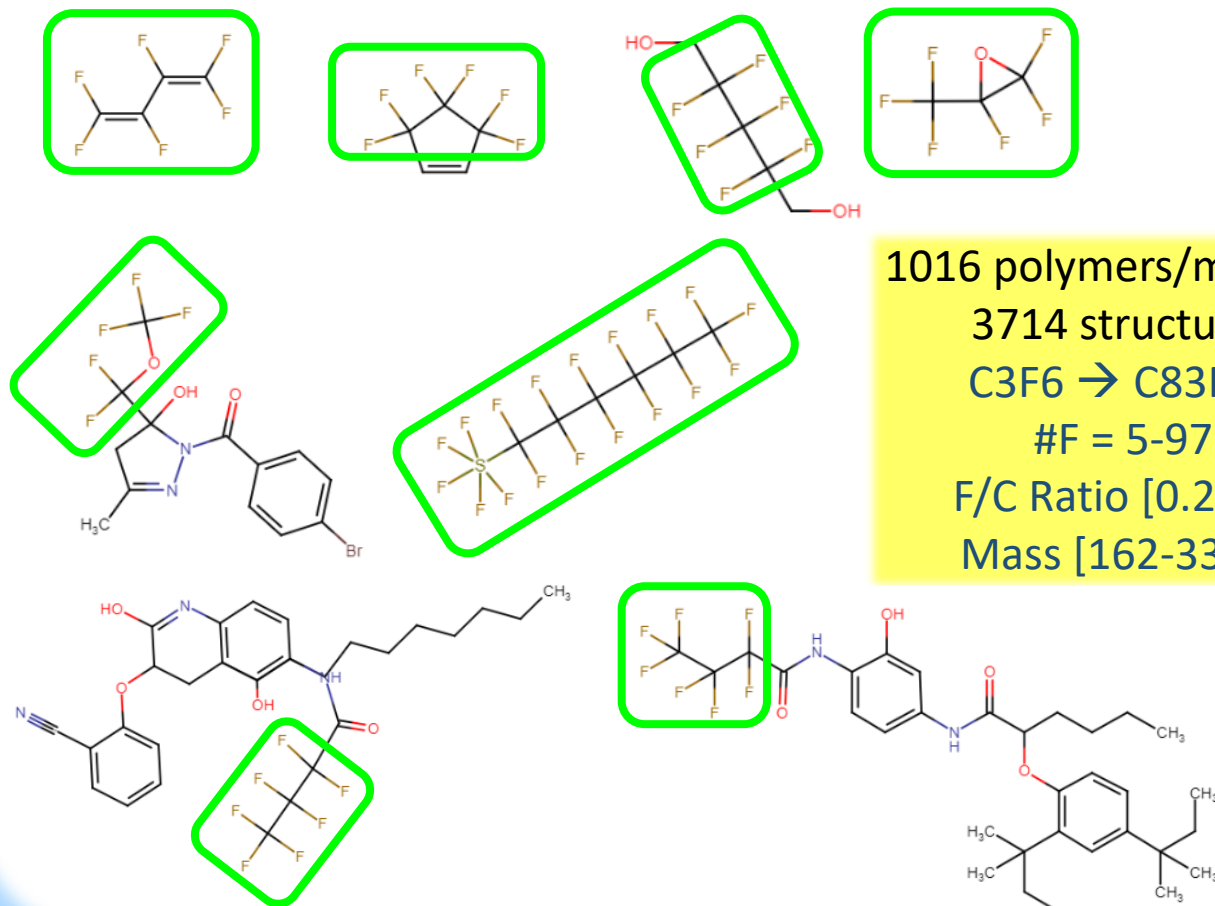
Expert-assigned OECD PFAS Categories, e.g.

- 4730 PFAS in list
- 173 expert-assigned categories under 8 general headings (bold)
- Broad “catch-all” terms (in red)
- Structural elements, but NOT structure-based
- Requires expert to assign new chemicals to categories

perfluoroalkyl carbonyl compounds	CnF2n+1_C(O)_R
perfluoroalkyl carbonyl halides	R = F/Cl/Br/I
perfluoroalkyl carboxylic acids (PFCAs), their salts and esters	R = OH, ONa, OCH3, etc.
other perfluoroalkyl carbonyl-based nonpolymers	to be refined
perfluoroalkyl carbonyl amides / amido ethanols and other alcohols	R = NH2, NH(OH), etc.
perfluoroalkyl carbonyl (meth)acrylate	R = R'_OC(O)CH=CH2
perfluoroalkyl carbonyl (meth)acrylate polymers	
1-H perfluoroalkyl carboxylic acids	H(CF2)nCOOH
perfluoroalkane sulfonyl compounds	CnF2n+1_S(O)(O)_R
perfluoroalkane sulfonyl halides	R = F/Cl/Br/I
perfluoroalkane sulfonic acids (PFASs), their salts and esters	R = OH, ONa, OCH3, etc.
perfluoroalkane sulfonyl-based nonpolymers	
per- and polyfluoroalkyl ether-based compounds	CnF2n+1_O_CmF2m+1_R
per- and polyfluoro alkyl ether sulfonic acids (PFESAs), their salts and esters, as well as derivatives	CnF2n+1_O_CmF2m+1_SO3H
fluorotelomer-related compounds	
perfluoroalkyl iodides (PFAIs)	CnF2n+1_I
n:2 fluorotelomer-based non-polymers	CnF2n+1_C2H4_R, to be refined

Definitions of PFAS

OECD Per & Polyfluorinated Substances (PFAS)



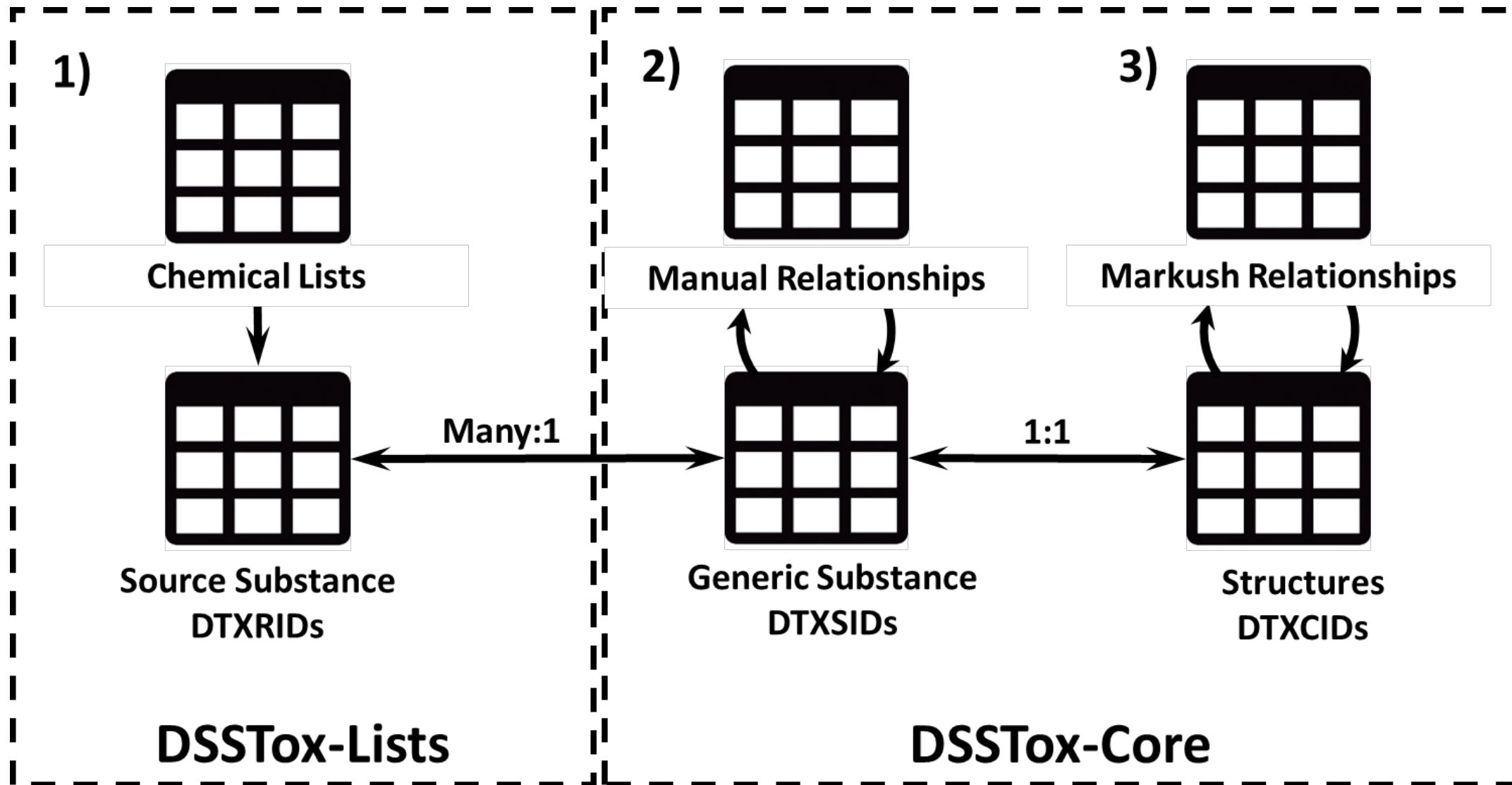
1016 polymers/mixtures
3714 structures
C3F6 → C83F97
#F = 5-97
F/C Ratio [0.22-3]
Mass [162-3378]

DSSTox Structure Filters

*Query DSSTox (>750K substances)
for procurements*

- no aromatic or cyclic moieties
- no metals or inorganics
- >3 Fluorines

Grouping and Linking Chemicals in DSSTox



DSSTox Chemical Lists

[View/Edit a Single Record](#)
[Structure Search](#)
[Browse/Curate Records](#)
[Export DSSTox](#)
[Chemotypes](#)
[Manage Chemical Lists](#)
[Manage Property Data](#)
[Add Deleted Casms](#)

Welcome aricha02

Welcome, Ann
Logout

Editing Listname: ECP_ADT

Duplicates: ✔

External Check Results

Description	Records
Valid Synonym matched; CAS-RN matched	121
Preferred Name matched; Other CAS-RN matched	1
Unique Synonym matched; CAS-RN matched	9
Structure connectivity matched; CAS-RN matched	3
Structure matched	4
Valid Synonym matched; CAS-RN matched; Unique Synonym matched other record	1
Mapped Identifier matched; CAS-RN matched	273
Preferred Name matched; CAS-RN matched; Valid Synonym matched other record	4
Preferred Name matched	3

Substance Mapping

(1 of 1) 1 25

	Source Casrn	Source Name	Hit Substance_ID	Hit Casrn	Hit Name	
▶	7786-30-3	Magnesium Chloride	DTXSID5034690	7786-30-3	Magnesium chloride	Other Hits
▶	1406-66-2	Tocopherols	DTXSID8021357	1406-66-2	Tocopherols	Other Hits
▶	108-95-2	phenol	DTXSID5021124	108-95-2	Phenol	Other Hits
▶	7733-02-0	zinc sulfate	DTXSID2040315	7733-02-0	Zinc sulfate	Other Hits

(1 of 1) 1 25

[Validate Selected List](#)
[Export Selected List](#)

Hits

	ssCAS-RN	ssName	Hit Desc	Hit Substance_ID	Hit Casrn	Hit Name
●	1406-66-2	Tocopherols	Preferred Name matched	DTXSID8021357	1406-66-2	Tocopherols
●	1406-66-2	Tocopherols	Unique Synonym matched	DTXSID9049031	54-28-4	(+)-gamma-Tocopherol

[Map hit](#)
[Cancel](#)

Hits

	ssCAS-RN	ssName	Hit Desc	Hit Substance_ID	Hit Casrn	Hit Name
●	7733-02-0	zinc sulfate	Preferred Name matched	DTXSID2040315	7733-02-0	Zinc sulfate
●	7733-02-0	zinc sulfate	Ambiguous Synonym matched	DTXSID0040175	7446-20-0	Zinc sulfate heptahydrate

[Map hit](#)
[Cancel](#)

PFAS Lists on the Dashboard

https://comptox.epa.gov/dashboard/chemical_lists/?search=PFAS

 EPA
United States
Environmental Protection
Agency

[Home](#) [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#)

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Search:

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Show entries

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	PFAS: EPA List of 75 Test Samples (Set 1)	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	PFAS: Registered DSSTox "category substances" representing Per- and Polyfluoroalkyl Substances (PFAS) categories	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.
EPAPFASINSOL	PFAS in EPA's Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS in EPA's ToxCast Chemical Inventory	2018-08-21	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL				
PFASKEMI				
PFASMASTER				
PFASOECD				
PFASTRIER				

[Download](#) [Columns](#)

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
C4PFAS	PFAS; C4-chain length chemicals	2018-11-19	291	List of C4F9 linear substructure containing chemicals
C6PFAS	PFAS; C6-chain length chemicals	2018-11-19	269	List of C6F13 containing chemicals
C8PFAS	PFAS; C8-chain length chemical	2018-11-19	248	List of C8F17 containing chemicals

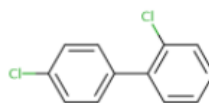
Showing 1 to 9 of 9 entries

Manually Defined Relationship Creation

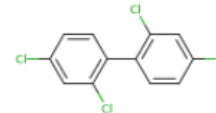
Successor Substances (209)

	CAS-RN	Relationship	
●	32774-16-6	is a Representative Isomer of this	STN
●	2051-60-7	is a Representative Isomer of this	Publ
●	2051-61-8	is a Representative Isomer of this	Publ
●	2051-62-9	is a Representative Isomer of this	Publ
●	13029-08-8	is a Representative Isomer of this	Publ
●	16605-91-7	is a Representative Isomer of this	Publ
●	25569-80-6	is a Representative Isomer of this	Publ
●	33284-50-3	is a Representative Isomer of this	Publ
●	34883-43-7	is a Representative Isomer of this	Publ
●	34883-39-1	is a Representative Isomer of this	Publ
●	33146-45-1	is a Representative Isomer of this	Publ
●	2050-67-1	is a Representative Isomer of this	Publ
●	2974-92-7	is a Representative Isomer of this	Publ
●	2974-90-5	is a Representative Isomer of this	Publ
●	34883-41-5	is a Representative Isomer of this	Publ
●	2050-68-2	is a Representative Isomer of this	Public ▼

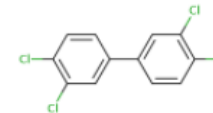
Download as: TSV Excel SDF



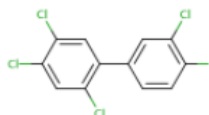
2,4-Dichlorobiphenyl
34883-43-7



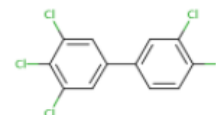
2,2',4,4'-Tetrachlorobiphenyl
2437-79-8



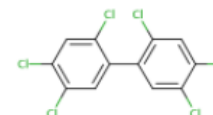
3,3',4,4'-Tetrachlorobiphenyl
32598-13-3



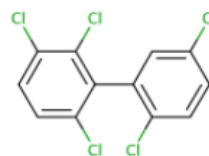
2,3',4,4',5-Pentachlorobiphenyl
31508-00-6



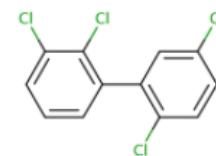
3,3',4,4',5-Pentachlorobiphenyl
57465-28-8



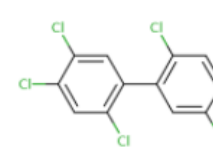
2,2',4,4',5,5'-Hexachlorobiphenyl
35055-27-1



2,2',3,5',6-Pentachlorobiphenyl
38379-99-6



2,2',3,5'-tetrachlorobiphenyl
41464-39-5



2,2,4,5,5'-Pentachlorobiphenyl
37680-73-2

Related Chemicals

Found 209 chemicals

Example Manual Linkages

← → ↻ ⓘ Not secure | comptox-prod.epa.gov/dashboard/dsstoxdb/results?search=68258-85-5#related-substances

Home Advanced Search Batch Search Lists ▾ Predictions Downloads

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Submit Comment

Search all data

1-Hexene, 3,3,4,4,5,5,6,6,6-nonafluoro-, polymer with ethene and 1,1,2,2-tetrafluoroethene

68258-85-5 | DTXSID50880596

Searched by CAS-RN.

DETAILS

RELATED SUBSTANCES

SYNONYMS

LINKS

BIOACTIVITY

► EXPOSURE

HAZARD

COMMENTS

PROPERTIES

► LITERATURE

4 chemicals

Select all

Download ▾

Send to Batch Search

Relationship ▾

⬆

DTXSID ✕

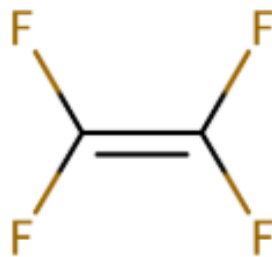
CASRN ✕

TOXCAST ✕ ▾

Hide chemicals that are: ▾

Filter by Name or CASRN

Monomer



[Tetrafluoroethylene](#)

DTXSID: DTXSID6021325

CASRN: 116-14-3

TOXCAST: -

Monomer



[Ethylene](#)

DTXSID: DTXSID1026378

CASRN: 74-85-1

TOXCAST: -

Monomer



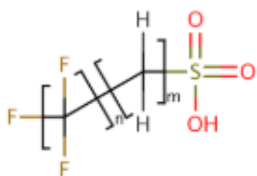
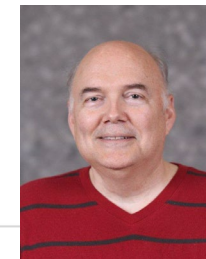
[1H,1H,2H-Perfluoro-1-hexene](#)

DTXSID: DTXSID6047575

CASRN: 19430-93-4

TOXCAST: -

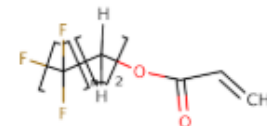
Markush Record Creation



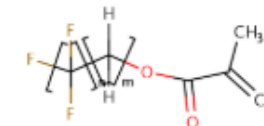
Fluorotelomer (linear) sulfonic acids
DTXSID: DTXSID50892558
CASRN: NOCAS_892558
TOXCAST: -



Fluorotelomer (linear) alcohols
DTXSID: DTXSID10893581
CASRN: NOCAS_893581
TOXCAST: -



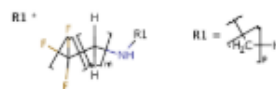
Fluorotelomer (linear) n:2 acrylates
DTXSID: DTXSID70893582
CASRN: NOCAS_893582
TOXCAST: -



Fluorotelomer (linear) n:2 methacrylates
DTXSID: DTXSID30893583
CASRN: NOCAS_893583
TOXCAST: -



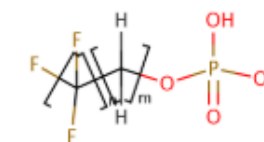
Fluorotelomer symmetric diols
DTXSID: DTXSID90893584
CASRN: NOCAS_893584
TOXCAST: -



Fluorotelomer (linear) amines (secondary)
DTXSID: DTXSID50893585
CASRN: NOCAS_893585
TOXCAST: -



Fluorotelomer (linear) carboxylic acids
DTXSID: DTXSID10893586
CASRN: NOCAS_893586
TOXCAST: -



Fluorotelomer (linear) phosphate esters ...
DTXSID: DTXSID30893588
CASRN: NOCAS_893588
TOXCAST: -

Notes:

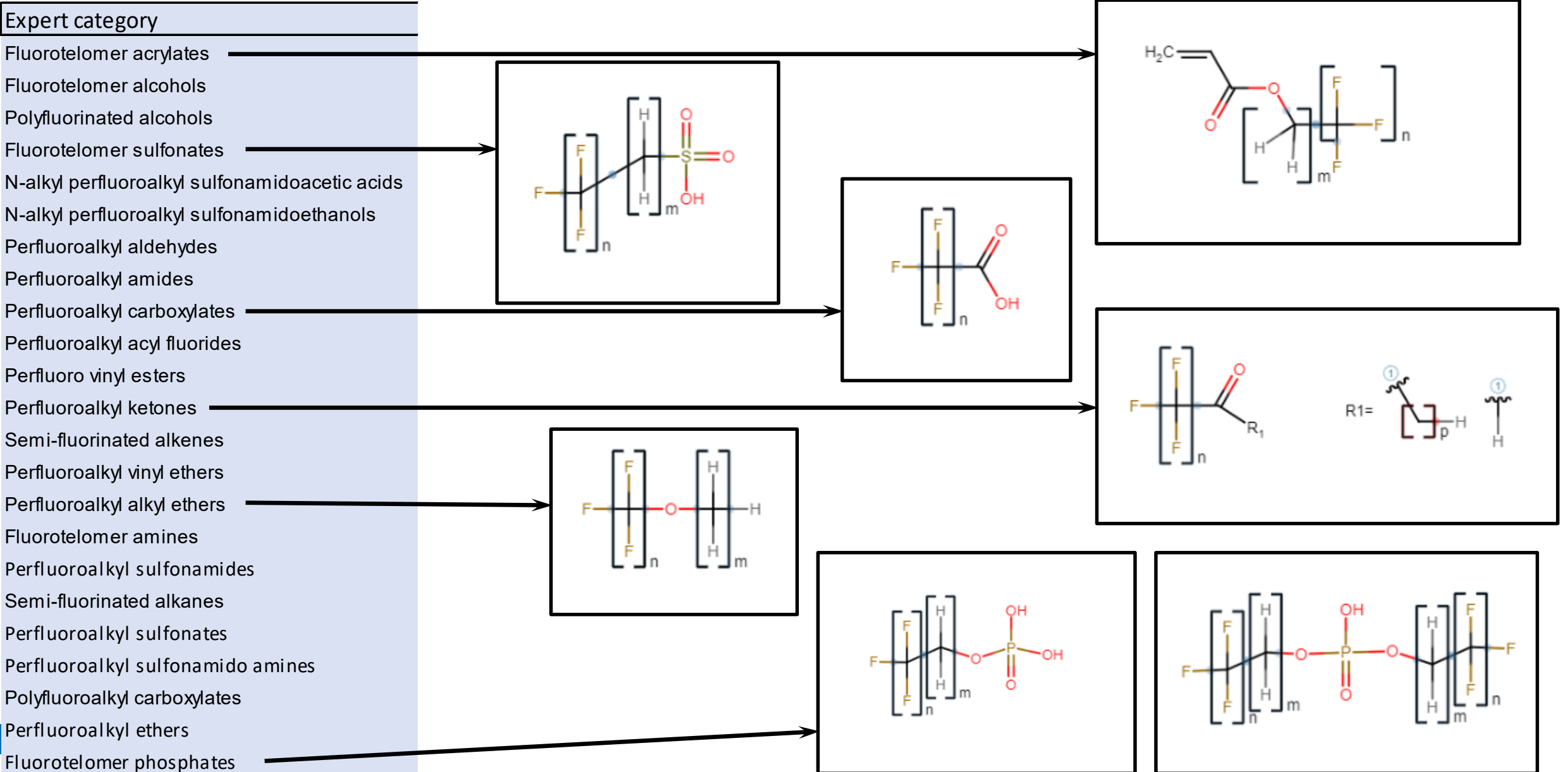
Name: C10-C16 alkyl alcohol

Chemical Form:

Organic Form:

Organic

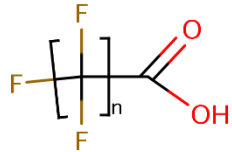
Translating Expert Categories to Markush



PFAS Markush Child Linking

Perfluoroalkyl (linear) carboxylic acids

DTXSID00893893

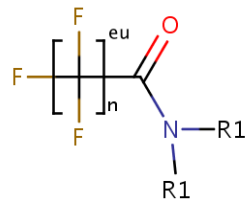
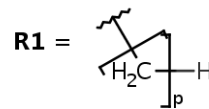


Markush_Child	DTXSID	Substance_Name	CASRN
DTXSID1037303	DTXSID1037303	Perfluoroheptanoic acid	375-85-9
DTXSID3031860	DTXSID3031860	Perfluorodecanoic acid	335-76-2
DTXSID3031862	DTXSID3031862	Perfluorohexanoic acid	307-24-4
DTXSID4059916	DTXSID4059916	Perfluorobutanoic acid	375-22-4
DTXSID6062599	DTXSID6062599	Perfluoropentanoic acid	2706-90-3
DTXSID8031863	DTXSID8031863	Perfluorononanoic acid	375-95-1
DTXSID8031865	DTXSID8031865	Perfluorooctanoic acid	335-67-1
DTXSID8047553	DTXSID8047553	Perfluoroundecanoic acid	2058-94-8
DTXSID8059970	DTXSID8059970	Perfluoropropanoic acid	422-64-0
DTXSID9041578	DTXSID9041578	Trifluoroacetic acid	76-05-1

Perfluoroalkyl (linear) amides (tertiary)

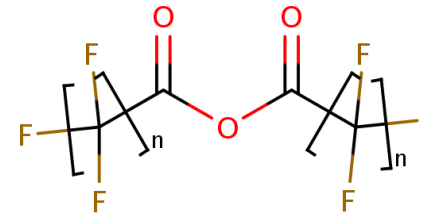
DTXSID30893886

R1 *

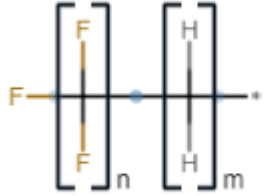


Perfluoroalkyl symmetric anhydrides

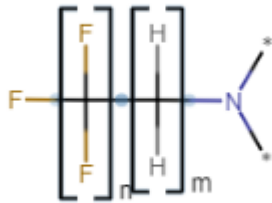
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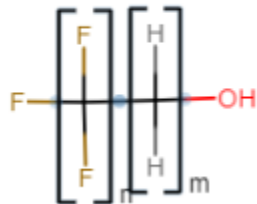
Nested Categories



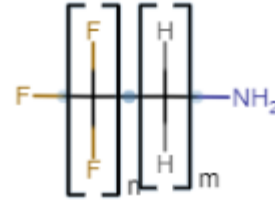
Fluorotelomers (linear)



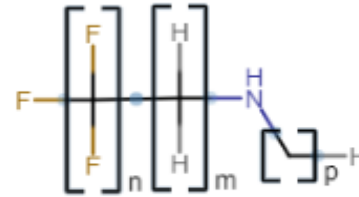
Fluorotelomer (linear) amines



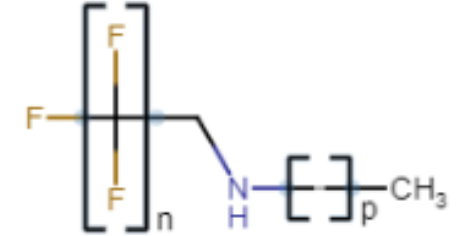
Fluorotelomer (linear) alcohols



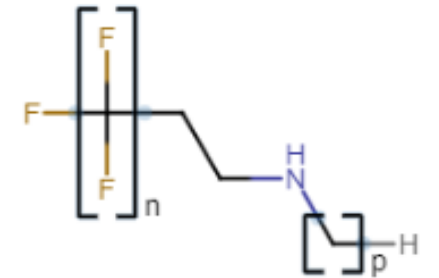
Fluorotelomer (linear)
amines (primary)



Fluorotelomer (linear)
amines (secondary)



Fluorotelomer (linear) n:1
amines (secondary)

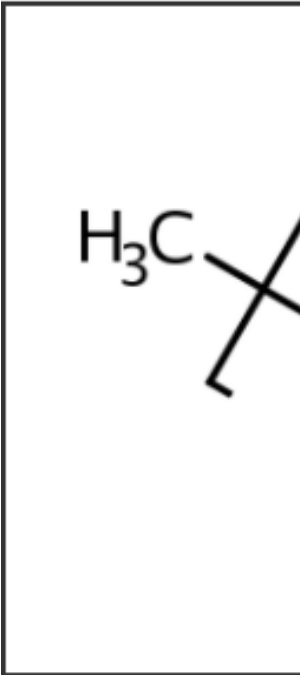


Fluorotelomer (linear) n:2
amines (secondary)

Difficult Substances/Categories

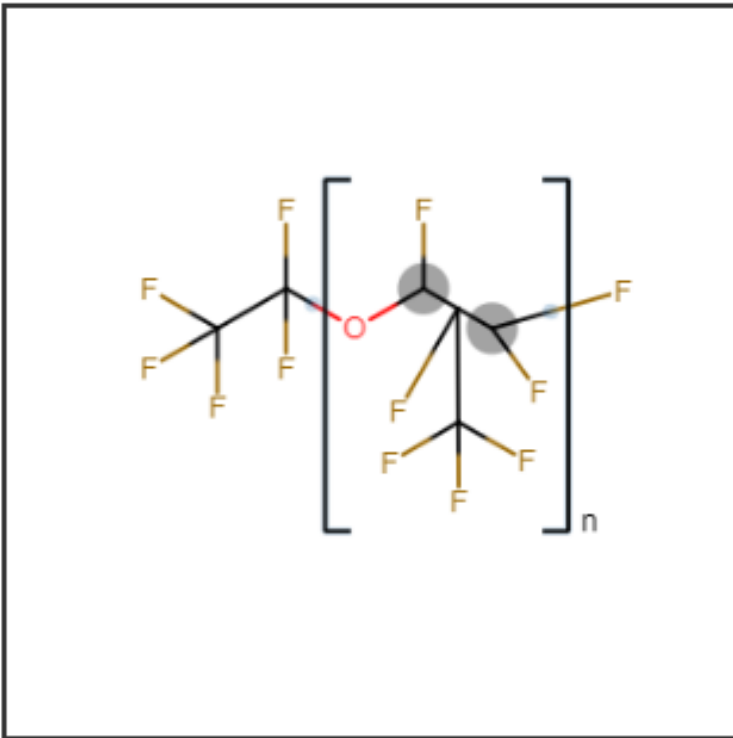
C10-16 A **Krytox 143**
67762-41-8 | 60164-51-4 | DTXSID70880513

© Searched by Approved Name: Found 1 result for 'krytox 143' 'C10-16 Alcohols'.



Krytox 143

© Searched by Approved Name: Found 1 result for 'krytox 143'.



Krytox oils

NOCAS_892470 | DTXSID30892470

© Searched by Approved Name: Found 1 result for 'krytox oils'.

Krytox™ Performance Lubricants Can Provide The Solutions You Need.

Industry	Krytox™ Product	Temperature Range	Optimum Use Range	ISO Viscosity	Properties
Chemical - including reactive gases (F, O2, Cl2, HF)					
Valves	GPL 204	-60°F to +355°F	-30°F to +300°F	68	Safe in all reactive gases including oxygen, chlorine, fluorine, and HF. Won't react with acids, bases or other harsh chemicals. Won't oxidize or coke up.
Valves	GPL 206	-33°F to +500°F	+40°F to +500°F	220	Safe in all reactive gases including oxygen, chlorine, fluorine, and HF. Won't react with acids, bases or other harsh chemicals. Won't oxidize or coke up.
Bearings	GPL 224	-60°F to +355°F	-30°F to +300°F	68	Safe for use with common acids, bases, solvents

A pie chart illustrating the distribution of data categories. The chart is divided into three segments: a large gray segment representing 'At least 1 Category' at 44%, an orange segment representing 'Uncategorized' at 35%, and a blue segment representing 'Unstructured' at 21%.

Category	Percentage
At least 1 Category	44%
Uncategorized	35%
Unstructured	21%



Conclusions

- Expert classification of PFAS is difficult to maintain
- Defining structure based classes for PFAS is achievable
- Structural classes provide unambiguous, reproducible assignments of substances to class
- Extension of available classes is necessary to achieve our desired coverage
- Several issues remain for addressing
 - Branched perfluorinated alkyl chains
 - Partially fluorinated chains
 - Unique functionalizations

Acknowledgements



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EPA NCCT Curation

Inthirany Thillainadarajah

Sakuntala Sivasupramaniam

Questions?