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TOWARD A NEW COMPREHENSIVE GLOBAL DATABASE OF PER- AND POLYFLUOROALKYL SUBSTANCES (PFASs):

SUMMARY REPORT ON UPDATING THE OECD 2007 LIST OF PER- AND POLYFLUOROALKYL SUBSTANCES (PFASs)

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IOMC

INTER-ORGANIZATION PROGRAMME FOR THE SOUND MANAGEMENT OF CHEMICALS

A cooperative agreement among **FAO, ILO, UNDP, UNEP, UNIDO, UNITAR, WHO, World Bank and OECD**

Environment Directorate
ORGANISATION FOR ECONOMIC COOPERATION AND DEVELOPMENT
Paris 2018

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OECD Environment Directorate,
Environment, Health and Safety Division
2 rue André-Pascal
75775 Paris Cedex 16
France

Fax: (33-1) 44 30 61 80

E-mail: ehscont@oecd.org

Executive summary

This study represents recent efforts by the OECD/UNEP Global PFC Group between January 2017 and February 2018 in updating the OECD “Lists of PFOS, PFAS, PFOA, PFCA, Related Compounds and Chemicals That May Degrade to PFCA”, which was last updated in 2007, to provide a comprehensive list of per- and polyfluoroalkyl substances (PFASs) that may have been on the global market. In particular, it focuses on those PFASs, including perfluorocarbons, that contain a perfluoroalkyl moiety with three or more carbons (i.e. $–C_nF_{2n}–$, $n \geq 3$) or a perfluoroalkylether moiety with two or more carbons (i.e. $–C_nF_{2n}OC_mF_{2m}–$, n and $m \geq 1$). The study utilises publicly accessible information sources, including (1) two lists of PFASs (and other highly fluorinated substances) by national or international regulatory bodies, (2) nine public national/regional inventories of chemicals, (3) two public national/regional inventories of chemicals in specific uses, (4) four public national/regional inventories of chemicals subject to specific regulations, and (5) one scientific database.

In total, 4730 PFAS-related CAS numbers have been identified and manually categorised in this study, including several new groups of PFASs that fulfil the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs. The identified PFASs are diverse in terms of structure and other categorisation elements. In addition, the number and type of identified PFASs vary considerably across sources. Several limitations, gaps and challenges were identified, including (1) information gaps within the information sources searched, (2) gaps associated with information sources that were included, (3) limitations associated with the format of the study (as a snap shot of the situation when the study was done, while information may continuously evolve), and (4) challenges associated with the vague description of some PFASs identified, the currently used terminology of PFASs, and the current state of knowledge about certain aspects such as the degradability of many PFASs. As such, it should be noted that while this list is comprehensive, it is not an exhaustive list.

Based on lessons learned from identified limitations, gaps and challenges, opportunities for future improvement have also been identified. In particular, there is a need for an intensified dialogue and cooperative actions across regions and sectors, designing and fostering new types of public-private partnerships to facilitate effective and efficient information exchange between public and private sectors within the field of PFASs. Additional recommendations include (1) expansion of the current terminology of PFASs to reflect all substances and resolve issues identified (e.g., no clear cut-off values between some substance groups), (2) development of a web-based knowledge base to share up-to-date information on PFASs across sectors and regions, and (3) continuous support to address critical knowledge gaps including the degradability of many non-studied PFASs.

1. Background, Aim and Scope

The OECD/UNEP Global PFC[1] Group was established to respond to the Resolution II/5 adopted at the second session of the UN International Conference on Chemicals Management (ICCM 2) in 2009, which calls upon intergovernmental organizations, governments and other stakeholders to "consider the development, facilitation and promotion in an open, transparent and inclusive manner of national and international stewardship programmes and regulatory approaches to reduce emissions and the content of relevant perfluorinated chemicals of concern in products and to work toward global elimination, where appropriate and technically feasible". Further work on this resolution was reaffirmed in Resolution III/3 adopted at ICCM 3 noting that a significant need remains for additional work to support implementation of Resolution II/5. This work is conducted within the framework of the OECD/ UNEP Global PFC Group.

This report summarizes recent efforts by the OECD/UNEP Global PFC Group between January 2017 and February 2018 in updating the OECD "Lists of PFOS, PFAS[2], PFOA, PFCA, Related Compounds and Chemicals That May Degrade to PFCA" that was last updated in 2007 (hereafter referred to as "*OECD 2007 List*") to provide a comprehensive list of per- and polyfluoroalkyl substances (PFASs) that may have been present on the global market. In particular, this report highlights (1) the methodology that was used to update the OECD 2007 List (Section 2), (2) the major findings with respect to the total numbers and types of PFASs identified (Section 3), and (3) the limitations, gaps and challenges identified in the development of the new list, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices (Section 4).

According to the currently most accepted terminology (Buck et al., 2011), per- and polyfluoroalkyl substances (PFASs) are a family of anthropogenic chemicals that "contain one or more C atoms on which all the H substituents (present in the nonfluorinated analogues from which they are notionally derived) have been replaced by F atoms, in such a manner that they contain the perfluoroalkyl moiety (C_nF_{2n+1}–)." In the past, PFASs were often referred to as "PFCs" (per- and polyfluorinated chemicals), but this term "PFCs" can also be understood as perfluorocarbons (e.g., under the Kyoto Protocol; UNFCCC, 2014), which contain only carbon and fluorine. In this study, the focus is on a much broader range of substances beyond only perfluorocarbons. To avoid confusion, the term "PFASs" and associated terminology as recommended by Buck et al. (2011) has been used instead of "PFCs".

Due to the high chemical and thermal stability and the water- and oil-repellency of the perfluoroalkyl moiety, many PFASs are effective surfactants or surface protectors, and

1 PFCs refer here to per- and poly-fluorinated chemicals, and not to perfluorocarbons.
2 Please note that the acronym "PFAS" in the "OECD 2007 List" referred to "perfluoroalkyl sulfonate". This terminology is no longer commonly used and is replaced by the acronym "PFSA" as recommended in Buck et al. (2011).

have therefore been widely produced and used in numerous commercial and consumer applications since the late 1940s (Banks et al., 1994; Kissa, 2001; Buck et al., 2011). Since the late 1990s and early 2000s, numerous studies have been conducted to understand and assess PFASs with a particular focus on so-called “long-chain” perfluoroalkyl acids (PFAAs)[3] and their precursors. Consequently, long-chain PFAAs have been identified as highly persistent (P), bioaccumulative (B), and toxic (T) (see scientific evidence reviewed by OECD, 2013). In addition, they have been detected to be ubiquitously distributed in the environment (e.g., Gawor et al., 2014; Rankin et al., 2016; Kaboré et al., 2017), biota (e.g., Giesy and Kannan, 2002; Houde et al., 2011; Ahrens and Bundschuh, 2014), and humans (e.g., Vestergren and Cousins, 2009), including in remote regions far from sources (e.g., Young et al., 2007; Butt et al., 2010). Hence, long-chain PFAAs have been recognised as global contaminants of high concern. Driven by concerns about undesired adverse effects on humans and the environment, regulatory measures, industry voluntary initiatives and risk management programmes (e.g., rules for use and voluntary controls) to restrict/eliminate releases of long-chain PFAAs and precursors have been initiated since 2000, particularly in many developed countries (OECD, 2015). In response to these actions, an industrial transition has taken place to replace long-chain PFAAs and their precursors with alternative chemicals, many of which are still PFASs (for examples, see Buck et al., 2011, Wang et al., 2013, 2016 and references therein). It is noted that there is an increasing interest by regulators[4] and scientists across the globe to assess legacy and novel PFASs other than long-chain PFASs.

However, in contrast to the continuous industrial development of diverse PFASs over the past decades, progress in the public domain in identifying and understanding production, use, releases and environmental presence of the various PFASs on the global market has been limited due to the complexity of the issue, data scarcity and fragmentation, and data confidentiality. In brief, two distinct but complementary approaches have been developed: Some scientists use a “bottom-up” approach that systematically identifies and studies the life-cycle of some PFASs based on public literature and surveys, whereas other scientists use a “top-down” approach that empirically measures, identifies and quantifies known and unknown PFASs in environmental media, biota, humans and other matrices (e.g., products, drinking water) using chemical analysis (e.g., Place and Field, 2012; Backe et al., 2013; Liu et al., 2015, Strynar et al., 2015; Newton et al., 2017). This study focuses on the “bottom-up” approach based on publicly available information, whereas readers may find more details on the “top-down” approach to empirically measuring and identifying unknown PFASs in Ruan and Jiang (2017) and references therein.

On the international level, several milestones have been reached in using “bottom-up” approaches to identifying PFASs, including the three OECD surveys on production and use of PFASs (OECD, 2005, 2006, 2011) and the OECD 2007 List (OECD, 2007). In particular, the OECD 2007 List of PFASs identified over 950 Chemical Abstract Service

[3] In this study, PFAAs also cover per- and polyfluoroalkylether acids, i.e. those acids with the acidic functional group(s) directly connecting to a perfluoroalkylether chain ($–C_nF_{2n}OC_mF_{2m}–$), or in some cases a polyfluoroalkylether chain (one or multiple fluorine atoms in the perfluoroalkylether chain may be substituted with atoms other than fluorine) (for examples, see Figure 4 below). Based on the commonly accepted OECD definition, long-chain PFAAs refer to perfluoroalkyl carboxylic acids (PFCAs) with $\geq$ 7 perfluorinated carbons and perfluoroalkane sulfonic acids (PFSAs) with $\geq$ 6 perfluorinated carbons.

[4] For example, multiple PFASs other than long-chain PFASs are listed in ECHA’s Public Activities Coordination Tool (PACT) to be assessed (https://echa.europa.eu/pact).

Registry Numbers (hereafter referred to as "CAS Nos." or "CAS numbers"). Recently, the Swedish Chemicals Agency (KEMI) systematically investigated national/regional chemical inventories and other public sources, identified PFASs and other highly fluorinated substances with over 2000 CAS numbers, and indicated that many more PFASs may be present on the global market with unknown CAS numbers (KEMI, 2015). The present study builds on and expands these major efforts in identifying PFASs that may have been on the market using a carefully designed methodology (see Section 2 below). The resulting list of PFASs is briefly summarized in Section 3 and provided in the accompanying Excel spreadsheets, which may be used as a resource for scientific and regulatory activities. It should be noted that this list is not an exhaustive list of all PFASs that have been on the market and/or may be detected in the environment; limitations, gaps and challenges within and beyond the current lists, and opportunities to address them, are summarized in Section 4.

2. Methodology

PFASs have been manufactured typically by one of the following three techniques: electrochemical fluorination, telomerization, or oligomerization; all of the three methods result in complex mixtures containing intended substances, unreacted raw material residuals, and/or byproducts, which may in some cases be purified through additional processing (Banks et al., 1994; Kissa, 2001; Buck et al., 2011). In addition, the polyfluorinated PFASs, i.e. PFASs in which for at least one, but not all, carbon atoms all hydrogen atoms have been replaced by fluorine atoms (Buck et al., 2011), may degrade during their life-cycle both within the products that contain them and in the environment to form various degradation intermediates and stable PFAAs (e.g., Young and Mabury, 2007; Liu and Avendaño, 2013; Butt et al., 2014; Wang et al., 2014). Therefore, PFASs that are on the global market and in the environment consist of intentionally produced substances and unintentionally generated substances (i.e. unreacted residuals, by-products, and degradation intermediates). The original intention of this study was to focus on identifying PFASs that have been produced for commercial uses (as registered under many national/regional chemical inventories). However, during the development of the list, it was noted that some sources do not have such a clear indication (for details, see Table 2 below). Therefore, a clear labelling of PFASs with respect to their origins (e.g., produced for commercial uses, produced for research purposes, unintentionally generated) cannot be made in this study; this is discussed further in Section 4 below.

It should also be noted that this study focuses on those PFASs that contain a perfluoroalkyl moiety with three or more carbons (i.e. $–C_nF_{2n}–$, $n \geq 3$)[5] or a perfluoroalkylether moiety with two or more carbons (i.e. $–C_nF_{2n}OC_mF_{2m}–$, n and $m \geq 1$). Some PFASs with shorter-chain perfluoroalkyl(ether) moieties have also been present in products as intended ingredients (e.g., lithium bis(trifluoromethylsulfonyl)imide (CAS number 90076-65-6) as electrolytes in the manufacture of batteries for electric vehicles or stationary applications; ECHA, 2018) or as impurities (e.g., Barzen-Hanson and Field, 2015), and/or in the environment (e.g., Barzen-Hanson and Field, 2015); however, they are not within the scope of this study.

The overall methodology is illustrated in Figure 1, and details on information sources, PFAS identification, and major information processing steps are summarized in the subsections below.

[5] Please note that in this study, the definition of a perfluoroalkyl moiety has been expanded from "(C_nF_{2n+1}–)" in Buck et al. (2011) to "$–C_nF_{2n}–$" so as to include PFASs with both ends of the perfluoroalkyl moiety connected to a functional group (e.g., perfluoroalkyl dicarboxylic acids, $HOOC–C_nF_{2n}–COOH$), including cyclic analogues of linear PFASs (e.g., $C_6F_{11}SO_3K$, CAS No. 3107-18-4).

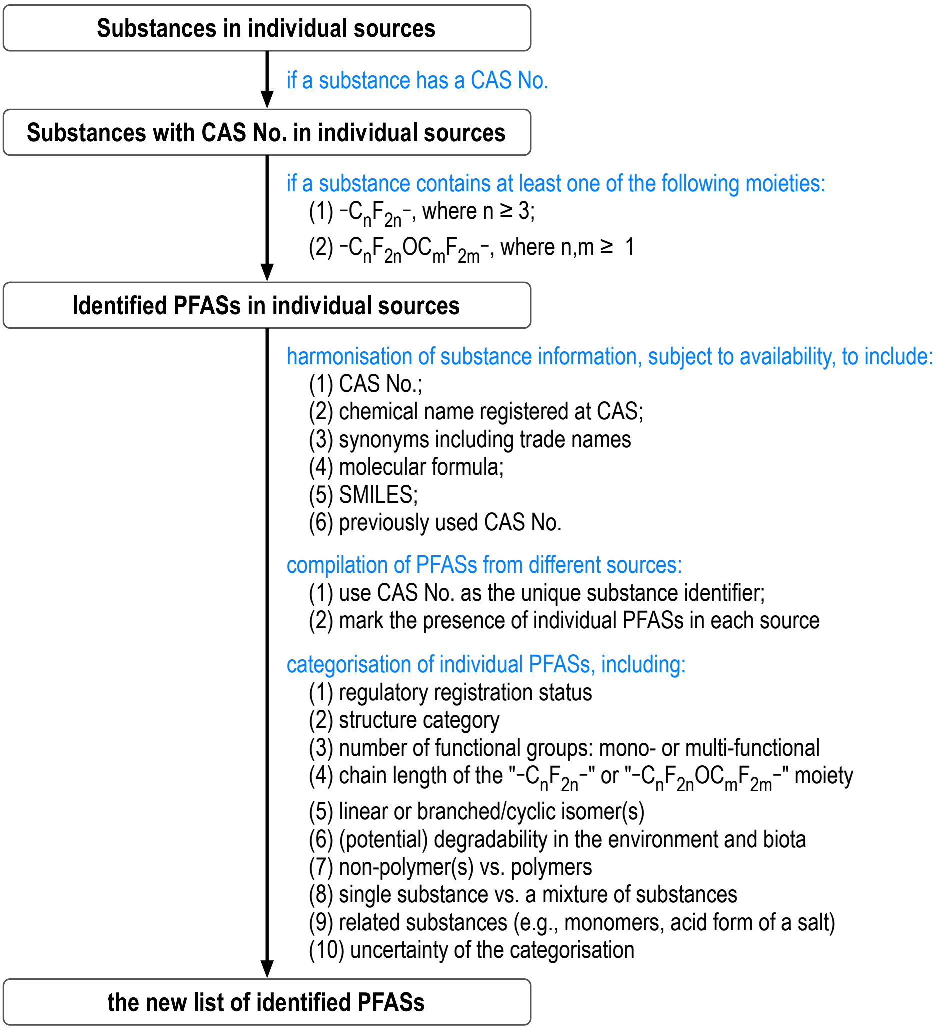

Figure 1. Schematic overview of the methodology used in this study

2.1. Information Sources and PFAS Identification

This study utilises publicly accessible information sources, consisting of the following categories: (1) lists of PFASs (and other highly fluorinated substances), (2) national/regional chemical inventories, (3) national/regional inventories of chemicals in specific uses, (4) national/regional inventories of chemicals subject to specific regulations, and (5) a scientific database. Details on information sources and PFAS identification (based on the common definition by Buck et al. (2011) and the chain length criteria as set above) are listed in Table 1.

Table 1. Overview of information sources used in this study

	Details	PFAS Identification
Existing Lists of PFASs (and Other Highly Fluorinated Substances)		
OECD 2007 List	Lists of PFOS, PFAS, PFOA, PFCA, Related Compounds and Chemicals That May Degrade to PFCA (http://oe.cd/2ah); Includes substances from the responses to the OECD surveys, listed on the inventories of OECD member countries (with a perfluorinated chain of four or more carbons), reviewed by international agencies or regulatory bodies, and identified from published literatures; Does not contain chemical substances listed in the confidential sections of the inventories, provisional PMN list of TSCA and inventories of non-OECD countries, chemical intermediates and R&D chemicals, chlorofluorocarbons (CFCs), hydrofluorocarbons (HFCs), hydrochlorofluorocarbons (HCFCs), perfluorocarbons (PFCs) and polymers with fluorinated backbone structures (e.g., fluoropolymers) Entries considered in the PFAS identification step: 993	Taken as they are in the List after filtering out substances without CAS numbers
KEMI 2015 Report	Occurrence and use of highly fluorinated substances and alternatives (https://www.kemi.se/global/rapporter/2015/report-7-15-occurrence-and-use-of-highly-fluorinated-substances-and-alternatives.pdf); Based on information from databases that the Swedish Chemicals Agency has access to (e.g., the Swedish Products Register and the ECHA database of registered substances), information in scientific articles, various reports on, and lists of, industrial chemicals from other countries (mainly North America and Asia), and information from industry; Includes both PFASs and other highly fluorinated substances; Entries considered in the PFAS identification step: 2542	Taken as they are in the Report after filtering out substances without a CAS number and substances that do not contain $-C_nF_{2n}-$ ($n \geq 3$) or $-C_nF_{2n}OC_mF_{2m}-$ (n and $m \geq 1$).
National/Regional Chemical Inventories		
AICS	Australian Inventory of Chemical Substances (https://www.nicnas.gov.au/chemical-inventory-AICS); A database of chemicals available for industrial use in Australia; Regularly updated; a list of substances containing the term "fluoro" in the chemical name was kindly provided by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) on October 3, 2017; Entries considered in the PFAS identification step: 903	Taken as they are in the respective sources after filtering out substances without a CAS number and substances that do not contain $-C_nF_{2n}-$ ($n \geq 3$) or $-C_nF_{2n}OC_mF_{2m}-$ (n and $m \geq 1$).
Canadian DSL	Canadian Domestic Substances List (https://pollution-waste.canada.ca/substances-search/Substance?lang=en); Includes Substances manufactured in, imported into or used in Canada on a commercial scale; Regularly updated, and last accessed on October 13, 2017 for this study; Entries considered in the PFAS identification step: 519	
Chinese IECSC	Inventory of Existing Chemical Substances Produced or Imported in China (https://chemicalwatch.com/asiahub/15187/existing-chemical-substances-inventory-2016-revisionchina/); Last updated in March 2016 (used in this study); Entries considered in the PFAS identification step: 621	
ECHA Pre-registered Substances	Pre-registration intentions submitted by companies planning to register phase-in (existing) substances to the European Chemicals Agency (ECHA) (https://echa.europa.eu/information-on-chemicals/pre-registered-substances); This list reflects only an intention to register, not actual registration of the substances; Regularly updated, and last accessed on October 3, 2017 for this study; Entries considered in the PFAS identification step: 5801	Taken as they are in the respective sources after filtering out substances without CAS numbers and substances that do not contain $-C_nF_{2n}-$ ($n \geq 3$) or $-C_nF_{2n}OC_mF_{2m}-$ (n and $m \geq 1$).

ECHA Registered Substances	Substances that are registered under the EU Chemicals Regulation, REACH (https://echa.europa.eu/information-on-chemicals/registered-substances); Regularly updated, and last accessed on October 3, 2017 for this study; Entries considered in the PFAS identification step: 1014	
Japanese ENCS	List of Existing and New Chemical Substances (http://www.nite.go.jp/en/chem/chrip/chrip_search/systemTop); Regularly updated, and last accessed on October 3, 2017 for this study; Entries considered in the PFAS identification step: 1589	
SPIN	Substances in Preparations in Nordic Countries (SPIN) database (http://spin2000.net); Includes quantities, industries in which it is used, and the function of chemicals that are used in the Nordic countries based on data from the Product Registries of Norway, Sweden, Denmark and Finland; Regularly updated, and last accessed on October 3, 2017 for this study; Entries considered in the PFAS identification step: 733	
US EPA TSCA Inventory	A list of each chemical substance that is manufactured or processed, including imports, in the United States for uses under TSCA (https://www.epa.gov/tsca-inventory/how-access-tsca-inventory); Regularly updated, and last updated in June 2017 (used in this study); Entries considered in the PFAS identification step: 2094	
US EPA CDR (formerly IUR) Inventories	US EPA Chemical Data Reporting (formerly Inventory Update Rule) Inventories (https://www.epa.gov/chemical-data-reporting); Basic exposure-related information on the types, quantities and uses of chemical substances produced domestically and imported into the United States when production volumes for the chemical are 25,000 pounds or greater at any single site for a specific reporting year (a reduced reporting threshold − 2,500 pounds − now applies to chemical substances subject to certain TSCA actions); Data collected in 1986, 1990, 1994, 1998, 2002, 2006, 2012 and 2016; Entries considered in the PFAS identification step: 1441	
National/regional Inventories of Chemicals in Specific Uses		
US FDA FCS	US FDA Inventory of Effective Food Contact Substance Notification (https://www.accessdata.fda.gov/scripts/fdcc/?set=FCN); effective premarket notifications for food contact substances that have been demonstrated to be safe for their intended use in the United States; Regularly updated, and last accessed on October 3, 2017 for this study; Entries considered in the PFAS identification step: 43	Taken as they are in the respective sources after filtering out substances without CAS numbers and substances that do not contain $-C_nF_{2n}-$ (n ≥ 3) or $-C_nF_{2n}OC_mF_{2m}-$ (n and m ≥ 1).
EU CosIng	European Commission database for information on cosmetic substances and ingredients (http://ec.europa.eu/growth/tools-databases/cosing/); Regularly updated, and last accessed on October 3, 2017 for this study; Entries considered in the PFAS identification step: 107	
National/regional Inventories of Chemicals Subject to Specific Regulations		
Canada PCTSR 2012	Non-exhaustive list of chemical abstracts service registry numbers for substances subject to the Prohibition Of Certain Toxic Substances Regulations, 2012; The list was kindly provided by the Government of Canada in November 2016; Entries considered in the PFAS identification step: 167	Taken as they are in the respective sources
Japan Examples for the Stockholm Convention	Examples of PFOA and related substances based on the discussion of POPRC12 under the Stockholm Convention (http://www.meti.go.jp/policy/chemical_management/int/2_besshi2.pdf); Prepared for domestic survey by the Ministry of Economy, Trade and Industry, Japan;	

	Entries considered in the PFAS identification step: 49	
US EPA TSCA 12b	Chemicals subject to TSCA Section 12(b) Export Notification Requirements (https://www.epa.gov/tsca-import-export-requirements/chemicals-subject-tsca-section-12b-export-notification-requirements); Entries considered in the PFAS identification step: 758	
Australia IMAP Tier 2	Substances that have been assessed at Tier II (individual chemical evaluation) under the Inventory Multi-tiered Assessment and Prioritisation (IMAP) by the NICNAS for the human health and environmental impacts of unassessed industrial chemicals listed on the Australian Inventory of Chemical Substances (AICS) (https://www.nicnas.gov.au/chemical-information/imap-assessments/imap-assessments); The list was kindly provided by the Government of Australia in December 2016 Entries considered in the PFAS identification step: 258	
Scientific Database		
SciFinder Database	A scientific search engine and database that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences, maintained by the Chemical Abstracts Service, a division of the American Chemical Society (https://scifinder.cas.org); This study used C_2F_5−, C_3F_7−, CF_3O−, C_2F_5O−, C_3F_7O−, iso-C_3F_7−, and iso-C_3F_7O− as sub-structures for substance search made on 9th February, 2017, and selected substances that have any references (e.g., peer-reviewed articles, patents, etc.) and commercial sources listed in the SciFinder for further PFAS identification; Entries considered in the PFAS identification step: 9290	Taken as they are in the respective sources after filtering out substances that do not contain $-C_nF_{2n}-$ ($n \geq 3$) or $-C_nF_{2n}OC_mF_{2m}-$ (n and $m \geq 1$).

2.2. Major Information Processing Steps

After PFASs in individual sources were identified and their associated information was collected, the information went through several major processing steps as outlined below.

Harmonisation of Substance Information. As a given PFAS may have different information, including different chemical names, in different sources, an extra step of harmonisation of substance information before compilation took place: Information related to a given CAS number (including chemical name registered at the CAS, synonyms including certain trade names, molecular formula, and previously used CAS numbers, subject to availability) was extracted from the SciFinder database, and used to replace and expand the information contained in individual sources. In particular, the CAS numbers in individual sources were revised to ensure that they are all up-to-date and consistent.

Information Compilation. After harmonisation, CAS numbers were used as the unique identifier to compile PFASs from individual sources into one list. The presence of PFASs in multiple sources was marked.

PFAS Categorisation. To obtain an overview of identified PFASs, and to ease the readers' search for specific individual, or groups of, PFASs, all substances were additionally categorised using the elements outlined in Table 2.

Table 2. Overview of elements considered in the PFAS categorisation

Elements	Details
Regulatory registration status (based on information in the SciFinder Database)	SciFinder contains a "Regulatory Information" section, which is an electronic collection of chemicals that are regulated in key markets across the globe, including information from many of the inventories that were considered in this study, but also beyond (for the list of sources used by SciFinder, see: http://support.cas.org/content/regulated-chemicals). 0 = there is no regulatory information found in the SciFinder database; 1 = there is regulatory information found in the SciFinder database
Structure category	Based on Buck et al. (2011) with an expansion developed in this study to accommodate PFASs that have not been detailed in Buck et al. (2011); Developed a two-level categorization system (for details, see in the accompanying Excel Spreadsheets): 1st level is a primary categorization (e.g., fluorotelomer-based substance) and 2nd level is a more refined categorization (e.g., fluorotelomer alcohols (FTOHs))
Number of functional groups	0 = the substance contains multiple functional groups; 1 = the substance contains one functional group
Chain length of perfluroalkyl (or perfluoroalkylether) moieties	3, 4, 5, or longer (elements other than carbon were highlighted, e.g., "O" for an ether linkage, "R" for a ring structure, and "DB" for a double bond)
Isomer	0 = branched or cyclic isomer; 1 = linear isomer
(Potential) degradability in the environment and biota	0 = the substance would likely not degrade into stable perfluoroalkyl acids (PFAAs) in the environment and biota (general assumption in this study: perfluorinated substances without reactive functional group(s), e.g., alkanes, PFCAs and PFSAs); 1 = the substance would likely degrade into stable PFAAs in the environment and biota (general assumption in this study: polyfluorinated substances + perfluorinated substances with one or more reactive functional groups (e.g., double bonds, aldehyde, triple bonds, etc.) + PFPiAs); The general assumption was made based on studies as reviewed in Young and Mabury (2007), Liu and Avendaño (2013), Butt et al. (2014), Wang et al. (2014) and others; Please note that the time scale of such degradation is not taken into consideration, i.e., it may take still years to decades or longer for a substance to degrade into stable PFAAs. In particular, side-chain fluorinated polymers, some fluoropolymers, and fluoroelastomers may first need a substantial amount of time to break down to much smaller fragments that would then be bioavailable and subject to further degradation.
Polymeric vs. non-polymeric	0 = non-polymeric; 1 = polymeric (e.g., when terms such as "polymer", "poly", "polymd.", "ethoxylated", or "telomere with" are mentioned in the chemical name; in addition, reaction products that may include polyurethane are taken into account.)
Constituent	0 = the CAS number refers to a single PFAS; 1 = the CAS number refers to a mixture
Related chemicals	CAS number(s) of related chemical(s) including monomers of the polymers, or acidic form of the salt, etc.
Uncertainty	0 = the PFAS categorisation is certain; 1 = the PFAS categorisation is uncertain (with details provided in the "Note" column)
Note	Notes qualifying the uncertainty in the PFAS categorization (e.g., structure categorisation uncertain, degradation uncertain, chain length of degradation products uncertain, etc.)

3. Overview of Identified PFASs and Major Findings

In total, 4730 PFAS-related CAS numbers have been identified in this study. Identified PFASs can be categorised as illustrated in Figure 2, whereas statistics of these identified PFASs are illustrated in Figures 3 to 5 below. In addition, major findings are summarized as follows:

- The identified PFASs are diverse in terms of structure (see Figure 3) and other categorisation elements listed in Table 2 (see Figure 4).
- About one-third of the identified PFASs (1616 CAS numbers) have been listed under at least one national/regional chemical inventory considered in the SciFinder database, including those listed in Table 1 and beyond. In addition, the number and type of identified PFASs vary considerably across the inventories (see Figure 5).
- There are PFASs that are or were commercially available, but were not found in the national/regional chemical inventories researched in this study, e.g., Surflon S 111 (CAS number 84932-01-4) and S 113 (CAS number 76199-70-7). This may be because (1) their production volumes were below reporting requirements, (2) they were registered with other CAS numbers, or (3) they were registered in the non-public section of those inventories. The number of such PFASs can currently not be quantified due to a lack of information in the public domain on the overview of all PFASs that have been on the global market.
- In addition to the commonly recognised groups of PFASs with an established general terminology as in Buck et al. (2011) (see Figure 2, a), new groups of PFASs have been identified (see Figure 2, b). These new groups fulfil the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety; Buck et al., 2011), including:

  (1) hydrofluorocarbons (HFCs) with a general structure of $C_nF_{2n+1}C_mH_{2m+1}$, hydrofluoroethers (HFEs) with a general structure of $C_nF_{2n+1}OC_mH_{2m+1}$, and hydrofluoroolefins (HFOs) with a general structure of $C_nF_{2n+1}C_mH_{2m-1}$,

  (2) perfluoroalkyl alkenes (C_nF_{2n}) and their derivatives,

  (3) perfluoroalkyl ketones ($C_nF_{2n+1}C(O)C_mF_{2m+1}$), semi-fluorinated ketones ($C_nF_{2n+1}C(O)C_mH_{2m+1}$), and their derivatives,

  (4) side-chain fluorinated aromatics (C_nF_{2n+1}–aromatic ring(s)), and

  (5) others such as perfluoroalkyl alcohols ($C_nF_{2n+1}OH$), silanes ($C_nF_{2n+1}Si$–), and amines (C_nF_{2n+1}–N–).

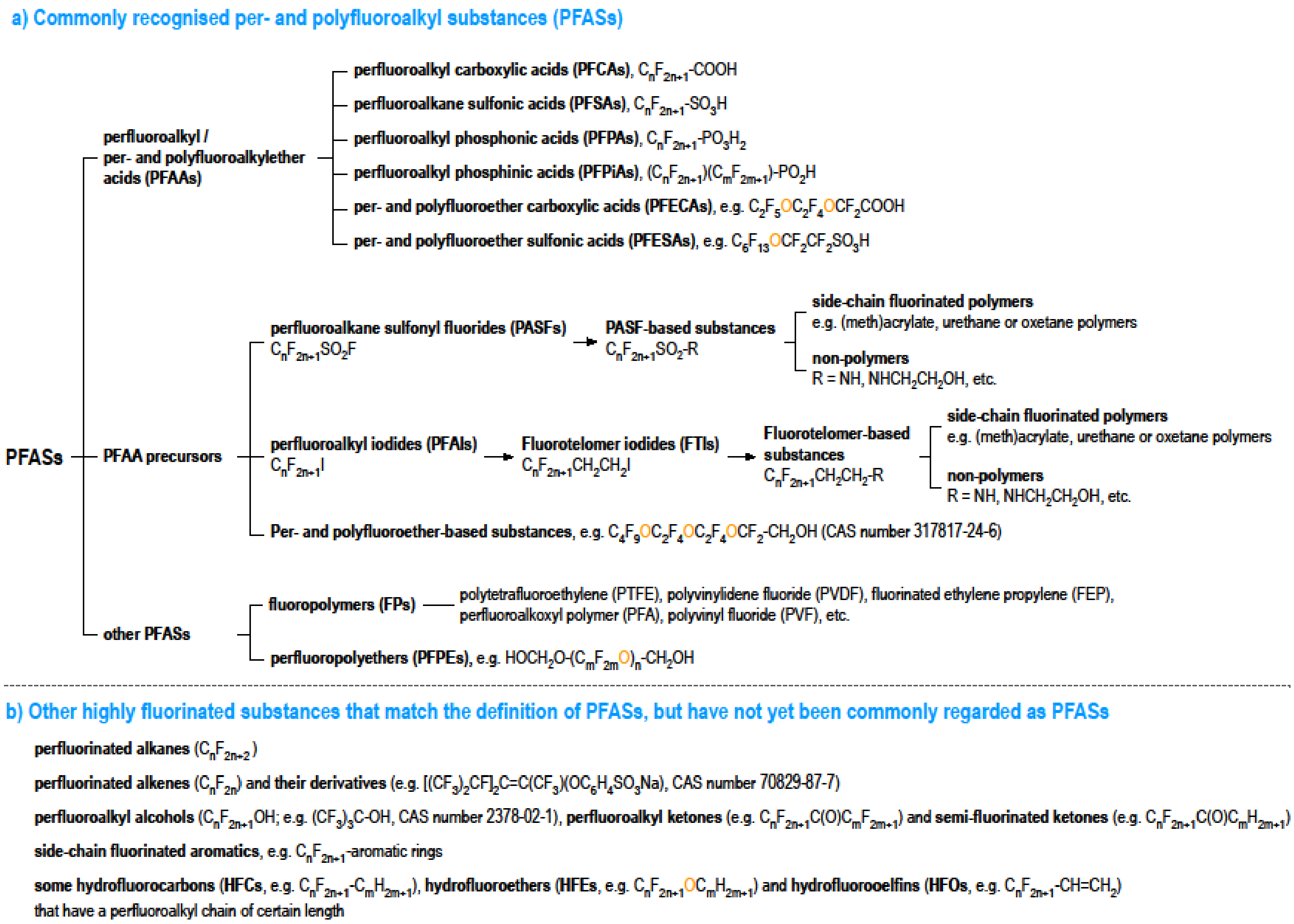

Figure 2. Schematic overview of the structure categories of identified PFASs

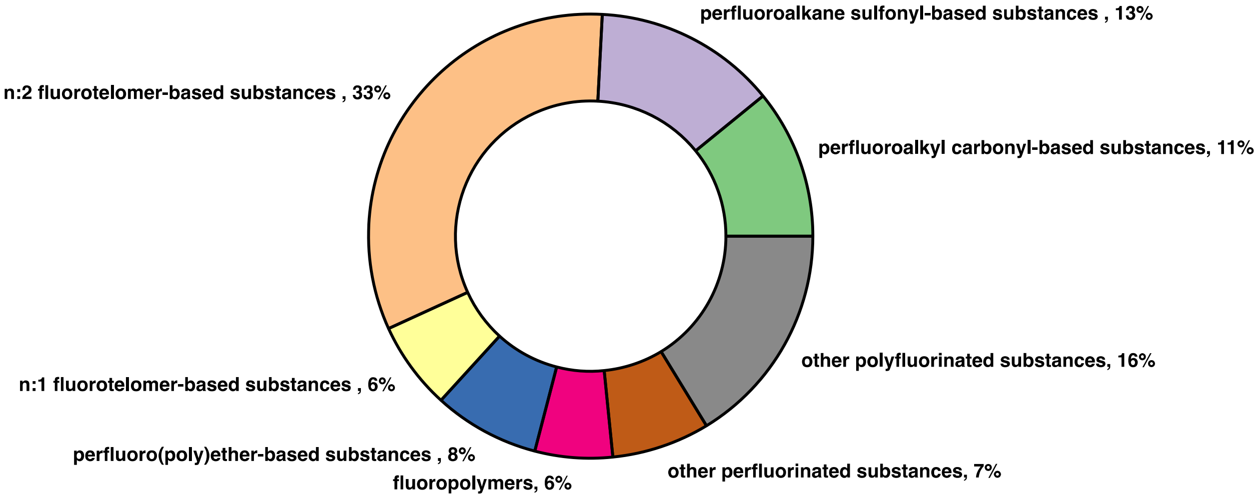

Figure 3. Overview of identified PFASs in this study, grouped by 1st level of structure

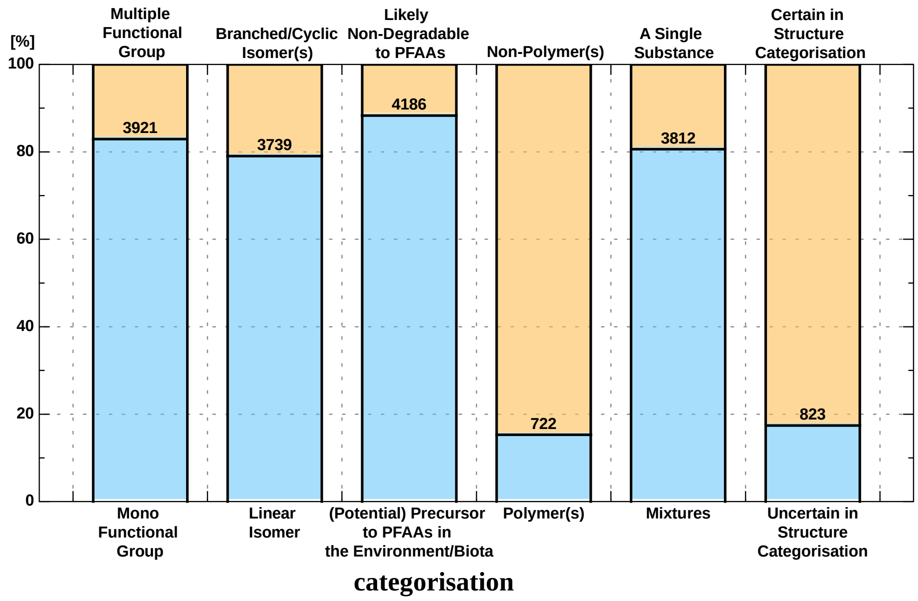

Figure 4. Overview of identified PFAS according to the other categorisation elements outlined in Table 2

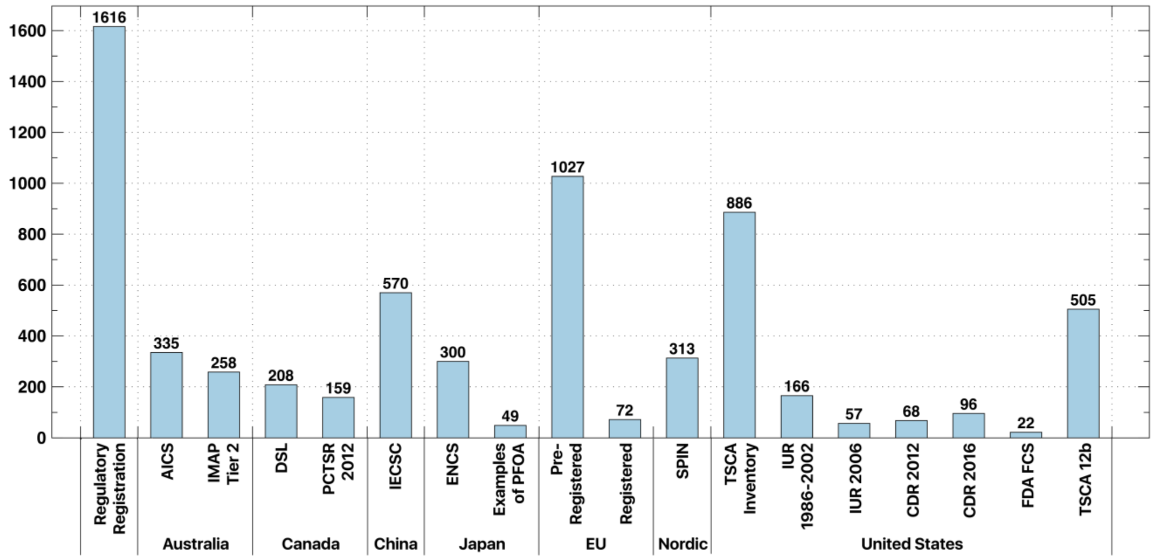

Figure 5. Numbers of identified PFASs having regulatory registration information in the SciFinder Database (see Table 2) and listed in individual sources

4. Limitations, Gaps, Challenges and Opportunities

During the development of the new list of PFASs, several limitations, gaps and challenges, as well as opportunities to address them to improve understanding of PFAS production, use on the global market, and their occurrence, were identified and summarized in Table 3. In particular, there is a need for intensified dialogue and cooperative actions across regions and sectors, designing and fostering new types of public-private partnerships to facilitate effective and efficient information exchange between public and private sectors without harming intellectual property within the field of PFASs and as a model for other fields.

Table 3. Overview of limitations, gaps, challenges, and opportunities identified during the course of this study

<table>
<tr><th colspan="2">Limitations, Gaps and Challenges</th><th>Example(s)</th><th>Opportunities</th></tr>
<tr><td colspan="4">Limitation and gaps in the current methodology (information sources as well as data collection and processing)</td></tr>
<tr><td rowspan="3">Information gaps within the information sources searched.</td><td>A number of substances registered in national/regional inventories have been claimed as confidential business information with no CAS number or molecular structure revealed. Such substances could not be added in this study.</td><td>The PMN section of the US EPA TSCA Inventory contains 312 substances with “fluoro” in their names (e.g., P120406 as “fluoroalkyl sulphonamide derivative”)</td><td>New types of partnerships to be fostered to ensure effective and efficient information exchange (at least chemical identity) across regions and sectors without harming intellectual property.</td></tr>
<tr><td>The current selection of PFASs from the SciFinder Database (labelled as having public references and commercial sources in the Database) may be limited and not yet complete.
Other PFASs excluded from this study due to a lack of information on molecular structure, references, and/or commercial sources in the Database may have also been on the market.</td><td>PFASs without clear molecular structures in the SciFinder Database could not be retrieved from the search.
Surflon (CAS No. 77752-25-1) was registered as “a fluorine-containing oligomer based on a perfluoroacrylate prepared from tetrafluoroethylene via a linear perfluoro alcohol” with 15 references but no commercial sources in the SciFinder Database.</td><td rowspan="2">The current list may be used as a first step to create a web-based database that may be regularly updated and expanded to include new PFASs identified on the global market and in the environment (as in peer-reviewed articles), as well as new information such as commercial availability, production and use volumes, country of manufacture, releases, and alternatives.
Further functions of such a web-based database may include a prediction tool for identifying unintentional PFASs (unreacted raw material residuals, by-products, degradation intermediates) related to the listed PFASs, and other relevant in silico tools for estimating properties.</td></tr>
<tr><td>Information presented in the current list is limited; in particular, information related to prioritization for action is missing, because it is either lacking or scattered over the public domain.</td><td>In many cases, information in the respective source does not reflect during what time periods, where, how, and how much of a PFAS has been produced and used for what purposes. In these cases, further categorization of the PFASs according to their origins/uses (e.g., produced for commercial uses, produced for research purposes, unintentionally generated) or based on commercial availability (e.g., in commerce, no longer in commerce) is not possible. Information on alternatives is also missing.</td></tr>
</table>

Gaps associated with information sources	Not all publicly available information sources have been included in this study.	Company websites, peer-reviewed articles, other technical reports from national and international bodies, and other publicly accessible inventories and lists are not included in this study.	
Limitations associated with the format of the final list compiled in this study	Information in the current list may be superseded over time (e.g., some PFASs may be no longer in commerce, or new PFASs may be put on the market), whereas the list reflects only a snapshot of the state when the research was conducted.	The CAS numbers may be updated or merged over the time: e.g., PFOA (CAS No. 335-67-1) had two other CAS numbers (65618-66-8; 71244-15-0).	

General challenges in PFAS categorisation

Challenges associated with the descriptions of identified PFASs	The descriptions of many PFASs in the public domain are unclear, including - described as "reaction products"; - described with unclear terms; or - registered with only trade names and general descriptions	As indicated by comments from the industry, CAS No. 69991-67-9 "1-propene, 1,1,2,3,3,3-hexafluoro-oxidized, polymd." is a perfluoropolyether, whereas CAS No. 161075-14-5 "1-propene, 1,1,2,3,3,3-hexafluoro-, oxidized, polymd., reduced, hydrolyzed" is a fluoropolymer. Another example is the use of "poly(difluoromethylene)" for PTFE or fluorotelomer-based substances. An additional example is using vague phrases such as "octafluoro-1-oxopentyl" and "heptadecafluorononyl" without clear indication of position(s) of the non-fluorinated carbon(s).	New types of partnerships to be fostered to ensure effective and efficient information exchange (at least chemical identity) across regions and sectors without harming intellectual property.
Challenges associated with the current terminology of PFASs	No common terminology for newly identified substance groups.	Side-chain fluorinated aromatics, perfluoroether-based substances, perfluoroalkyl alkenes and derivatives, PFASs with multiple functional groups.	The common terminology in Buck et al. (2011) may be discussed and expanded, e.g., by a group of international experts (e.g., major manufacturers, academic scientists, regulators, civil society representatives) to address these gaps.
	The distinction between certain groups is not clear as they have the same general molecular formula; the cut-off values have not been defined. Similarly, there are no common cut-off values for the differentiation between telomers and polymers.	Certain HFCs and semi-fluorinated alkanes (SFAs) have the same general structure of $C_nF_{2n+1}C_mH_{2m+1}$; Certain HFOs and fluorotelomer olefins (FTOs) have the same general structure of $C_nF_{2n+1}CH=CH_2$	
	Some fluoropolymers may contain other halogens than fluorine on the backbone; it is unclear if they should be considered as PFASs or not.	Polychlorotrifluoroethylene (PCTFE)	
Challenges associated with the current state of knowledge	The degradability of many identified PFASs other than PFAAs and their major precursors including perfluoroalkanesulfonyl fluoride (PASF) derivatives and fluorotelomer-based substances, and the chain length of their degradation products, remain unclear.	Perfluoroalkyl alkenes, perfluoroether-based halides	Continuous support for degradation studies will be needed.

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