



POPFREE

Promotion of PFAS-free alternatives

Deliverable Report



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Deliverable summary

This report is a deliverable from task 4.4 of the POPFREE project (stage 3). Based on the OECD Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs) more than 4700 substances have been categorised for their current regulatory status in Sweden, the EU and globally. For example, more than 1000 substances were categorised as covered by the Regulation (EU) No 2019/1021 of the European Parliament and of the Council concerning Persistent Organic Pollutants (POPs) for Perfluorooctanoic acid (PFOA), its salts and PFOA-related compounds. The categorisations are associated with a high level of uncertainty due to the limited size of this project. Substance by substance evaluations have not been possible and all categorisations are based on group level criteria. Next steps forward are discussed, including the development of digital tools, to support the manufacture and use of products without PFAS.

This report is a deliverable from task 4.4 of the UDI stage 3 project “POPFREE – Promotion of PFAS-free alternatives. POPFREE is funded by Vinnova, the Swedish Innovations Agency and coordinated by RISE. Among the tasks is 4.4, which is led by IVL Swedish Environmental Research Institute and executed in collaboration with Volvo Cars, RISE and the Swedish Chemicals Agency. The POPFREE project ran from 2020 to 2022.

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Abbreviations

Terms and abbreviations used in this report are listed in the table below. For naming of substances, priority was given to the terms used at www.kemi.se. The naming of the substances in the database associated with this report (based on the OECD PFAS database) was not adjusted to align with the table below. Neither was the naming adjusted in lists taken from different databases (i.e., lists in appendices to this report). Hence, a substance might have different names in different tables of this report and its associated database.

Abbreviation	Explanation
APFO	Ammonium pentadecafluorooctanoate
CLP	Classification, Labelling and Packaging
FTOH	Fluorotelomer alcohol
GADSL	Global Automotive Declarable Substance List
GenX	2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propionic acid, its salts and its acyl halides (HFPO-DA, GenX)
GHS	United Nations' Globally Harmonized System of Classification and Labelling of Chemicals
HFPO-DA	See GenX
PACT	EU Public Activities Coordination Tool
PFAA	Perfluoroalkyl acid
PFAS	Per- and polyfluoroalkyl substances
PFBS	Perfluorobutanesulfonic acid
PFCA	Perfluoroalkyl carboxylic acid
PFDA	Perfluorodecanoic acid
PFDoDA	Tricosfluorododecanoic acid
PFHpA	Perfluoroheptanoic acid
PFHxA	Perfluorohexanoic acid
PFHxS	Perfluorohexanesulfonic acid
PFNA	Perfluorononan-1-oic-acid
PFOA	Perfluorooctanoic acid

PFOS	Perfluorooctanesulfonic acid
PFSA	Perfluoroalkane sulfonic acids
PFTeDA	Heptacosaf fluorotetradecanoic acid
PFTTrDA	Pentacosaf fluorotridecanoic acid
PFUnDA	Henicosaf fluoroundecanoic acid
POP	Persistent Organic Pollutants
POPRC	Persistent Organic Pollutants Review Committee
REACH	Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)
SVHC	Substances of Very High Concern

1. Introduction

Per- and polyfluoroalkyl substances (PFAS) is a large substance group. The latest OECD “Comprehensive global database of PFASs” (hereafter termed the OECD PFAS database; available at <https://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/>) contained 4730 individual CAS numbers (OECD 2018). Since current chemical legislation covers different subsets of PFAS, industrial actors need to identify which PFAS are covered by the different legislations, in order to ensure legal compliance and to make a prioritization for substitution. A traffic light categorisation of PFAS according to their regulatory status is reported herein as a support to industry. The scope of this categorisation is PFAS legislation in Sweden, the EU and globally. Country specific legislation in other countries than Sweden and region-specific legislation other than in the EU are not covered. The scope is further limited to legislation in place in March 2022.

The categorisation of PFAS according to their regulatory status (as described above) was added to the OECD PFAS database (OECD 2018). This report accompanies this derivative PFAS database and includes a brief background on PFAS and relevant regulations, a method description for the categorisation and finally, a summary of how the PFAS are covered by the legislations in scope.

This report is intended as a support for industrial actors in their work to phase out all application areas of PFAS that are not essential. This report and the associated database are not intended as strict legal advice.

2. Background

2.1 Per- and polyfluoroalkyl substances

PFAS is a complex substance group. PFAS are used in a wide array of application areas (Glüge *et al.* 2020) and PFAS belong to many different chemical structural categories (Buck *et al.* 2011). PFAS are extremely persistent or degrade to extremely persistent terminal degradation products, usually the perfluoroalkyl acids (PFAA) (Wang *et al.* 2017). PFAS that degrade to PFAAs are called PFAA precursors. Further descriptions of PFAS can be found elsewhere and detailed descriptions will not be given herein, see e.g. Buck *et al.* (2011), OECD (2021).

PFAS definitions have expanded over time. The definition of a perfluoroalkyl moiety has in OECD (2018) been expanded from “(C_nF_{2n+1}-)” (Buck *et al.* 2011) to “-C_nF_{2n}-” (with a focus on PFAS with perfluorinated chain length ≥ 3 ¹). And according to the OECD in their recent terminology reconciliation: “any chemical with at least a perfluorinated methyl group (-CF₃) or a perfluorinated methylene group (-CF₂-) is a PFAS” (OECD 2021).

¹ Or a perfluoroalkylether moiety with two or more carbons (i.e. -C_nF_{2n}OC_mF_{2m}-, n and m ≥ 1)

Long-chain PFAs are perfluoroalkyl carboxylic acids (PFCA) with ≥ 7 perfluorinated carbons and perfluoroalkane sulfonic acids (PFSA) with ≥ 6 perfluorinated carbons (Buck *et al.* 2011).

2.2 Current PFAS regulations

PFAS as a group is currently not regulated. Sweden, together with three other member states in the EU and Norway, is working on a broad restriction proposal for PFAS in Annex XVII to the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) regulation (www.kemi.se).

2.2.1 Global

The Stockholm Convention on Persistent Organic Pollutants

Perfluorooctane sulfonic acid (PFOS) and its derivatives, and perfluorooctanoic acid (PFOA), its salts and PFOA-related compounds (which include substances that can degrade to PFOA) are listed in the Stockholm Convention and implemented in the EU by Regulation (EU) No 2019/1021 of the European Parliament and of the Council concerning Persistent Organic Pollutants (POPs).

In regulation (EU) 2019/1021 of the European parliament and of the council (hereafter the POPs regulation) molecular structure criteria are stipulated:

“Perfluorooctanoic acid (PFOA), its salts and PFOA-related compounds’ means the following: (i) perfluorooctanoic acid, including any of its branched isomers; (ii) its salts; (iii) PFOA-related compounds which, for the purposes of the Convention, are any substances that degrade to PFOA, including any substances (including salts and polymers) having a linear or branched perfluoroheptyl group with the moiety (C₇F₁₅)C as one of the structural elements.”

“Perfluorooctane sulfonic acid and its derivatives (PFOS) C₈F₁₇SO₂X (X = OH, Metal salt (O-M⁺), halide, amide, and other derivatives including polymers)”

One challenge here is to identify all substances meeting the above criteria with due considerations to the relevant exceptions, see further in the methods section. The Persistent Organic Pollutants Review Committee (POPRC) Annex II to document UNEP/POPS/POPRC.16/INF/12 contains an indicative list of 185 PFOA- and PFOA-related substances and Annex UNEP/POPS/POPRC.17/INF/14/Rev.1 contain an updated indicative list of substances covered by the listing of PFOA, its salts and PFOA-related compounds (ver. February 2022) with 454 substances.

Perfluorohexanesulfonic acid (PFHxS), its salts and related substances, are under evaluation for inclusion in the Stockholm Convention during spring 2022. In January 2022 there was a proposal to list long-chain perfluorocarboxylic acids, their salts and related compounds in Annexes A, B and/or C of the Stockholm Convention.

The Rotterdam Convention

PFOS and a number of related compounds (sulfonates, sulfonamides and sulfonyls) are listed under the Rotterdam Convention Annex III and PFOA, its salts and PFOA-related compounds, are recommended for listing in the same annex. This convention list is not considered further herein.

2.2.2 EU

Classification, Labelling and Packaging (CLP) Regulation

The Classification, Labelling and Packaging (CLP) Regulation ((EC) No 1272/2008) is based on the United Nations' Globally Harmonised System (GHS). At present (March 2022), PFOS, PFOA, Perfluorononan-1-oic-acid (PFNA), perfluorodecanoic acid (PFDA) and ammonium pentadecafluorooctanoate (APFO) have harmonised classifications and are listed in Annex VI of the CLP. A proposal for the addition of perfluoroheptanoic acid (PFHpA) and 6:2 fluorotelomer alcohol (FTOH) into Annex VI is in progress. In the Swedish PRIO database (see further in 2.3), there are a few additional inclusions of PFAS listed in Annex VI (see Appendix 3: CLP, Annex VI).

Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)

Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) restricts PFAS (March 2022):

- More than 10 PFAS are identified as substances of very high concern (SVHC) and are listed on the Candidate List of substances of very high concern for Authorisation (<https://www.echa.europa.eu/web/guest/candidate-list-table>).
- Currently (March 2022) no PFAS are included in Annex XIV, the authorisation list.
- Since August 2021, PFCA C9-C14 and their precursors are included in Annex XVII, restriction that are to be implemented by February 2023.
- In addition, several PFAS are listed in the Public Activities Coordination Tool (PACT) as they are under evaluation. Restrictions are underway for perfluorohexanoic acid (PFHxA) (restrictions are not relevant for PFHxS anymore due to its coming inclusion in the Stockholm Convention).
- The Stockholm Convention's restrictions on PFOS and PFOA and related compounds have been implemented by Regulation (EU) No 2019/1021 of the European Parliament and of the Council concerning Persistent Organic Pollutants (POPs). Hence, restrictions on PFOA in REACH has ceased to apply.

2.2.3 Sweden

The Swedish Chemicals Agency has developed a national strategy on PFAS (KEMI 2016). PFAS that are deliberately added to chemical products are required to be reported to the Swedish Chemicals Agency's Products Register. This statutory requirement applies to those who manufacture or import notifiable products, irrespective of the percentage of the substance in that product. This is in contrast to the REACH regulation, where levels below a defined threshold do not have to be reported.

2.2.4 Summary table PFAS regulations

Table 1: Summary table of PFAS regulations (based on information at www.kemi.se; (KEMI 2022))

Substance	CAS-no.	Legislation			
		REACH: Annex XVII	REACH: Cand. List	CLP: Annex VI	POPs*
Perfluorobutane sulfonic acid (PFBS) and its salts	375-73-5, and others		X		
PFHxS and its salts	355-46-4, and others		X		
PFOA, its salts and PFOA-related compounds	335-67-1, and others		X (335-67-1)	X (335-67-1)	X
APFO**	3825-26-1			X	X
PFOS and its derivatives	1763-23-1, and others			X	X
C9-C14 PFCA-related substances		X (Feb 2023)			
PFNA and its sodium and ammonium salts	375-95-1, and others	X	X	X	
PFDA and its sodium and ammonium salts	335-76-2, and others	X	X	X	
Henicosaflluoroundecanoic acid (PFUnDA)	2058-94-8	X	X		
Heptacosaflluorotetradecanoic acid (PFTeDA)	376-06-7	X	X		
Pentacosaflluorotridecanoic acid (PFTrDA)	72629-94-8	X	X		
Tricosaflluorododecanoic acid (PFDoDA)	307-55-1	X	X		
HFPO-DA (GenX)***	13252-13-6, and others		X		
<p>* Implemented by Regulation (EU) No 2019/1021 of the European Parliament and of the Council concerning Persistent Organic Pollutants (POPs)</p> <p>** APFO is a PFOA salt</p> <p>*** 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propionic acid, its salts and its acyl halides (HFPO-DA, GenX)</p>					

2.3 PRIO

The Swedish Chemicals Agency provides the PRIO tool (<https://www.kemi.se/prioguiden/start>) that helps industries and other actors to identify and replace or reduce the risk of particularly hazardous substances in articles or chemical products. The OECD PFAS database (OECD 2018) has been incorporated in the PRIO tool and it can be used to identify e.g. PFOA related substances and other sub-groups of PFAS in the database. However, as an example, a search in June 2022 for the substance group “Perfluorooctanoic acid (PFOA) and its derivatives” and reference “PFAS, OECD 2018” generated only 178 hits even though it is likely that many more substances would qualify for the criteria set by the PRIO tool. Hence, the additional categorisation of the OECD PFAS database in this work also poses a relevant input to the PRIO tool.

2.4 Substance list for the automotive industry

The Global Automotive Declarable Substance List (GADSL; <https://www.gadsl.org/>) covers substances that are expected to be present in a material or a part that remains in a vehicle at point of sale. The GADSL is the result of the efforts of a global team from the automotive, automotive parts supplier (tier supplier) and chemical/plastics industries who have organized the Global Automotive Stakeholders Group (GASG). The GASG’s purpose is to facilitate communication and exchange of information regarding the use of certain substances in automotive products throughout the supply chain. The GADSL will be updated and published at least once a year according to the latest stage of knowledge.

In the GADSL reference list 828 substances (with CAS no’s) were listed in Index for “PFOA, perfluorooctanoic acid, its salts and PFOA related compounds” in February 2022.

2.5 The OECD PFAS database

The OECD PFAS database (OECD 2018) contains 4730 PFAS related CAS-numbers (only PFAS with CAS-numbers are included). Each PFAS related CAS-number has been described for the following characteristics and parameters:

- Structure Category (incl. uncertainty of this classification)
- Number of Functional Groups
- Perfluoroalkyl Chain Length
- Linear vs. Branched Isomer
- (Potential) precursor to PFAAs in the environment/biota
- Polymer/Non-polymer
- Mixture/Individual substance
- Related Chemicals
- Regulatory Status

3. Method

3.1 Development of a traffic light list

The further categorisation of the substances in the OECD PFAS database was done by defining a traffic light system according to Table 2.

Table 2: The traffic light system

Colour	Substances categorised [#]
RED	Substances regulated by any or several of the following: - REACH: Annex XVII, - REACH: Candidate List of SVHC, - CLP: Annex VI and - POPs*
ORANGE	Substances or mixtures of uncertain identity or of uncertain relevance for the legislations
YELLOW	Substances not covered to date by any of the legislations
* Implemented by Regulation (EU) No 2019/1021 of the European Parliament and of the Council concerning Persistent Organic Pollutants (POPs)	
# Categorisation was coded as: (1) REACH: Annex XVII (2) REACH: Candidate List (3) CLP: Annex VI (4) POPs	

The traffic light system was developed in a two-step procedure:

1. Matching database entries with CAS-number specified in the relevant legislations (i.e. legislations as listed in Table 1 with CAS-numbers as listed in Table A 1-Table A 4).
2. Identification of substances matching a specified combination of criteria as outlined in Table 3 (in addition to those identified in step 1) and further in Appendix 5: Criteria for PFOA, its salts and PFOA-related compounds in the POPs regulation.

Table 3: Criteria for identification of a substance in the OECD PFAS database to be covered by the POPs legislation. Criteria categories are from the OECD PFAS database (i.e. column names in tab 3. "overview with CAS" in said database)

Legislation	Substance	Criteria		Comment
		Red	Orange	
POPs*	PFOA, its salts and PFOA-related compounds	Perfluoroalkyl chain length: ≥ 7 or ≥ 8 (see Appendix 5: Criteria for PFOA, its salts and PFOA-related compounds in the POPs regulation)	Same as for red but also: Chain lengths with insertions R/O/H/DB/Cl/Br/I # or perfluoroalkyl chain length "unclear".	Substances covered by exceptions removed, see specific criteria list in Appendix 5: Criteria for PFOA, its salts and PFOA-related compounds in the POPs regulation.
POPs*	PFOS and its derivatives	Structure category: 200 Perfluoroalkyl chain length: 8	Same as for red but also: Chain lengths with insertions R/O/H/DB/Cl/Br/I # or perfluoroalkyl chain length "unclear".	Cat. 206, 207, 208, 209 removed due to functional groups in both ends (no hits). Note CAS-numbers with several chain lengths including also 8 were included.
* Implemented by Regulation (EU) No 2019/1021 of the European Parliament and of the Council concerning Persistent Organic Pollutants (POPs)				
# DB= double bond, R=undefined chemical structure, O, H, Cl, Br, I are elements				
Notes on these criteria:				
<ul style="list-style-type: none"> The exception (ii) in the POPs regulation (2019/1021) was interpreted as to cover only fluoropolymers as defined by Buck <i>et al.</i> (2011): "[...]carbon-only polymer backbone with F atoms directly attached to it[...]" Categorisation for the PFOA and PFOS POPs regulation was made in a stepwise procedure, first including all substances meeting the criteria for inclusion and then removing substances meeting criteria for exception. Categorisation was made per structure category separately. 				

PubChem (<https://pubchem.ncbi.nlm.nih.gov/>) was used as the primary database to explore substance identities, i.e., chemical structures.

3.1.1 Limitation of scope

The applied method has a limited scope:

- Exceptions for intermediate use, concentration thresholds and other specifications made in the regulations are not considered in the traffic light categorisation. Therefore, some uses may still be allowed for a limited period or for cases a substance is used under certain concentration thresholds despite the substance being covered by the legislation.
- It should be noted that the OECD PFAS database contains a category for “(Potential) precursor to PFAAs in the environment/biota”. Since this categorisation was used in the further categorisations herein (see Table 3) the scope of the present study is environmental degradation. Therefore, a strict interpretation, meaning that all substances with a perfluorinated heptyl group ((C₇F₁₅)C) except the exceptions are PFOA related, was not applied.
- With regards to potential precursors to PFAAs it should further be noted that there are uses of PFAS that could render degradation that would not take place in the environment. For example, if a substance is heated or placed under high pressure. These types of conditions that are more extreme than environmental conditions (e.g. during production processes) are not covered herein. Hence, a substance categorised as not being a PFAA precursor in the lists presented here could possibly be a PFAA precursor when exposed to extreme conditions (non-environmental).
- The C9-C14 PFCA regulation under REACH, implemented by February 2023, was not considered in the categorisations.
- Only for PFOS and PFOA in the POPs regulation unspecified CAS numbers were considered. Hence, in all other cases where PFAS are covered by the legislation but do not have complete lists of CAS numbers specified, categorisation herein did not go beyond CAS-number listings in Table A 1, A 2 and A 3.
- CLP Annex VI was not searched beyond the CAS numbers included in the PRIO database.
- Tables with CAS-numbers in GADSL, PRIO and POPRC indicative lists (see 2.2.1) have not been matched to the database.

- For some filter criteria (see Table 3 and Appendix 5: Criteria for PFOA, its salts and PFOA-related compounds in the POPs regulation) hits were many (e.g. PFOA >800) and substance by substance evaluation was not possible.

3.2 Exploration of the use of an automatized workflow

To explore the use of an automatized workflow the KNIME software (<https://www.knime.com/>) was used to set up the workflow as specified above for PFOS under the EU POPs regulation.

4. Results and discussion

4.1 Summary of the PFAS categorisations in the Traffic light system

The outcome of the categorisations in the traffic light system is summarised in Table 4. PFOA, its salts and PFOA-related compounds as covered by the POPs regulation rendered by far the most amount of hits (in both red and orange category).

Note that the limitations of the scope (see 3.1.1) affect the outcome. As an example, for PFNA under REACH Annex XVII only one hit is noted in Table 4, which is simply due to the fact that only one CAS number was specified and herein considered.

Table 4: Summary of traffic light categorisations of PFAS based on the OECD PFAS database (n=4730). Number of CAS numbers meeting the criteria in categories red (top cell) and orange (bottom cell). Empty cells in case the legislation is not applicable.

Substance	CAS-number	Legislation				Comment
		REACH: Annex XVII	REACH: Cand. List [#]	CLP: Annex VI [□]	POPs*	
PFBS and its salts	375-73-5, and others		9 0			
PFHxS and its salts	355-46-4, and others		6 0			
PFOA, its salts and PFOA-related compounds	335-67-1, and others		1	1	1272	
			0	0	192	
APFO	3825-26-1			1 0	*	* APFO is a PFOA salt
PFOS and its derivatives	1763-23-1, and others			5	249	
				0	9	
C9-C14 PFCA-related substances		X (Feb 2023)				
PFNA and its sodium and ammonium salts	375-95-1, and others		1	3	3	
			0	0	0	

PFDA and its sodium and ammonium salts	335-76-2, and others	1	3	3		
		0	0	0		
PFUnDA	2058-94-8	1	1			
		0	0			
PFTeDA	376-06-7	1	1			
		0	0			
PFTrDA	72629-94-8	1	1			
		0	0			
PFDoDA	307-55-1	1	1			
		0	0			
HFPO-DA (GenX)	13252-13-6, and others		4			
			0			
<p>* Implemented by Regulation (EU) No 2019/1021 of the European Parliament and of the Council concerning Persistent Organic Pollutants (POPs)</p> <p># Several CAS-numbers on the candidate list could not be found in the OECD PFAS database, these are annotated in Appendix 2: REACH, Candidate List.</p> <p>□ Include only PFAS categorised as included in the CLP Annex VI in the PRIO tool (www.kemi.se). Four of the CAS-numbers did not fall under any of the substance groups in this table and were not included herein.</p> <p>Note: The limitations of the scope of this work limit the number of hits in several of the legislation categories above. Only for the POPs legislation were substances with unspecified (i.e. not specifically listed) CAS-numbers considered.</p>						

4.2 Uncertainty and effect of limitations

It is necessary to highlight the limitations and associated uncertainties connected to the regulatory categorisations made herein. Only PFAS with a CAS-number are included in the OECD PFAS database and hence also in the derivative database associated with this report. The limitations of scope (3.1.1) limit the number of hits in several of the legislation categories, i.e. the actual coverage may well be larger than captured herein. In addition, the lack of substance-by-substance assessment results in a high uncertainty associated with the categorisations, especially in the broad scope legislations such as the POPs regulation on PFOA, its salts and related compounds. Finally, it must be considered that the original OECD PFAS database or other databases used may include errors (see e.g. Sha *et al.* (2019)).

4.3 Practical application of the traffic light list

The aim of the categorisations of PFAS according to their regulatory status was to give a simplified and practical tool to actors who have to comply to PFAS regulations. Unfortunately, the uncertainty of the regulatory categorisations strongly limits the use of the derived database as a tool for regulatory compliance check.

To exemplify this, it can be noted that the traffic light list contains more than 1000 substances (1272 substances, see Table 4) that were categorised to be covered by the POPs regulation for PFOA and PFOA related substances (categorisation red). Another set of almost 200 substances (192) were categorised as being potentially covered by the legislation (categorisation orange). In total, almost double as many substances were identified as PFOA and PFOA related substances compared to the often referred to “800 substances”. The higher number herein could partly be associated with uncertainties, i.e., mis-categorisations, but nevertheless it shows the very broad scope of the new PFAS regulations.

Despite the limitations in use of the traffic light list for regulatory compliance check, this report and the appended database can serve as a practical guidance for industry to handle the regulations on PFAS in general and the complex PFOA regulation specifically.

4.4 The applicability of an automatized workflow

By use of the KNIME software an automatized workflow was set up to categorise substances in the OECD PFAS database for their regulatory status and subsequently count the entries in the respective categories. The categorisation was verified for PFOS in the POPs regulation by comparing the result with the result of a manual categorisation according to criteria in Table 3. It was beyond the scope of the present project to set up such automated workflows for all regulatory categorisations. However, an automated workflow is recommended as it: a) reduces the risk of human error and enables b) a fast review and c) an easy update of the categorisations following regulation changes and d) an easy match of databases with existing lists, such as the POPRC indicative lists (see 2.2.1).

4.5 Looking ahead: New tools and their relevance in the future following new PFAS regulations

Based on experience as reported herein, it can be recommended to set up automatized workflows for categorisations. Such approaches will be adaptable, robust, and easy to review. Tools for such automatization are available and their applicability in this context was demonstrated herein by one tool. In a long-time perspective, it is recommended to derive tools based on cheminformatics to support substance categorisation based on molecular structural traits (see e.g. Sha *et al.* (2019), OECD (2021)). Such a tool would further not be limited to substances with CAS numbers, and it would allow for a more flexible substance evaluation as it would not be limited to existing lists and databases. Such a cheminformatics tool could for example draw any molecular structure from e.g. a SMILES code (Simplified Molecular Input Line Entry Specification) and look for structure moieties as stipulated in the regulatory text. As

an example, the cheminformatics tool could look for the $C_7F_{15}C$ moiety in any molecular structure. Finally, the cheminformatics tool would inform the user on whether the substance of interest matches regulatory criteria or not, i.e., if it is restricted or not.

With new, broader, PFAS regulations foreseen to be implemented in the relatively near future, regulatory categorisation of PFAS may become obsolete as all PFAS might become banned. Any PFAS that is not for essential use should then be substituted. Many actors affected by this broad PFAS regulation may still have the need for practical support. The cheminformatics tool proposed above could then be set to identify if a substance is a PFAS at all by answering the general question: “does the structure contain a perfluorinated methyl group ($-CF_3$) or a perfluorinated methylene group ($-CF_2-$)?”, and by that provide support to meet potential future regulations.

5. References

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Appendices

Appendix 1: REACH, Annex XVII

Table A 1: REACH Annex XVII. This table contains only PFAS and CAS numbers listed as regulated under REACH: Annex XVII on www.kemi.se, KEMI (2022; Table "PFAS that are regulated in the EU chemicals legislation"). Inclusion of C9-C14 PFCA-related substances that apply from February 25 2023 is not included.

Substance name	CAS number
PFNA and its sodium and ammonium salts	375-95-1, and others
PFDA and its sodium and ammonium salts	335-76-2, and others
PFUnDA	2058-94-8
PFTeDA	376-06-7
PFTTrDA	72629-94-8
PFDoDA	307-55-1

Appendix 2: REACH, Candidate List

Table A 2: Entries in the REACH Candidate List of substances of very high concern for Authorisation (extracted from the ECHA website where the list is published in accordance with Article 59(10) of the REACH Regulation; <https://echa.europa.eu/sv/candidate-list-table>), for PFAS listed as regulated under REACH: Candidate List on www.kemi.se, KEMI (2022; Table "PFAS that are regulated in the EU chemicals legislation").

Substance	Substance sub-category	CAS-no
Pentadecafluorooctanoic acid (PFOA)		335-67-1
Perfluorohexane-1-sulphonic acid and its salts		-
	tridecafluorohexanesulphonic acid, compound with 2,2'-iminodiethanol (1:1)	70225-16-0
	ammonium perfluorohexane-1-sulphonate	68259-08-5

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	potassium perfluorohexane-1-sulphonate	3871-99-6
	perfluorohexane-1-sulphonic acid	355-46-4
	Ethanaminium, N-[4-[[4-(diethylamino)phenyl][4-(ethylamino)-1-naphthalenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-ethyl-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	1310480-24-0#
	Methanaminium, N-[4-[[4-(dimethylamino)phenyl][4-(ethylamino)-1-naphthalenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methyl-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	1310480-27-3#
	Methanaminium, N-[4-[[4-(dimethylamino)phenyl][4-(phenylamino)-1-naphthalenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methyl-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	1310480-28-4#
	Beta-Cyclodextrin, compd. with 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonic acid ion(1-)(1:1)	1329995-45-0#
	Gamma-Cyclodextrin, compd. with 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonic acid ion(1-)(1:1)	1329995-69-8#
	Sulfonium, triphenyl-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	144116-10-9#
	Quinolinium, 1-(carboxymethyl)-4-[2-[4-[4-(2,2-diphenylethenyl)phenyl]-1,2,3,3a,4,8b-hexahydrocyclopent[b]indol-7-yl]ethenyl]-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	1462414-59-0#

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	Iodonium, diphenyl-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	153443-35-7#
	Methanaminium, N,N,N-trimethyl-, salt with 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonic acid (1:1)	189274-31-5#
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, compd.with 2-methyl-2-propanamine (1:1)	202189-84-2#
	Iodonium, bis[4-(1,1-dimethylethyl)phenyl]-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	213740-81-9#
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, zinc salt	70136-72-0#
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, lithium salt (1:1)	55120-77-9
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, sodium salt	82382-12-5
	Iodonium, bis[(1,1-dimethylethyl)phenyl]-, salt with 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonic acid (1:1) (9CI)	866621-50-3#
	Sulfonium, (4-methylphenyl)diphenyl-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	910606-39-2#
	Sulfonium, [4-[(2-methyl-1-oxo-2-propen-1-yl)oxy]phenyl]diphenyl-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	911027-68-4#
	Sulfonium, [4-[(2-methyl-1-oxo-2-propenyl)oxy]phenyl]diphenyl-, salt with 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonic acid (1:1), polymer with 2-ethyltricyclo[3.3.1.1 ^{3,7}]dec-2-yl 2-methyl-2-propenoate, 3-	911027-69-5#

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	hydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl 2-methyl-2-propenoate and tetrahydro-2-oxo-3-furanyl 2-methyl-2-propenoate	
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, cesium salt (1:1)	92011-17-1#
	Dibenzo[k,n][1,4,7,10,13]tetraoxathiacyclopentadecinium, 19-[4-(1,1-dimethylethyl)phenyl]-6,7,9,10,12,13-hexahydro-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	928049-42-7#
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, gallium salt (9CI)	341035-71-0#
	Sulfonium, bis(4-methylphenyl)phenyl-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	341548-85-4#
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, scandium(3+) salt (3:1)	350836-93-0#
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, neodymium(3+) salt (3:1)	41184-65-0#
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, yttrium(3+) salt (3:1)	41242-12-0#
	Sulfonium, (thiodi-4,1-phenylene)bis[diphenyl]-, salt with 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonic acid (1:2)	421555-73-9#
	Iodonium, bis[4-(1,1-dimethylpropyl)phenyl]-, salt with 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonic acid (1:2)	421555-74-0#
	Sulfonium, tris[4-(1,1-dimethylethyl)phenyl]-, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	425670-70-8#
	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, compd. With pyrrolidine (1:1)	1187817-57-7#

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	N,N,N-triethylethanaminium sulfonate	tridecafluorohexane-1-	108427-55-0#
	N,N,N-tributylbutan-1-aminium sulfonate	tridecafluorohexane-1-	108427-54-9#
	Phosphonium, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonate (1:1)	triphenyl(phenylmethyl)-,	1000597-52-3#
	1-Hexanesulfonic acid, tridecafluoro-, compd. with N,N-diethylethanamine (1:1)	1,1,2,2,3,3,4,4,5,5,6,6,6-	72033-41-1#
Perfluorononan-1-oic-acid and its sodium and ammonium salts			-
	Perfluorononan-1-oic-acid		375-95-1
	Sodium salts of perfluorononan-1-oic-acid		21049-39-8
	Ammonium salts of perfluorononan-1-oic-acid		4149-60-4
Nonadecafluorodecanoic acid (PFDA) and its sodium and ammonium salts			
	Nonadecafluorodecanoic acid		335-76-2
	sodium nonadecafluorodecanoate		3830-45-3
	Ammonium nonadecafluorodecanoate		3108-42-7
Henicosafleuroundecanoic acid			2058-94-8
Heptacosafleurotetradecanoic acid			376-06-7
Pentacosafleurotridecanoic acid			72629-94-8
Tricosafleurododecanoic acid			307-55-1
2,3,3,3-tetrafluoro-2- (heptafluoropropoxy)propionic acid, its salts and its acyl halides*			-
	potassium (heptafluoropropoxy)propionate	2,3,3,3-tetrafluoro-2-	67118-55-2

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	2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propionyl fluoride	2062-98-8
	ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	62037-80-3
	2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propionic acid	13252-13-6
	Propanoic acid, 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)-, (-)-	75579-40-7#
	Propanoic acid, 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)-, (+)-	75579-39-4#
Perfluorobutane sulfonic acid (PFBS) and its salts		-
	Potassium 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonate	29420-49-3
	1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonic acid	375-73-5
	Ammonium 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonate	68259-10-9
	bis(4-t-butylphenyl)iodonium perfluorobutanesulfonate	-
	tetrabutyl-phosphonium nonafluoro-butane-1-sulfonate	220689-12-3
	morpholinium perfluorobutanesulfonate	503155-89-3#
	1-(4-butoxy-1-naphthalenyl)tetrahydrothiophenium 1,1,2,2,3,3,4,4,4-nonafluoro-1-butanesulfonate	-
	Triphenylsulfanium perfluorobutane sulfonate	144317-44-2
	N,N,N-triethylethanaminium 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate	25628-08-4
	magnesium perfluorobutanesulfonate	507453-86-3
	lithium perfluorobutanesulfonate	131651-65-5
	dimethyl(phenyl)sulfanium perfluorobutanesulfonate	220133-51-7
* HFPO-DA (GenX)		
# CAS-number not found in the OECD PFAS database (column "CAS number" in tab "overview with CAS")		

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Appendix 3: CLP, Annex VI

Table A 3: PFAS categorised as included in the CLP Annex VI in the PRIO tool (<https://www.kemi.se/prioguiden/start>).

Substance	CAS-no
Heptadekafluorooktan-1-sulfonsyra	1763-23-1
1-[3-[4-(Heptadekafluornonyloxi)-benzamido]propyl]-N,N,N-trimetylammoniumjodid	59493-72-0
5-(N-Metylperfluoroktylsulfonamido)metyl-3-oktadecyl-1,3-oxazolidin-2-on och 5-(N-metylperfluorheptylsulfonamido)metyl-3-oktadecyl-1,3-oxazolidin-2-on, blandning	
1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Heptadekafluoro-1-oktansulfonsyra, kaliumsalt	2795-39-3
Perfluoroktansulfonsyra, ammonium salt	29081-56-9
Perfluoroktansulfonsyra, litium salt	29457-72-5
Perfluoroktansulfonsyra, dietanolaminsalt	70225-14-8
Trifenyl(fenylmetyl)fosfonium 1,1,2,2,3,3,4,4,4-nonafluoro-N-metyl-1-butansulfonamid (1:1)	332350-93-3
Ammonium pentadekafluoroktanoat	3825-26-1
Pentadekafluoroktansyra	335-67-1
Natrium-1,1,2,2,3,3,4,4,4-nonafluor-1-butansulfinat	102061-82-5
3-Etoxi-1,1,1,2,3,4,4,5,5,6,6,6-dodekafluoro-2-(trifluorometyl)hexan	297730-93-9
Perfluornonansyra	375-95-1
Nonansyra, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadekafluor-, natrium salt	21049-39-8
Nonansyra, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadekafluor-, ammonium salt	4149-60-4
Nonadekafluorodekansyra	335-76-2
Ammonium nonadekafluorodekanoat	3108-42-7
Natrium nonadekafluorodekanoat	3830-45-3

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Appendix 4: POPs

Table A 4: Text from the consolidated version of the POPs regulation, Regulation (EU) 2019/1021 of the European Parliament and of the Council of 20 June 2019 on persistent organic pollutants, Current consolidated version: 07/09/2020 ELI:

<http://data.europa.eu/eli/reg/2019/1021/oj>, Annex I, Part A.

Substance	CAS-no	Specific exemption on intermediate use or other specification
Perfluorooctane sulfonic acid and its derivatives (PFOS) C ₈ F ₁₇ SO ₂ X (X = OH, Metal salt (O-M ⁺), halide, amide, and other derivatives including polymers)	1763-23-1 2795-39-3 29457-72-5 29081-56-9 70225-14-8 56773-42-3 251099-16-8 4151-50-2 31506-32-8 1691-99-2 24448-09-7 307-35-7 and others	<p>1. For the purposes of this entry, point (b) of Article 4(1) shall apply to concentrations of PFOS equal to or below 10 mg/kg (0,001 % by weight) where it is present in substances or in mixtures.</p> <p>2. For the purposes of this entry, point (b) of Article 4(1) shall apply to concentrations of PFOS in semi-finished products or articles, or parts thereof, if the concentration of PFOS is lower than 0,1 % by weight calculated with reference to the mass of structurally or micro-structurally distinct parts that contain PFOS or, for textiles or other coated materials, if the amount of PFOS is lower than 1 µg/m² of the coated material.</p> <p>3. Use of articles already in use in the Union before 25 August 2010 containing PFOS shall be allowed. Article 4(2), third and fourth subparagraphs shall apply in relation to such articles.</p> <p>► M2</p> <p>4. If the quantity released into the environment is minimised, manufacturing and placing on the market shall be allowed until 7 September 2025 for use as mist suppressant for non-decorative hard chromium (VI) plating in closed loop systems. Provided that those Member States where PFOS is used report</p>

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		<p>to the Commission by 7 September 2024 on progress made to eliminate PFOS and justify the continuing need for this use, the Commission shall review the need for a prolongation of the derogation for this use of PFOS for a maximum of five years by 7 September 2025. ◀</p> <p>Where such a derogation concerns production or use in an installation within the scope of Directive 2008/1/EC of the European Parliament and of the Council (4), the relevant best available techniques for the prevention and minimisation of emissions of PFOS described in the information published by the Commission pursuant to Article 17(2), second subparagraph, of Directive 2008/1/EC shall apply.</p> <p>▶ M2 _____ ◀</p> <p>5. Once standards are adopted by the European Committee for Standardisation (CEN) they shall be used as the analytical test methods for demonstrating the conformity of substances, mixtures and articles to points 1 and 2. Any other analytical method for which the user can prove equivalent performance could be used as an alternative to the CEN standards.</p>
<p>Perfluorooctanoic acid (PFOA), its salts and PFOA-related compounds</p> <p>‘Perfluorooctanoic acid (PFOA), its salts and PFOA-related compounds’ means the following:</p> <p>(i) perfluorooctanoic acid, including any of its branched isomers;</p> <p>(ii) its salts;</p>	335-67-1 and others	<p>1. For the purposes of this entry, point (b) of Article 4(1) shall apply to concentrations of PFOA or any of its salts equal to or below 0,025 mg/kg (0,000025 % by weight) where they are present in substances, mixtures or articles.</p> <p>2. For the purposes of this entry, point (b) of Article 4(1) shall apply to concentrations of any individual PFOA-related compound or a combination of PFOA-related compounds equal to or below 1 mg/kg (0,0001 % by weight) where they are present in substances, mixtures or articles.</p>

<p>(iii) PFOA-related compounds which, for the purposes of the Convention, are any substances that degrade to PFOA, including any substances (including salts and polymers) having a linear or branched perfluoroheptyl group with the moiety (C₇F₁₅)C as one of the structural elements.</p> <p>The following compounds are not included as PFOA-related compounds:</p> <ul style="list-style-type: none"> (i) C₈F₁₇-X, where X = F, Cl, Br; (ii) fluoropolymers that are covered by CF₃[CF₂]_n-R', where R'=any group, n> 16; (iii) perfluoroalkyl carboxylic acids (including their salts, esters, halides and anhydrides) with ≥ 8 perfluorinated carbons; (iv) perfluoroalkane sulfonic acids and perfluoro phosphonic acids (including their salts, esters, halides and anhydrides) with ≥ 9 perfluorinated carbons; (v) perfluorooctane sulfonic acid and its derivatives (PFOS), as listed in this Annex. 		<p>3. For the purposes of this entry, point (b) of Article 4(1) shall apply to concentrations of PFOA-related compounds equal to or below 20 mg/kg (0,002 % by weight) where they are present in a substance to be used as a transported isolated intermediate within the meaning of Article 3 point 15(c) of Regulation (EC) No 1907/2006 and fulfilling the strictly controlled conditions set out in Article 18(4)(a) to (f) of that Regulation for the production of fluorochemicals with a carbon chain equal to or shorter than 6 atoms. This exemption shall be reviewed and assessed by the Commission no later than 5.7.2022.</p> <p>4. For the purposes of this entry, point (b) of Article 4(1) shall apply to concentrations of PFOA and its salts equal to or below 1 mg/kg (0,0001 % by weight) where they are present in polytetrafluoroethylene (PTFE) micropowders produced by ionising irradiation of up to 400 kilograys or by thermal degradation as well as in mixtures and articles for industrial and professional uses containing PTFE micropowders. All emissions of PFOA during the manufacture and use of PTFE micropowders shall be avoided and, if not possible, reduced as far as possible. This exemption shall be reviewed and assessed by the Commission no later than 5.7.2022.</p> <p>5. By way of derogation, the manufacturing, placing on the market and use of PFOA, its salts and PFOA-related compounds shall be allowed for the following purposes: (a) photolithography or etch processes in semiconductor manufacturing, until 4 July 2025; (b) photographic coatings applied to films, until 4 July 2025;</p>
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		<p>(c) textiles for oil- and water-repellency for the protection of workers from dangerous liquids that comprise risks to their health and safety, until 4 July 2023;</p> <p>(d) invasive and implantable medical devices, until 4 July 2025;</p> <p>(e) manufacture of polytetrafluoroethylene (PTFE) and polyvinylidene fluoride (PVDF) for the production of:</p> <p>(i) high-performance, corrosion-resistant gas filter membranes, water filter membranes and membranes for medical textiles;</p> <p>(ii) industrial waste heat exchanger equipment,</p> <p>(iii) industrial sealants capable of preventing leakage of volatile organic compounds and PM2.5 particulates; until 4 July 2023.</p> <p>6. By way of derogation, the use of PFOA, its salts and PFOA-related compounds shall be allowed in fire-fighting foam for liquid fuel vapour suppression and liquid fuel fire (Class B fires) already installed in systems, including both mobile and fixed systems, until 4 July 2025, subject to the following conditions:</p> <p>(a) fire-fighting foam that contains or may contain PFOA, its salts and/or PFOA-related compounds shall not be used for training;</p> <p>(b) fire-fighting foam that contains or may contain PFOA, its salts and/or PFOA-related compounds shall not be used for testing unless all releases are contained;</p> <p>(c) as from 1 January 2023, uses of fire-fighting foam that contains or may contain PFOA, its salts and/or PFOA-related compounds shall only be allowed in sites where all releases can be contained;</p>
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	<p>(d) fire-fighting foam stockpiles that contain or may contain PFOA, its salts and/or PFOA-related compounds shall be managed in accordance with Article 5.</p> <p>7. By way of derogation, the use of perfluorooctyl bromide containing perfluorooctyl iodide for the purpose of producing pharmaceutical products shall be allowed, subject to review and assessment by the Commission by 31 December 2026, every four years thereafter and by 31 December 2036.</p> <p>8 Use of articles already in use in the Union before 4 July 2020 containing PFOA, its salts and/or PFOA-related compounds shall be allowed. Article 4(2), third and fourth subparagraphs shall apply in relation to such articles.</p> <p>9. ►C2 By way of derogation, the manufacturing, placing on the market and use of PFOA, its salts and PFOA-related compounds shall be allowed until 3 December 2020 for the following purposes: ◄</p> <ul style="list-style-type: none">(a) medical devices other than implantable ones, within the scope of Regulation (EU) 2017/745 (8);(b) latex printing inks;(c) plasma nano-coatings.
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Appendix 5: Criteria for PFOA, its salts and PFOA-related compounds in the POPs regulation

Table A 5: Criteria applied to manually filter out CAS numbers covered by the POPs regulation. “Structure category” is an already existing categorisation in the OECD PFAS database. The columns “Selection” and “Comment” describe the further categorisations made herein.

POPs: Regulation (EU) 2019/1021 of the European Parliament and of the Council of 20 June 2019 on persistent organic pollutants (Text with EEA relevance.)		
Criteria for categorisation of PFOA, its salts and PFOA-related compounds		
Structure category	Selection	Comment
Cat. 100 Perfluoroalkyl carbonyl compounds	<ol style="list-style-type: none"> 1. Included: perfluoroalkyl chain ≥ 7 <i>Uncertainty: Chain lengths with R/O/H/DB/Cl/Br/I or “unclear”</i> 2. Removal from above (1): <ol style="list-style-type: none"> a. (exception iii) PFCA+salt+ester cat. 102 perfluoroalkyl chain ≥ 8 (not including “unclear”); <i>Uncertainty: Chain lengths with R/O/H/DB/Cl/Br/I</i> b. (exception iii) Halides cat. 101 perfluoroalkyl chain ≥ 8 <i>Uncertainty: Chain lengths with R/O/H/DB/Cl/Br/I (no hits)</i> c. Not PFAA precursor: (Potential) precursor to PFAAs in the environment/biota “0”, in all cat. but 102 	<p>Note that 2c was not applied to cat. 102 as that would remove PFOA.</p> <p>Note no anhydride in 2a.</p> <p>Note 2c means all esters are assumed to degrade to PFAA.</p>
Cat. 200 Perfluoroalkane sulfonyl compounds	<ol style="list-style-type: none"> 1. Included: perfluoroalkyl chain ≥ 8 <i>Uncertainty: Chain lengths with R/O/H/DB/Cl/Br/I or “unclear”</i> 	<p>Note 8 perfluorinated carbon atoms to achieve (C₇F₁₅)C structure.</p>

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	<ol style="list-style-type: none"> 2. Removal from above (1): <ol style="list-style-type: none"> a. (exception iv) Halides cat. 201 perfluoroalkyl chain ≥ 9 b. (exception iv) PFSA+salt+ester cat. 202 perfluoroalkyl chain ≥ 9 c. (exception v) Cat. 200 perfluoroalkyl chain = 8 <i>Uncertainty: Chain lengths with R/O/H/DB/Cl/Br/I</i> d. Cat. 206, 207, 208, 209 e. Not PFAA precursor: (Potential) precursor to PFAAs in the environment/biota "0" 	<p>Note no anhydride in 2b.</p> <p>Note that 2c includes CAS-numbers covering several perfluorinated chain lengths including 8.</p> <p>Removal 2d. justified by functional groups in both ends of structure.</p> <p>Note Removal 2e overwrites some previous removals.</p>
Cat. 300 Perfluoroalkyl phosphate compounds	<ol style="list-style-type: none"> 1. Included: perfluoroalkyl chain ≥ 8 <i>Uncertain: Chain lengths with R/O/H/DB/Cl/Br/I or "unclear"</i> 2. Removal from above (1): <ol style="list-style-type: none"> a. (exception iv) Cat. 302 perfluoroalkyl chain ≥ 9 b. Not PFAA precursor: (Potential) precursor to PFAAs in the environment/biota "0". 	<p>Note 8 perfluorinated carbon atoms to achieve (C₇F₁₅)C structure.</p> <p>Note Removal 2b overwrites some previous removals.</p>
Cat. 400 Fluorotelomer-related compounds	<ol style="list-style-type: none"> 1. Included: perfluoroalkyl chain ≥ 7 <i>Uncertainty: Chain lengths with R/O/H/DB/Cl/Br/I or "unclear"</i> 2. Removal from above (1): <ol style="list-style-type: none"> a. Cat. 401, if perfluoroalkyl chain is = 7 it is not a C₇F₁₅C b. Not PFAA precursor: (Potential) precursor to PFAAs in the environment/biota "0" (no hits) 	<p>Note CAS-numbers with several chain lengths including also 7 were not excluded in 2a.</p>

<p>Cat. 500 Per- and polyfluoroalkyl ether-based compounds</p>	<ol style="list-style-type: none"> 1. Included: perfluoroalkyl chain ≥ 7 <i>Uncertainty: All categorised as perfluoroalkylether chains are generally very stable</i> 2. Removal from above (1): <ol style="list-style-type: none"> a. Substances with ether bonds in the $C_7F_{15}C$ structure (perfluorinated chain length 7-8) b. Substances categorised not to be (potential) precursor to PFAAs in the environment/biota, "0" 	<p>Beyond scope to study the structure of each individual compound included (n=94) Note CAS-numbers with several chain lengths including also 7-8 were not excluded in 2a. Note Removal 2b overwrites some previous removals.</p>
<p>Cat. 600 Other PFAA precursors and related compounds - perfluoroalkyl ones</p>	<ol style="list-style-type: none"> 1. Included: perfluoroalkyl chain ≥ 7 <i>Uncertainty: Chain lengths with R/O/H/DB/Cl/Br/I or "unclear"</i> 2. Removal from above (1): <ol style="list-style-type: none"> a. Perfluoroalkyl chain =7 in cat. 601, 602, 612, 613, 614, not $C_7F_{15}C$ b. Substances categorised not to be (potential) precursor to PFAAs in the environment/biota, "0" 	<p>Note CAS-numbers with several chain lengths including also 7 were not excluded in 2b.</p>
<p>Cat. 700 other PFAA precursors or related compounds - semifluorinated</p>	<ol style="list-style-type: none"> 1. Included: perfluoroalkyl chain ≥ 7 <i>Uncertainty: Chain lengths with R/O/H/DB/Cl/Br/I or "unclear"</i> 2. Removal from above (1): <ol style="list-style-type: none"> a. Cat. 702.1 and cat. 702.3 if perfluorinated chain =7, not $C_7F_{15}C$ b. Substances categorised not to be (potential) precursor to PFAAs in the environment/biota, "0" (no hits) 	

Cat. 800 Fluoropolymers	<ol style="list-style-type: none"> 1. Included: perfluoroalkyl chain ≥ 7 <i>Uncertainty: C₇F₁₅C moiety in cat. 800, cat. 803, cat. 804, cat. 810</i> 2. Removal from above (1): <ol style="list-style-type: none"> a. (exception ii) CF₃[CF₂]_n-R n>16, i.e., perfluorinated chain length n>18 b. Removal from above (1): Cat. 802, cat. 805, cat. 806, 807, 808, 809 as not C₇F₁₅C 	<p>Note Removal 2a assumes CF₃ end on PTFE.</p> <p>Note removal 2b overwrites some 2a.</p> <p>Note that all included was also excluded with 2a.</p>
<p>Notes:</p> <ul style="list-style-type: none"> • Exceptions are compounds identified in the legal text as not included as PFOA-related compounds, herein referred to within brackets as exception i-v referring to definitions in the legal text. • Categorisation for substances with chain lengths with R/O/H/DB/Cl/Br/I or “unclear” was set to uncertain, i.e., “orange”. The O/H/DB/Cl/Br/I insertion may interrupt a consecutive perfluorinated chain length as in PFOA. Chain lengths with “R” is the cyclic isomer and it was assessed as uncertain how it is covered by the legislation. • Cat. 800 fluoropolymers was included herein for completeness but did not generate any hits. 		

Appendix 6: Derivative PFAS database

The derivative PFAS database based on the OECD PFAS database (OECD 2018) is appended as the file POPFREE-D4.3-database.xlsx (<https://www.diva-portal.org/smash/get/diva2:1715096/FULLTEXT07.zip>)

Note that this derivative database contains the OECD Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs) and that the categorisations as explained in this report were only added on top of this comprehensive database.