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Technical work: process for the evaluation of perfluorooctane sulfonic acid, its salts and perfluorooctane sulfonyl fluoride pursuant to paragraphs 5 and 6 of part III of Annex B to the Stockholm Convention on Persistent Organic Pollutants

Report on the assessment of alternatives to perfluorooctane sulfonic acid, its salts and perfluorooctane sulfonyl fluoride

Note by the Secretariat

1. At its tenth meeting, the Persistent Organic Pollutants Review Committee completed the assessment of alternatives to perfluorooctane sulfonic acid (PFOS), its salts and perfluorooctane sulfonyl fluoride (PFOSF) in accordance with paragraph 3 of decision SC-6/4.

2. By decision POPRC-10/4, the Committee decided to submit the summary of the report on the assessment of alternatives to PFOS, its salts and PFOSF set out in the annex to that decision, together with the full report on the assessment of alternatives to PFOS, its salts and PFOSF set out in the annex to the present note, and the fact sheets on alternatives to those chemicals set out in the annex to document UNEP/POPS/POPRC.10/INF/8/Rev.1, to the Conference of the Parties for consideration at its seventh meeting. The present note, including its annex, has not been formally edited.

* Reissued for technical reasons on 12 December 2014.

Annex

Report on the assessment of alternatives to perfluorooctane sulfonic acid, its salts and perfluorooctane sulfonyl fluoride

Persistent Organic Pollutants Review Committee

30 October 2014

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Disclaimer

1. In conducting assessment of potential alternatives that are suitable substitutes for persistent organic pollutants (POPs), the criteria in paragraph 1 of Annex D to the Stockholm Convention on POPs should be taken into consideration to ensure that an alternative does not lead to the use of other chemicals that may be a POP. This report provides hazard-based information on the alternatives to perfluorooctane sulfonic acid (PFOS), its salts and perfluorooctane sulfonyl fluoride (PFOSF). The results of assessment in this report are based on an analysis on a screening level as to whether or not the identified alternatives to PFOS meets the numerical thresholds in Annex D, but does not analyze monitoring data or other evidence as provided for in Annex D. It should be noted that the assessment is not equivalent to the work undertaken by the Committee in examining proposals submitted by Parties for listing of chemicals under the Convention in accordance with paragraph 3 of Article 8 of the Convention.

2. Selection of the alternatives is described in section 3.1. More alternative substances might be commercially available but detailed information on them was not provided from primary sources. The assessment of the alternatives in this report should not be seen as a comprehensive and in depth assessment of all available information as only a limited number of databases and a limited amount of primary sources have been consulted

3. Parties may use this report when choosing alternatives to PFOS, its salts and PFOSF as an initial source of information. It should be noted that substances which have been identified in this report as not likely to be a POP, may still exhibit hazardous characteristics. As indicated in the General guidance[1] on considerations related to alternatives and substitutes for POPs, where possible, efforts should be made to collect information to ensure that alternatives do not exhibit hazardous properties and that the risk of alternatives is considerably lower than that of the POP they replace. It is therefore strongly recommended that further assessment of alternatives to PFOS, its salts and PFOSF identified in this report is carried out by Parties within their national framework of authorization before considering such substances as suitable alternatives.

1 Background

4. Perfluorooctane sulfonic acid, its salts and perfluorooctane sulfonyl fluoride are listed in Annex B to the Convention.

5. Paragraph 5 of part III of Annex B to the Convention provides that the Conference of the Parties shall evaluate the continued need for PFOS, its salts and PFOSF for the various acceptable purposes and specific exemptions listed in Annex B on the basis of available scientific, technical, environmental and economic information. As stated in paragraph 6 of part III of Annex B to the Convention, the evaluation shall take place no later than in 2015 and every four years thereafter, in conjunction with a regular meeting of the Conference of the Parties.

6. By decision SC-6/4, the Conference of the Parties adopted a process to enable it to undertake the evaluation of PFOS, its salts and PFOSF in accordance with paragraphs 5 and 6 of part III of Annex B to the Convention. In this decision, the Conference of the Parties requested the Persistent Organic Pollutants Review Committee, with the support of the Secretariat, to prepare a report on the assessment of alternatives to PFOS, its salts and PFOSF to assist it in undertaking the evaluation. The report is to be developed on the basis of information on the availability, suitability and implementation of such alternatives and any other relevant information.

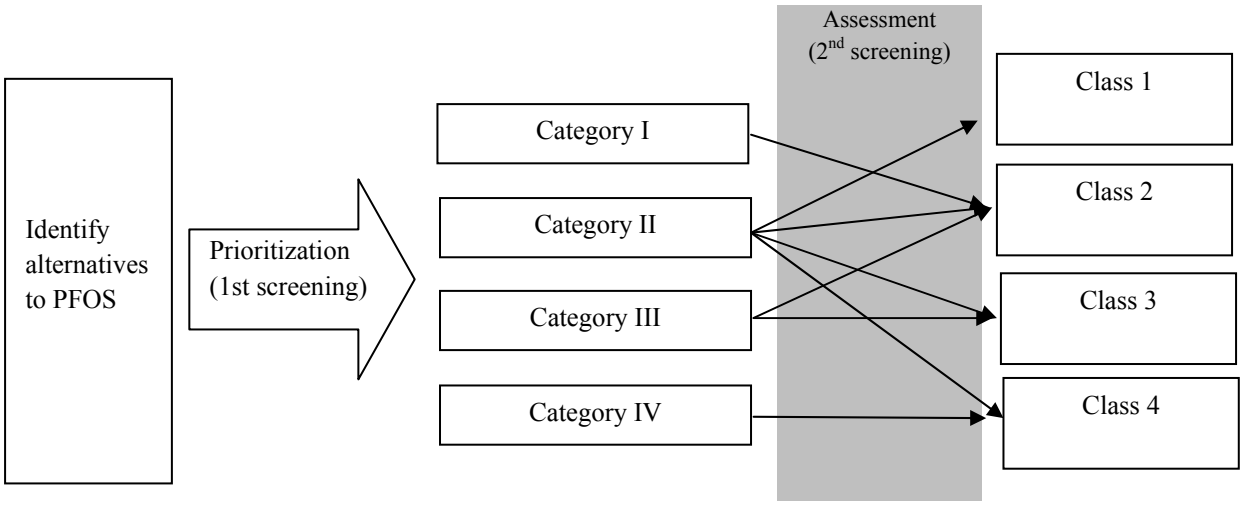
7. By decision POPRC-9/5, the Committee adopted terms of reference[2] for the assessment of alternatives to PFOS, its salts and PFOSF and the preparation of a report for the evaluation of information on PFOS, its salts and PFOSF. A working group was established by the Committee to undertake the activities assigned to it in the terms of the reference. The current report was prepared by the working group, with the support of the Secretariat, for consideration by the Committee at its tenth meeting.

8. In accordance with the terms of reference, the assessment of alternatives to PFOS, its salts and PFOSF has been undertaken by applying the methodology used by the Committee in the assessment of alternatives to endosulfan.[3] This methodology consists of a two-step screening process. In the first step, the alternatives to PFOS were subject to prioritization to screen for those alternatives that had a potential to be POPs and to identify those that were unlikely to be POP substances. To prioritize the alternatives, bioaccumulation (B) and persistence (P) (i.e., criteria (c) and (b) of Annex D to the Convention) were used. The second step consisted of a more detailed assessment of the POPs characteristics of alternatives that had been identified as having a potential to be POPs. Substances that had been identified as unlikely to be POP substances were not further analysed in the second step. In the assessment step, alternatives to PFOS were classified according to their likelihood to meet all the criteria of Annex D. The methodology used for the current report is summarised in graphical form in the figure below.

[1] UNEP/POPS/POPRC.5/10/Add.1.

[2] Annex to decision POPRC-9/5.

[3] UNEP/POPS/POPRC.8/INF/28.



9. The results of assessment are based on an analysis on a screening level as to whether or not the identified alternatives to PFOS meets the numerical thresholds in Annex D but does not analyze monitoring data or other evidence as provided for in Annex D. The assessment is not equivalent to the work undertaken by the Committee in examining proposals submitted by Parties for listing of chemicals under the Convention in accordance with paragraph 3 of Article 8 of the Convention.

10. In accordance with the terms of reference, the assessment of alternatives to PFOS, its salts and PFOSF was based on information on alternatives to PFOS, its salts, PFOSF and their related chemicals.[4] This assessment also includes information on manufacturing intermediates used in the manufacture of certain PFOS alternatives. It should be understood that these manufacturing intermediates are not in of themselves alternatives to PFOS. However, as some of these manufacturing intermediates present evidence of harmful characteristics, it is believed that this information may be of assistance in considering alternatives.

2 Identification of alternatives

2.1 Sources of information

11. In accordance with decision POPRC-9/5, information on alternatives to PFOS was collected from parties and observers using the format developed by the Committee.[5] The information submitted by parties (11) and others (3) is available on the website of the Stockholm Convention.[6]

12. In addition, information on the identity of alternatives to PFOS was compiled from the Guidance on alternatives to PFOS, its salts and PFOSF and their related chemicals[7] and the Technical paper on the identification and assessment of alternatives to the use of PFOS, its salts and PFOSF and their related chemicals in open applications.[8] Both documents had been developed on the basis of information about alternatives to PFOS provided by parties and observers. Information was also obtained from recent publications on this topic.[9]

13. In identifying alternatives to POPs, the list of alternatives should include not only alternative chemicals that can be used without major changes in products or processes in which they are used, but also innovative changes in the design of products, industrial processes and other practices that do not require the use of POPs.[10] Available information on such changes and practices to substitute for the use of PFOS in a number of applications is summarized in appendix 5 to this report. These alternatives are not further considered in this report since the methodology used for the current assessment is applicable to chemical substances only and a comprehensive

[4] Related chemicals are chemicals that contain the structural element PFOS in their molecular structure and are or were produced with PFOSF as a starting or intermediate material.

[5] UNEP/POPS/POPRC.9/INF/10/Rev.1.

[6] http://chm.pops.int/TheConvention/POPsReviewCommittee/Meetings/tabid/3565/Default.aspx

[7] UNEP/POPS/POPRC.9/INF/11/Rev.1.

[8] UNEP/POPS/POPRC.8/INF/17/Rev.1.

[9] ENVIRON, Assessment of POP Criteria for Specific Short-Chain Perfluorinated Alkyl Substances, project number: 0134304A, (2014) ; OECD, "Synthesis paper on per- and polyfluorinated chemicals (PFCs)", (2013) ; Nordic Council of Ministers, Per- and polyfluorinated substances in the Nordic Countries,Use, occurence and toxicology", TemaNord 2013:542, ISBN: 978-92-893-2562-2, (2013), http://dx.doi.org/10.6027/TN2013-542

[10] Guidance on considerations related to alternatives and substitutes for listed persistent organic pollutants and candidate chemicals indicates (UNEP/POPS/POPRC.5/10/Add.1).

assessment of the suitability of non-chemical alternatives was beyond the resources and time available for its preparation of the current report.

2.2 Description of alternatives to PFOS

14. In total 58 alternatives were identified (see appendix 1 to this report). The alternatives to PFOS can be classified according to their occurrence as components of commercial products that are used in the applications listed as specific exemptions and acceptable purposes in Annex B to the Convention (44 alternatives, thereinafter referred to as commercial products), manufacturing intermediates (10 alternatives), or transformation products (4 alternatives). For the purposes of this report, manufacturing intermediates are defined as chemicals used in the manufacture and/or synthesis of other alternatives to PFOS. Transformation products are substances that are formed as a result of abiotic or biotic transformation of another substance.

15. As described in the table in appendix 1 to this report, the alternatives are used in wide range of applications that are listed as specific exemptions and acceptable purposes in Annex B to the Convention. Alternatives could be identified from the sources described in section 3.1 for most of these applications, except for chemically driven oil production, photo-imaging, etching agent for compound semiconductors and ceramic filters, photo masks in the semiconductor and liquid crystal display industries, electric and electronic parts for some printers and colour copy machines and certain medical devices. Additional information may be found in document UNEP/POPS/POPRC.10/INF/10. Given the range of applications, the alternatives have diverse functions and can have quite different properties. The alternatives include both fluorinated and non-fluorinated substances.

16. Chemical Abstract Service (CAS) numbers could not be obtained for a number of alternatives listed in the table in appendix 1 to this report. This was an impediment for obtaining information about these alternatives as CAS numbers are essential for retrieving substance-specific information from the majority of databases. 11 of the alternatives are commercialised under brand names by various companies. While some are described as polymers by the companies that sell them, information about the exact composition of these products is not publicly available and commercial brands could therefore not be assessed..

2.3 Information on the availability, suitability and implementation of alternatives.

17. As described in section 3.1 above, alternatives to PFOS were identified on the basis of information provided by parties about those substances that were available and implemented in their country for substituting the use of PFOS in the applications listed in Annex B to the Convention as specific exemptions and acceptable purposes. Material safety data sheets could be identified for the majority of alternatives to PFOS listed in appendix 1 to this report, indicating that they are commercialised.The majority of alternatives to PFOS identified as commercial products are also commercialised under brand names by various companies. However, some alternatives may be available only in some countries and may not be accessible globally. Pesticides in particular are subject to registration requirements before being allowed on the market in most countries.

18. In assessing potential alternatives that are suitable substitutes for POPs, it should be confirmed that an alternative does not lead to the use of other chemicals that may have the properties of POPs as defined by the criteria in Annex D of the Convention.[10] Accordingly, this report provides an assessment of POPs properties for alternatives to PFOS. Alternatives also need to be technically and economically feasible. The commercial availability of an alternative is an important indicator of technical feasibility.[10] As described above, the majority of alternatives to PFOS identified in this report are known to be commercially available.

19. The technical and economic feasibility of an alternative are heavily influenced by the specific requirements of the user (a company, an industry or sector) of the alternative and the conditions prevailing in the country where the user operates. In addition, determining the technical feasibility of an alternative requires detailed information about the performance of the alternative for a specific use and the expertise to assess this information. For example, in the case of the use of PFOS in fire-fighting foams, PFOS has been applied in aqueous film forming foams that are used to put out fires involving flammable liquids (class B fires). While a number of fire fighting foams are commercially available that do not contain PFOS, detailed information about their effectiveness specifically in quenching class B fires is necessary for assessing their technical feasibility. Although some information was provided by parties and observers regarding the implementation of alternatives to PFOS in their country and cost considerations associated with the use of such alternatives,[11] the information provided was not sufficient to support a detailed assessment of their technical and economic feasibility.

[11] Summarised in the Technical paper on the identification and assessment of alternatives to the use of PFOS, its salts and PFOSF and their related chemicals in open applications ; see also http://chm.pops.int/TheConvention/POPsReviewCommittee/Meetings/tabid/3775/Default.aspx

3 Prioritization of chemical alternatives to PFOS with respect to the persistent organic pollutant characteristics

3.1 Introduction

20. This chapter addresses the prioritization of alternatives to PFOS to identify those that should be further assessed with respect to their POPs characteristics as defined by the criteria in paragraph 1 of Annex D to the Convention. Given the limited time and resources available to prepare this report, this step was also applied to screen out alternatives that are unlikely to be bioaccumulative or persistent and thereby restrict the detailed assessment to a smaller number of alternatives. The methodology used for the prioritization is adapted from the report on the assessment of chemical alternatives to endosulfan[12] as indicated in the terms of reference[13] for this report.

21. The following four transformation products were not considered in the prioritization step or further analyzed in this report: perfluorohexanoic acid, perfluorohexanoic acid sodium salt, perfluorobutanoic acid, perfluoroheptanoic acid. Although consideration of transformation products may be relevant for the assessment of some alternatives to PFOS, their inclusion is outside of the mandate and scope of the current assessment which is intended to be a rapid screening of alternatives and not an extensive analysis of all possible degradation products of those alternatives.

22. The remaining identified 54 substances classified as commercial products or manufacturing intermediates, were included in the prioritization analysis. Components of commercial products that are used in the applications listed as specific exemptions and acceptable purposes in Annex B to the Convention are considered to be functional alternatives to PFOS, its salts, PFOSF and their related chemicals. Furthermore, as set out in Part I of Annex B to the Convention, the production and use of PFOS, its salts and PFOSF are allowed for production , or as an intermediate in the production of other chemicals to be used in the applications listed as acceptable purposes and specific exemptions. Accordingly, alternatives to PFOS classified as manufacturing intermediates (see appendix 1 to this report) were also included in the prioritization analysis.

23. Among the commercial products, the following 8 pesticides were previously included in the assessment of alternatives to endosulfan: abamectin, cypermethrin, chlorpyrifos, deltamethrin, fenitrothion, fipronil, imidacloprid, pyriproxyfen. Data for bioaccumulation, persistence and other hazard endpoints for these substances were obtained from the report on the assessment of alternatives to endosulfan. However, PB-scores (see section 4.3.2) were generated for these substances as part of the current assessment, as a new version of EPISUITE had become available since the endosulfan report was developed, thus leading to slightly different model outcomes.

3.2 Endpoint and data selection for prioritisation

24. To obtain a reliable database for prioritization, experimental as well as QSARs/modelled data were collected for each chemical to address bioaccumulation (B) and persistence (P) (i.e., criteria (b) and (c) of Annex D to the Convention). The two criteria were used in combination to reduce the uncertainty in selecting for substances that have a potential to be POPs.

25. Experimental data on persistence (P) (degradation half life in soil, water and sediment) and bioaccumulation (B) (aquatic bioconcentration factor (BCF) and log Kow) were compiled where available from publicly available databases and sources provided by parties and observers. In addition, for fluorinated substances, a search for data on biomagnification potential (biomagnification factor (BMF) or trophic magnification factor (TMF)) was conducted. For alternatives to PFOS, the information collected is presented in the table in appendix 2 to this report, whereas the manufacturing intermediates for alternatives to PFOS are presented in appendix 3 to this report.

3.3 Sources of information

3.3.1 Experimental information

26. The main databases consulted were eChemPortal,[14] Pesticide Properties DataBase (PPDB) and ChemSpider.[15]

27. eChemPortal provides free public access to information on chemical properties and direct links to collections of information prepared for government chemical review programmes at national, regional, and international levels. Access to information on existing chemicals, new industrial chemicals, pesticides and biocides is provided. eChemPortal also makes available national/regional classification results according to national / regional hazard

[12] UNEP/POPS/POPRC.8/INF/28.

[13] Decision POPRC-9/5.

[14] OECD Global Portal to Information on Chemical Substances; http://www.echemportal.org/echemportal

[15] Chem-phys data Chemspider; http://www.chemspider.com/

classification schemes or according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS).[16] In addition, eChemPortal provides also exposure and use information on chemicals.

28. The PPDB (Pesticide Properties Data Base) is a comprehensive relational database of pesticide physicochemical, toxicological, ecotoxicological and other related data. Reliable sources of information for pesticide properties are monographs produced as part of the EU review process and published by EFSA (European Food Safety Agency). These documents have been used in priority for putting together the data in the PPDB. Where EFSA documents are not available, alternative sources are used (e.g. data published by national government departments, peer-reviewed scientific publications, other databases). PPDB was consulted for data on hydramethylnon as this database was also used for the assessment of alternatives to endosulfan. Given that the majority of PFOS alternatives are not pesticides, the PPDB was relevant for hydramethylnon only.

29. ChemSpider is a free chemical database, owned by the Royal Society of Chemistry. This database is a useful instrument to find physical and chemical properties of substances and to find the valid Simplified Molecular Input Line Entry Specifications (SMILES) for further calculating parameters by EPIWEB 4.1.

3.3.2 Modelling information

30. In cases where experimental data were not available modelled data for persistence and bioaccumulation were based on QSAR estimates. Such data were generated using EPIWEB 4.1[17] and the PB-score tool.[18]

31. EPIWB 4.1 with the Estimation Programs Interface Suite (EPI Suite^{TM}) software is developed by US EPA and publicity available on the internet. This modelling programme is used to estimate properties related to a chemical's environmental transport and fate. This information is used to support regulatory decisions in the new chemicals program and in other existing chemical assessment activities. Governmental and private organizations within the United States and elsewhere make extensive use of this software in supporting decisions regarding new and existing chemicals. The widespread use of this software for a number of different purposes stems, in part, from its utilization and integration of available science in combination with its ease of operation, transparency, and cost-effectiveness. There are other modelling programmes available, but EpiSuite is publicly accessible and a widely referenced modelling programme.

32. The PB-score tool, developed at RIVM,[19] uses QSAR estimations for screening on persistence and bioaccumulation and generates a score, which reflects the chance that a certain substance is persistent in the environment, and bioaccumulating. It is developed as a first tier in the evaluation of PBT[20] and POP substances. It should be noted that the bioaccumulation potential of fluorinated chemicals might not be estimated correctly by the tool as it mainly focuses on passive bioaccumulation in fatty tissues, relevant for hydrophobic substances. However, the underlying US-EPA models have been updated for the fluorinated substances recently,[21] Furthermore, the PB-score screening is conservative, as it is considered preferable to end up with false positives than with false negatives. Those false positives should be screened out as a result of more in depth assessment based on experimental data whenever available.

33. The overall PB-score varies between 0 and 2. Cut-off values complying with the formal screening criteria in Annex D are ≥0.5 for the P-score as well as the B-score. Thus substances with a PB score of ≥1.5 will have individual P or B-scores of 0.5 or higher and comply with both criteria, whereas substances with a PB-score between 1 and 1.5 might fulfil both criteria or not.

3.4 Data quality and uncertainties

34. The main source of information on the name and identity of alternatives to PFOS was the reports submitted by parties and observers about the use of alternatives in their countries in the intersessional period, along with the documents referred to in paragraph 12. The accuracy and comprehensiveness of the information presented in appendix 1 to this report therefore depend on the ability of parties and observers to make such information available. Alternatives to PFOS were not reported for a number of applications listed in part I of Annex B to the Convention. Additional information may be found in document UNEP/POPS/POPRC.10/INF/10. In some cases, only the brand names, and not the chemical identity, of the alternatives to PFOS were reported, making it difficult to further obtain data on the properties of these alternatives.

[16] http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html" \t "_blank

[17] EPIWB 4.1 (US EPA, 2011). Estimation Programs Interface Suite Programs Interface Suiteep://www.United States Environmental Protection Agency, Washington, DC, USA.

[18] http://www.rivm.nl/bibliotheek/rapporten/601356001.html.

[19] Rijksinstituut voor Volksgezondheid en Milieu

[20] Persistent, Bioaccumulative and Toxic (PBT)

[21] http://www.epa.gov/oppt/exposure/pubs/updates_episuite_v4.11.revised.htm

35. When available, experimental data were used in the analysis for the prioritization of alternatives to PFOS. However, one major limitation of this exercise was the scarcity of data in public databases about many of the alternatives. For fluorinated substances, no data on BMF or TMF was available from the sources consulted. For chemicals for which experimental data for persistence were not available, modelled data were considered in the prioritization.

36. Available modelling tools are not ideal for generating estimated data on persistence and bioaccumulation for all PFOS alternatives. A number of estimation programs are available in EPI Suite™. These programs use the so-called fragment method and for organic substances, generate estimates of physical/chemical property and environmental fate based on the contribution of the hydrocarbon chains ($–CH_2-$ or $-CH_3$ fragments). These programs are thus most suitable for estimating data for PFOS alternatives that are pure hydrocarbons such as the aromatic substances. The United States Environmental Protection Agency has recently updated EPI Suite to improve the prediction of persistence and bioaccumulation of fluorinated substances[22]. However, these programs are still less accurate for generating modelled data for fluorinated organic alternatives than for the non-fluorinated organic alternatives.

3.5 Data analysis

37. In the next step, the collected numerical data were compared to benchmarks/cut off values in order to classify the substances within four categories. Cut off values were selected for the four categories to allow a ranking from a higher likelihood to be a POP (category I) to a lower likelihood to be a POP (category IV).

38. The methodology for data analysis used in this report is based on the one used in the assessment of alternatives to endosulfan. As described below, some modifications were made to the methodology used for endosulfan to account for the diverse range of properties of alternatives to PFOS, the low availability of relevant data about these alternatives contained in databases and the properties specific to alternatives that are fluorinated.

39. For the assessment of alternatives to endosulfan, the main criterion considered for bioaccumulation was experimental bioconcentration factor (BCF) and in its absence, log Kow values. For the current analysis, due to the scarcity of experimental BCF data, it was necessary to also include experimental log Kow as a main criterion for bioaccumulation when assessing non-fluorinated alternatives to PFOS. It has been argued that log Kow is not the best method to determine bioaccumulation of fluorinated chemicals because a considerable number of the fluorinated chemicals are surfactants. However, Webster & Ellis (2011)[23] compared measured and modelling data and concluded that for the perfluorinated carboxylic and sulfonic acids, the existing standard equilibrium models, using log Kow, are shown to be applicable. In practice, various authors have used log Kow in modeling the bioaccumulation potential of the fluorinated chemicals (e.g. Howard and Muir, 2010,[24] Rorije et al., 2011,[25] Strempel et al., 2012).[26]

40. Fluorinated chemicals tend to bind to proteins rather than to lipids. The fluorinated chemicals that have been evaluated internationally so far showed biomagnification rather than bioaccumulation. In the proposal to list PFOS under the Stockholm Convention it was indicated that BCFs were smaller than 5000, but biomagnification factors between two trophic levels were between 22 and 160. Howard and Muir (2010) concluded in their modelling study that there might be fluorinated chemicals that do not show to be bioaccumulative according to criteria (c)(i) of Annex D to the Convention (BCF < 5000 or log Kow < 5), but with a relatively high predicted biomagnification in air-breathing organisms. This indicates that, for the prioritization step, substances with BCF < 5000 and/or Log Kow < 5 should still be examined for their potential to bioaccumulate based on biomagnification factor (BMF) or trophic magnification factor (TMF).

41. Nevertheless, screening substances based on BMF or TMF potential is hindered by two factors. First, such data are scarce and are often not incorporated in publicly available databases. Thus, a more labour-intensive detailed search of available data is usually necessary for each individual fluorinated substance. Secondly, biomagnification has not been set as a standard routine in substance risk assessment and thus their determination is characterized by a

[22] http://www.epa.gov/oppt/exposure/pubs/updates_episuite_v4.11.revised.htm

[23] Webster E.M. & Ellis D.A. (2011). Equilibrium modeling: a pathway to understanding observed perfluorocarboxylic and perfluorosulfonic acid behavior. Environ Toxicol Chem. 30:2229-2236.

[24] Howard, P.; Muir, D. C. G. (2010). Identifying new persistent and bioaccumulative organics among chemicals in commerce. Environ. Sci. Technol. 44: 2277merce.

[25] Rorije, E., Verbruggen, E. M. J., Hollander, A., Traas, T. P., Janssen, M. P. M. Identifying potential POP and PBT substances: Development of a new persistence/bioacumulation-score. RIVM report 601356001, 2011. http://rivm.nl/bibliotheek/rapporten/601356001.html

[26] Strempel S., Scheringer M., Ng C.A., Hungerbühler K. (2012). Screening for PBT Chemicals among the ler K. (2012). 6001.html"bstances: Develo Environ. Sci. Technol. 46:5680g the

variable experimental approach. Often a proper definition of the endpoint is lacking and statistical strength of the approach is not always clear (Krop & DeVoogd, 2008;[27] Borgå et al, 2012).[28]

42. Based on the rationale in the preceding paragraphs, for the prioritization step in the current report, BCF > 5000 and/or a log Kow > 5 are included as criteria for bioaccumulation for fluorinated substances in category I. For fluorinated chemicals not meeting these criteria, a search for data on biomagnification potential (BMF or TMF >1) would be carried out and a decision on the likelihood of the substance to bioaccumulate would be made thereafter, consistent with criteria c (ii) of Annex D to the Convention.

43. The categories and cut-off values for the prioritization step are as follows:

Category I: Potential persistent organic pollutants

Cut-offs: bioaccumulation: experimental BCF > 5000 and/or experimental log Kow > 5 and/or biomagnification factor or trophic magnification factor (BMF/TMF) > 1(for fluorinated substances). Persistence: half-life (experimental) in water greater than two months (60 days), in soil greater than six months (180 days) or sediment greater than six months (180 days).

Category II: Candidates for further assessment

Cut-offs: bioaccumulation: experimental BCF >1000 and/or experimental log Kow > 4 and/or BMF/TMF > 0.5 (for fluorinated substances).

Persistence: A PB-score >1 (P-score >0.5) and/or half life (experimental and/or estimated) in water greater than two months (60 days), in soil greater than six months (180 days) or in sediment greater than six months (180 days). The reason for the selection of a BCF>1000 is that the Annex D criteria for bioaccumulation includes the consideration of other reasons for concern.

Category III: Candidates for further assessment with limited data

Cut-offs: bioaccumulation: no experimental data for BCF and log Kow and for BMF/TMF (for fluorinated substances).

Category IV: Not likely to fulfil the criteria on persistence and bioaccumulation in Annex D

Cut-offs: bioaccumulation: experimental BCF< 1000 and/or experimental log Kow < 4.0 (for non-fluorinated substances) and BMF/TMF values ≤0.5 (for fluorinated substances) and/or persistence: half life (experimental) in water less than 2 month (60 days), in soil less than six months (180 days) and sediment less than six months (180 days).

3.6 Results of the prioritization of the alternatives to PFOS

44. Of the 58 alternatives to PFOS, 54 substances were subject to prioritization, since the four transformation products were not assessed. One substance was selected as category I, 13 substances as category II, 34 substances were category III and 6 substances were selected as category IV. Details to be found in appendix 4 to the present report.

45. Substances in categories I, II and III were subject to further assessment as described in section 5.1. Substances in category IV were not further analyzed.

46. The results of the prioritization are set out below and the list of alternatives to PFOS with data for each endpoint is reported in the table in appendix 2 to this report, with the occurrence of manufacturing intermediates as an example reported in appendix 1 and appendix 3.

(a) Category I. Potential persistent organic pollutants (1 substance):

Fluorinated alternatives

2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl ester (6:2 FMA)**.

[27] Krop H & DeVoogd P. (2008). PERFORCE 2. Task 1. Physicochemical parameters and source markers of PFAS. Amsterdam, IVAM UvA b.v. and IBED. dare.uva.nl/document/129892.

[28] Borguva.nl/doc(2012). Trophic Magnification Factors: Considerations of Ecology, Ecosystems, and Study Design. IAEM 8:64-84.

(b) Category II. Candidates for further assessment (13 substances):

Fluorinated alternatives

1-chloro-perfluorohexyl phosphonic acid;

Non-fluorinated alternatives

Decamethyl cyclopentasiloxane (D5)**;

Dodecamethyl cyclohexasiloxane (D6**);

Octamethyl cyclotetrasiloxane (D4)**;

Octamethyl trisiloxane (MDM)**;

Decamethyl tetrasiloxane (MD2M)**;

Diisoproplynaftalene;

Triisopropylnaftalene;

1-Isopropyl-2-phenyl-benzene;

Diisopropyl-1,1'-biphenyl;

Pesticides

Chlorpyrifos;*

Cypermethrin;*

Deltamethrin;*

*Categorization of these pesticides is based on the results of the assessment of alternatives to endosulfan.

(c) Category III. Candidates for further assessment with limited data: 34 substances:

Fluorinated alternatives

Tris(octafluoropentyl) phosphate;

Tris(heptafluorobutyl) phosphate;

Sodium bis(perfluorohexyl) phosphinate;

Carboxymethyldimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]propylammonium hydroxide;

Tris(trifluoroethyl) phosphate;

Methyl nonafluorobutyl ether;

Methyl nonafluoro isobutyl ether;

3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctane-1-sulphonate potassium salt;

1*H*,1*H*,2*H*,2*H*-Perfluorohexanol or 3,3,4,4,5,5,6,6,6-nonafluorobutyl ethanol**;

2-(6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyloxy)-1,1,2,2-tetrafluoroethane sulfonate;

1,1,2,2,-tetrafluoro-2-(perfluorohexyloxy)-ethane sulfonate;

perfluorohexane ethyl sulfonyl betaine;

Dodecafluoro-2-methylpentan-3-one;

Perfluorohexyl phosphonic acid;

Perfluorobutane sulfonate potassium salt;

Perfluorohexanesulfonate potassium salt**;

3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanol**;

3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctane-1-sulphonate;

Non-fluorinated alternatives

(Hydroxyl) Terminated polydimethylsiloxane;

Di-2-ethylhexyl sulfosuccinate, sodium salt;

Stearamidomethyl pyridine chloride;

Dodecamethyl pentasiloxane (MD3M)**;

Hexamethyl disiloxane (MM or HMDS);

Commercial brands

Polyfox®;

Emulphor® FAS;

Enthone®;

Zonyl®;

Capstone®;

Nuva®;

Unidyne®;

Rucoguard®;

Oleophobol®;

Asahiguard®;

Solvera®.

(d) Category IV. Not likely to fulfil the criteria on persistence and bioaccumulation in Annex D: 6 substances:

Pesticides

Pyriproxyfen;*

Imidacloprid;*

Fipronil;*

Fenitrothion;*

Abamectin;*

Hydramethylnon;

*Categorization of these pesticides are based on the results of the assessment of alternatives to endosulfan.

** Manufacturing intermediate for alternatives to PFOS

3.6.1 Comments on selected alternative substances

47. Twelve of the alternatives to PFOS are commercialized under brand names and described as polymers by the companies that market them (see appendix 1 to this report). Due to their large molecular weight[29] and low mobility in the environment, polymers are thought not to bioaccumulate. It should be noted also that polymers are generally not subject to in-depth exposure and risk assessment. In some countries a registration is not required for polymers in many jurisdictions and that, if registration is judged appropriate, the test information burdens are reduced.[30] Information about the exact composition of the brand name products listed in appendix 1 to this report and the molecular weight of the substances they may contain is however not publicly available. These products were therefore placed in category III and were not further analysed. However, there are ongoing developments, e.g. in the US and the EU, to bring polymers under registration regime. This would generate new information that could be used for future assessments of polymer alternatives.

[29] A polymer has a number-average molecular weight (NAVG MW) in a range that is greater than or equal to 1,000 daltons and less than 10,000 daltons; http://www.epa.gov/oppt/newchems/pubs/polyguid.pdf

[30] Risk and policy analysts limited. Review of REACH with regard to the Registration Requirements on Polymers. 2012. http://ec.europa.eu/enterprise/sectors/chemicals/files/reach/review2012/registr-req-final-report-part-a_en.pdf

4 Methodology for the assessment of persistent organic pollutant characteristics and identification of other hazard indicators for the assessment of alternatives to PFOS

4.1 Introduction

48. Depending on the category in which they had been placed in the prioritization step, the alternatives to PFOS were further assessed and consequently assigned to one of the four classes based on their likelihood to meet all the criteria in Annex D to the Convention. The four classes are as follows:

Class 1: Substances that the committee considered met all Annex D criteria;

Class 2: Substances that the committee considered might meet all Annex D criteria but remained undetermined due to equivocal or insufficient data;

Class 3: Substances that are difficult for classification due to insufficient data;

Class 4: Substances that are not likely to meet all Annex D criteria (b), (c), (d) and (e).

49. The following approach was used for the assessment of substances in each category:

(a) Category I and II: an assessment of POPs characteristics and other hazard indicators (toxicity and ecotoxicity). Compile a detailed fact sheet on the properties selected for assessment when feasible;

(b) Category III: a more exhaustive search for experimental data on bioaccumulation. If such data is obtained, determine if the substance meets the Annex D c) (i) criterion or if it biomagnifies (TMF/BMF>1). If these criteria are met and the substance is considered likely to be bioaccumulative, proceed as described in (a). If no data was obtained, no factsheet is compiled and the substance is **assigned to class 3**;

(c) Category IV: no further action, substances are **assigned to class 4**.

4.2 Properties to be considered

50. The following priorities were considered:

(a) **Substance identity:** CAS no, IUPAC name, molecular weight, chemical structure, chemical group;

(b) **Physical-chemical properties:** vapour pressure, water solubility, partition coefficient;

(i) n-octanol/water (log value), partition coefficient air/water (log value), partition coefficient;

(ii) air/octanol (log value), Henry's Law Constant;

(c) **Bioaccumulation:** experimental BCF and log Kow data (Annex D (c) (i) criterion). For fluorinated substances, data on biomagnification (BMF or TMF). The evidence for assessment was considered reliable when at least two data points were available;

(d) **Persistence:** experimental data when available; modelling data on half-life in water, soil and sediment (Annex D (b) (i) criterion). The evidence for assessment was considered reliable when at least two data points were available;

(e) **Long-range transpor**t: Gather information on experimental and/or estimated half-life data in air (EpiSuite) (Annex D (d) (ii) criterion);

(f) **Ecotoxicity** (Annex D (e) criterion): GHS (global harmonization system) classification[31] (only harmonized classifications were considered) on aquatic toxicity, rated as follows:

Classification	Hazard statement	Ecotoxicity level	Acute effect conc. [mg/L]	Chronic effect conc. [mg/L]
Aquatic chronic 1	H410	Severe	1	0,1
Aquatic chronic 2	H411	High	>1-10	> 0,1 - 1
Aquatic chronic 3	H412	Moderate	>10-100	>1-10
Aquatic chronic 4 Aquatic acute 1	H413	Low	>100	>10

[31] http://www.unece.org/fileadmin/DAM/trans/danger/publi/ghs/ghs_rev04/English/ST-SG-AC10-30-Rev4e.pdf

(i) **Toxicity** (Annex D (e) criterion)**:** GHS [classification31] (only harmonized classifications were considered) on toxicity on humans, rated as follows:

Classification	Hazard statement	Toxicity level
Muta 1A/1B Carc. 1A/1B Repro. 1A/1B Carc 2+STOT RE Skin corr	H340 H350 H360	Severe
Muta 2. Carc 2. Repro 2. Skin irrit. Resp. sens. STOT RE1	H341 H351 H361	High
STOT RE 2 Acute tox 1 Acute tox 2		Moderate
Acute tox 3 Acute tox 4		Low

Additionally, the following hazards were considered:

(a) Acute toxicity;

(b) Mutagenicity;

(c) Carcinogenity;

(d) Toxicity for reproduction;

(e) Neurotoxicity;

(f) Immunotoxicity;

(g) Endocrine disruption;

(h) Mode of action;

(i) Acceptable exposure levels.

4.3 Information sources

51. In order to assess selected alternative substances for PFOS and related substances within the given time frame and resources, preference was given to governmental reports, relevant databases and evaluated peer review data. When information was not available from such sources, a search in the primary literature was carried out, where recent sources were consulted.

4.3.1 Databases consulted as references:

(a) ESIS: http://esis.jrc.ec.europa.eu/index.php?PGM=cla

(i) C&L (Classification and Labelling, Annex VI to EU CLP Regulation 1272/2008)

(ii) Risk Assessment Reports (RAR)

(b) CLP inventory (for endpoints not covered by ESIS):

(i) http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database

(c) EFSA: http://www.efsa.europa.eu/en/search.htm

(d) EU Endocrine Disruption Database:

(i) http://ec.europa.eu/environment/chemicals/international_conventions/index_en.htm

(e) WHO/EPS: http://www.who.int/publications/en/

(f) EPI SUITE: http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

(g) IARC: http://monographs.iarc.fr/ENG/Monographs/PDFs/index.php

(h) International limit values (working place): http://limitvalue.ifa.dguv.de/Webform_gw.aspx

(i) ECETOC: http://www.ecetoc.org/index.phpECOTOX

(j) TOXNET: http://toxnet.nlm.nih.gov/index.html

(k) ECHA information on chemicals: http://echa.europa.eu/nl/information-on-chemicals

4.3.2 Database for peer-reviewed literature:

52. The following database for peer-reviewed literature was used:

Scopus: http://www.scopus.com/

5 Results of the assessment of the persistent organic pollutant characteristics and other hazard indicators of the alternatives to PFOS

53. There were 14 substances identified during the first screening assigned to category I and II. Three of these substances, the pesticides, Chlorpyrifos, Cypermethrin, Deltamethrin, were already considered during the assessment of alternatives to endosulfan. For these substances we refer to document UNEP/POPS/POPRC.8/INF/13. For two fluorinated substances, 6:2 FMA, (CAS No.: 2144-53-8) in category I and 1-chloro-perfluorohexyl phosphonic acid in category II, it was expected, based on past experience, that data limitations would lead to a very incomplete fact sheet. In a prescreening, the availability on bioaccumulation data was checked and as these were not readily available during drafting the current document, these were assigned to class 3. Therefore, nine factsheets have been developed (see document UNEP/POPS/POPRC10/INF/8).

54. The summary factsheets provide an indication as to whether or not the alternative substance meets the numerical thresholds in Annex D to the Convention, but do not analyze monitoring data or other evidence in depth so failure to meet the thresholds should not be taken as a determination that the alternative substance is not a POP. Furthermore, not all criteria of Annex D were considered for the assessment such that the conclusions regarding certain alternatives may change in light of information for other Annex D criteria. As an overview, a table summarizing the data contained in the factsheets for the endpoints considered in the assessment is set out in appendix 4 to this report.

55. For substances in category III, a search was performed for experimental data on bioaccumulation. If such data were not available, which was expected for a considerable number of substances, no further assessment was carried out and substances were assigned to class 3. This methodology was also applied to the fluorinated chemicals in category I (6:2 FMA, CAS No.: 2144-53-8) and category II (1-chloro-perfluorohexyl phosphonic acid). The results are presented in table 1 below. For 5 substances in category III and for 6:2 FMA, registration dossiers under REACH[32] were available in ECHA's database on information on chemicals. Experimental data on bioaccumulation could be obtained for five of the substances. None of the dossiers contained information on BMF/TMF, which was considered to be essential to make a proper judgement for the fluorinated chemicals. The non-fluorinated substances for which the Annex D (c) (i) criterion was not met were assigned to class 4. The fluorinated substances for which no BMF/TMF data were available were assigned to class 3.

[32] Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals.

Table 1: Results of the assessment of the bioaccumulation potential of substances in category III for which a REACH registration dossier was available.

Substance name	Cas. No.	Bioaccumulation Experimental BCF	Reference	Class assigned
1-Octanol, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro- (6:2 FTOH)	647-42-7	BCF: 29, 8.4-58, 24-99, 46, ≤ 36, no data on BMF/TMF	http://echa.europa.eu/information-on-chemicals	3
2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl ester (6:2 FMA)	2144-53-8	BCF: 268, no data on BMF/TMF	http://echa.europa.eu/information-on-chemicals	3
Perfluoro-2-methylpentan-3-one	756-13-8	BCF < 1, no data on BMF/TMF	http://echa.europa.eu/information-on-chemicals	3
Di-2-ethylhexyl sulfosuccinate, sodium salt	577-11-7	No data available on BCF, no data on BMF/TMF	http://echa.europa.eu/information-on-chemicals	3
Hexamethyl disiloxane (MM or HMDS)	107-46-0	BCF: 776, 1290, 1660 and 2410	http://echa.europa.eu/information-on-chemicals	4
Dodecamethyl pentasiloxane (MD3M)	141-63-9	BCF: 1240 and 1430	http://echa.europa.eu/information-on-chemicals	4

5.1 Data availability and uncertainties

56. Consistent with the methodology used for the assessment of alternatives to endosulfan, the assessment of the 9 substances in category II was based on data available from databases and governmental reports and additional information from parties and observers. However, the availability of such data for alternatives to PFOS, which are in majority industrial chemicals, is relatively low and comparatively much lower than for pesticides. The number of peer-reviewed studies from primary literature that was available as second-line references was also limited for the assessed alternatives to PFOS. The conclusions on some of the alternatives may thus change when more data become available.

57. The scarcity of data on alternatives to PFOS has been one of the major limitations for their assessment as undertaken in this report. A large number of substances were assigned to category III at the prioritization step and could not be further analysed due to lack of data.

58. For bioaccumulation, persistence and long-range transport, the factsheets compiled for the substances in category II provide an analysis of whether the substances meet the numerical thresholds in Annex D but not of other evidence as provided for in Annex D such as monitoring data (see section 5.2). Therefore consideration of data on other Annex D criteria might change the conclusions on some substances. Moreover, failure to meet the thresholds should be considered as likelihood rather than as evidence that the substance is not a POP.

6 Conclusions of the screening assessment on persistent organic pollutants characteristics of alternatives to PFOS

59. Based on the results of the screening assessment the conclusions below are suggested. However, the assessment provides only an indication as to whether or not the alternative substances meet the numerical threshold in Annex D to the Convention, and does not analyse monitoring data or other evidence as provided for in Annex D, so failure to meet the thresholds should not be taken as a determination that the alternative substance is not a POP. Furthermore this work is only a first screening indicating the likelihood and not a definite classification of the substances concerning their POP characteristics.

Class 1: Substances that the committee considered met all Annex D criteria

Non florinated alternatives (1 substance)	
CAS No	**Substance**
556-67-2	Octamethyl cyclotetrasiloxane (D4)*

Class 2: Substances that the committee considered might meet all Annex D criteria but remained undetermined due to equivocal or insufficient data

Pesticides (1 substance)	
CAS No	**Substance**
2921-88-2	Chlorpyrifos

Class 3: Substances that are difficult for classification due to insufficient data

Fluorinated alternatives (20 substances)	
CAS No	**Substance**
29420-49-3	Perfluorobutane sulfonate potassium salt
3871-99-6	Perfluorohexanesulfonate potassium salt[33]
647-42-7	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanol*
27619-97-2	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctane-1-sulfonate
355-86-2	Tris(octafluoropentyl) phosphate
563-09-7	Tris(heptafluorobutyl) phosphate
40143-77-9	Sodium bis(perfluorohexyl) phosphinate
34455-29-3	Carboxymethyldimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]propylammonium hydroxide
358-63-4	Tris(trifluoroethyl) phosphate
163702-07-6	Methyl nonafluorobutyl ether
163702-08-7	Methyl nonafluoro isobutyl ether
59587-38-1	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctane-1-sulphonate potassium salt
2043-47-2	1*H*,1*H*,2*H*,2*H*-Perfluorohexanol or 3,3,4,4,5,5,6,6,6-nonafluorobutyl ethanol*
	2-(6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyloxy)-1,1,2,2-tetrafluoroethane sulfonate
	1,1,2,2,-tetrafluoro-2-(perfluorohexyloxy)-ethane sulfonate
	Perfluorohexane ethyl sulfonyl betaine
756-13-8	Dodecafluoro-2-methylpentan-3-one
40143-76-8	Perfluorohexyl phosphonic acid
	1-chloro-perfluorohexyl phosphonic acid
2144-53-8	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl ester*
Non fluorinated alternatives (4 substances)	
541-02-6	Decamethyl cyclopentasiloxane (D5)[34]*
577-11-7	Di-2-ethylhexyl sulfosuccinate, sodium salt
4261-72-7	Stearamidomethyl pyridine chloride

[33] This chemical is subject to a Significant New Use Rule in the U.S. since November 2007.

[34] There is ongoing work through which new information is becoming available to further support the assessment of these substances.

67674-67-3	(Hydroxyl) Terminated polydimethylsiloxane
Commercial brands (11 brands)	
	Polyfox®
	Emulphor® FAS
	Enthone®
	Zonyl®[35]
	Capstone®
	Nuva®
	Unidyne®
	Rucoguard®
	Oleophobol®
	Asahiguard®
	Solvera®

Class 4: Substances that are not likely to meet all Annex D criteria (b), (c), (d) and (e)

It should be noted that the following substances, which are not likely to be a POP, may exhibit hazardous characteristics (e.g. mutagenicity, carcinogenicity, reproductive and developmental toxicity, endocrine disruption, immune suppression or neurotoxicity) that should be assessed by parties before considering such substances as a suitable alternative.

Non fluorinated alternatives (9 substances)	
CAS No	**Substance**
540-97-6	Dodecamethyl cyclohexasiloxane (D6)**Error! Bookmark not defined.***
107-46-0	Hexamethyl disiloxane (MM or HMDS)*
107-51-7	Octamethyl trisiloxane (MDM)*
141-62-8	Decamethyl tetrasiloxane (MD2M)*
141-63-9	Dodecamethyl pentasiloxane (MD3M)*
25640-78-2	1-Isopropyl-2-phenyl-benzene
38640-62-9	Diisoproplynaftalene (DIPN)
35860-37-8	Triisopropylnaftalene /TIPN)
69009-90-1	Diisopropyl-1,1'-biphenyl
Pesticides (2 substances)	
CAS No	**Substance**
52315-07-8	Cypermethrin
52918-63-5	Deltamethrin

In addition, the following 6 substances in category IV of the results of the prioritization step (see section III) are not likely to meet the Annex D criteria (b), (c), (d) and (e)

Pesticides (6 substances)	
CAS No	**Substance**
95737-68-1	Pyriproxyfen

[35] According to FluoroCouncil, production of Zonyl® will be discontinued in 2014.

138261-41-3, 105827-78-9	Imidacloprid
120068-37-3	Fipronil
122-14-5	Fenitrothion
71751-41-2	Abamectin
67485-29-4	Hydramethylnon

* Manufacturing intermediates for alternatives to PFOS

60. In summary, 54 chemical alternatives to PFOS were analysed following a methodology previously used for the assessment of alternatives to endosulfan. 1 substance (octamethyl cyclotetrasiloxane (D4)) was identified as being likely to meet all the Annex D criteria. Chlorpyrifos was identified as a substance that may meet all of the Annex D criteria but have equivocal data. A further 17 substances were classified as unlikely to be POPs. These 17 substances have been reported as alternatives to PFOS for the following applications: carpets, leather and apparel, textiles and upholstery, coating and coating additives, insecticides for control of red imported fire ants and termites and insect bait for control of leaf-cutting ants from *Atta spp.* and *Acromyrmex spp.* (see appendix 1to this report). Additionally 35 of the alternatives to PFOS could not be classified since experimental data on their potential to bioaccumulate was not available. Of these 35 substances, modelled data for three substances (tris(octafluoropentyl) phosphate, tris(heptafluorobutyl) phosphate and sodium bis(perfluorohexyl)) suggest that they may be of concern with respect to bioaccumulation and persistence.

7 Information gaps

61. According to the terms of reference in the annex to decision POPRC-9/5, the screening process as used for the assessment of alternatives to endosulfan was used in the present assessment. The methodology used for the assessment of alternatives to endosulfan, which was adapted for the current assessment, had been developed for a group of chemicals that are all pesticides. Because pesticides are subject to a process of registration and risk assessment in many countries, reliable information about their properties is readily available in a number of public databases. In contrast, the alternatives to PFOS are in majority industrial chemicals on which much less information is made publicly available. In many cases, the information is classified as confidential business information. The low availability of data presented one of the main difficulties in undertaking the assessment of alternatives to PFOS, as evidenced by the large number of chemicals that could not be classified due to insufficient data.

62. The scarcity of experimental data about alternatives to PFOS also made it necessary to rely more heavily on modelled data for their assessment than in the case of alternatives to endosulfan. Existing modelling tools provide estimates of bioaccumulation based on log Kow values. Although modelling tools have in recent years shown some improvement in accurately predicting the properties of fluorinated substances, further development of tools more suited for estimating bioaccumulation and biomagnification values for this group of chemicals should facilitate their assessment.

63. The identification of alternatives to PFOS in the report is based largely on information provided by parties and observers. Alternatives to PFOS that are not likely to meet all Annex D criteria were identified for several of the applications listed as specific exemptions and acceptable purposes in part I of Annex B to the Convention (see paragraph 57 and appendix 1 to this report). Alternatives to PFOS were, however, not reported for a number of applications listed in part I of Annex B to the Convention (see paragraph 15). The information provided by parties and others on the technical feasibility, cost-effectiveness, efficacy, availability and accessibility of the alternatives to PFOS did not include enough data to enable a comprehensive assessment related to the availability, suitability and implementation of such alternatives. While more information on the identity of alternatives to PFOS and their properties may be available in open sources, obtaining such information was beyond the scope of this report and the resources and time available for its preparation.

64. As pointed out in the Guidance on considerations related to alternatives and substitutes for listed persistent organic pollutants and candidate chemicals,[36] in identifying and evaluating alternatives to POPs, it is important to describe the specific use and functionality of POPs as specifically as possible. In the case of PFOS, the various specific exemptions and acceptable purposes listed in Annex B to the Convention describe broad use categories (e.g. fire fighting foams) , articles (e.g. electric and electronic parts for some colour printers and colour copy machines) and processes (e.g. chemically driven oil production) for which PFOS can have a variety of uses. The lack of information about the precise use and function of PFOS in these applications makes it difficult to identify

[36] UNEP/POPS/POPRC.5/10/Add.1.

corresponding alternatives with a high degree of certainty. Where possible, the functionality and application of alternative substances have been indicated in the table in appendix 1 to this report.

65. As highlighted in the preceding paragraphs, obtaining precise and detailed information about alternatives to the use of PFOS and their properties is necessary for the assessment of these alternatives by the Committee. It is recommended that the format for collecting information from parties and others be revised to facilitate the provision of such information by, e.g., specifying the functionality of PFOS under the use categories listed as specific exemptions and acceptable purposes. Parties and others should also be encouraged to provide further information to support the assessment of alternatives to PFOS. Information on four transformation products was submitted for the present assessment. It was acknowledged that degradation products may be relevant in a future screening. However, considering the complexity related to the degradation products, these were set aside.

Appendix 1 Alternatives to PFOS, their occurrence and applications

Compound			Functionality	Occurrence	Applications[37]	Class (results of the assessment)
CAS no	Name	Abbr.				
29420-49-3	Perfluorobutane sulfonate potassium salt	PFBS K	Fluorosurfactant[38]	commercial product	Coating and coating agents, carpets, leather and apparel, textiles and upholstery, paper and packaging, rubber and plastics. [A,B]	3
3871-99-6	Perfluorohexanesulfonate potassium salt	PFHxS K	Fluorosurfactant[39]	commercial product	Carpets, leather and apparel, textiles and upholstery [B],	3
307-24-4	Perfluorohexanoic acid	PFHxA		transformation product	Not applicable	
2923-26-4	Perfluorohexanoic acid sodium salt	PFHxA Na		transformation product	Not applicable	
375-22-4	Perfluorobutanoic acid	PFBA		transformation product	Not applicable	
375-85-9	Perfluoroheptanoic acid	PFHpA		transformation product	Not applicable	
2043-47-2	1*H*,1*H*,2*H*,2*H*-Perfluorohexanol or 3,3,4,4,5,5,6,6,6-nonafluorobutyl ethanol	4:2 FTOH	Raw material for surfactant and surface protection products[40]	manufacturing intermediate	Carpets, leather and apparel, textiles and upholstery [A],	3
647-42-7	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-	6:2 FTOH	Raw material for	manufacturing	Carpets, leather and	3

[37] Applications listed in part I of Annex B to the Convention for which the alternative is relevant.(A) Information from the Guidance on alternatives to PFOS, its salts and PFOSF and their related chemicals (UNEP/POPS/POPRC.9/INF/11/rev1); (B) Information from the technical paper on the identification and assessment of alternatives to the use of PFOS, its salts and PFOSF and their related chemicals in open applications UNEP/POPS/POPRC.8/INF/17.

[38] Buck et al. "Perfluoroalkyl and polyfluoroalkyl Substances in the Environment: Terminology, Classification and Origins", Integrated Environmental Assessment and Management, Vol 7, Number 4 – pp 513-541 (2011)

Buck et al. "Perfluoroalkyl and polyfluoroalkyl Substances in the Environment: Terminology, Classification and Origins", Integrated Environmental Assessment and Management, Vol 7, Number 4 – pp 513-541 (2011)

[39] Buck et al. "Perfluoroalkyl and polyfluoroalkyl Substances in the Environment: Terminology, Classification and Origins", Integrated Environmental Assessment and Management, Vol 7, Number 4 – pp 513-541 (2011)

[40] Buck et al. "Perfluoroalkyl and polyfluoroalkyl Substances in the Environment: Terminology, Classification and Origins", Integrated Environmental Assessment and Management, Vol 7, Number 4 – pp 513-541 (2011)

Compound			Functionality	Occurrence	Applications[37]	Class (results of the assessment)
CAS no	Name	Abbr.				
	octanol		surfactant and surface protection products[41]	intermediate	apparel, textiles and upholstery [A,B]	
2144-53-8	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl ester	6:2 FMA	Raw material for surfactant and surface protection products[42]	manufacturing intermediate	Carpets, leather and apparel, textiles and upholstery [A]	3
756-13-8	Dodecafluoro-2-methylpentan-3-one		Fluorosurfactant	commercial product	Fire fighting foams [A,B]	3
	Perfluorohexane ethyl sulfonyl betaine		Fluorosurfactant	commercial product	Fire fighting foams [A,B]	3
34455-29-3	Carboxymethyldimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]propylam monium hydroxide		Fluorosurfactant	commercial product	Fire fighting foams [A,B]	3
163702-07-6	Methyl nonafluorobutyl ether		Fluorosurfactant	commercial product	Coating and coating additives [A,B]	3
163702-08-7	Methyl nonafluoro isobutyl ether		Fluorosurfactant	commercial product	Coating and coating additives [A,B]	3
27619-97-2	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctane-1-sulphonate	6:2 FTS	Fluorosurfactant	commercial product	Metal plating [A,B].	3
59587-38-1	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctane-1-sulphonate potassium salt	6:2 FTS K	Fluorosurfactant	commercial product	Metal plating [A,B].	3
	1,1,2,2,-tetrafluoro-2-(perfluorohexyloxy)-ethane sulfonate	F-53	Fluorosurfactant	commercial product	Metal plating [A,B]	3
	2-(6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyloxy)-1,1,2,2-tetrafluoroethane sulfonate	F-53B	Fluorosurfactant	commercial product	Metal plating [A,B]	3
355-86-2	Tris(octafluoropentyl) phosphate	POFPP (PAPs)	Fluorosurfactant	commercial product	Paper and packaging [A,B]	3
563-09-7	Tris(heptafluorobutyl) phosphate	PHFBP (PAPs)	Fluorosurfactant	commercial product	Paper and packaging [A,B]	3
358-63-4	Tris(trifluoroethyl) phosphate	PTEHP	Fluorosurfactant	commercial product	Paper and packaging [A,B]	3

[41] Buck et al. "Perfluoroalkyl and polyfluoroalkyl Substances in the Environment: Terminology, Classification and Origins", Integrated Environmental Assessment and Management, Vol 7, Number 4 – pp 513-541 (2011)

[42] Buck et al. "Perfluoroalkyl and polyfluoroalkyl Substances in the Environment: Terminology, Classification and Origins", Integrated Environmental Assessment and Management, Vol 7, Number 4 – pp 513-541 (2011)

Compound			Functionality	Occurrence	Applications[37]	Class (results of the assessment)
CAS no	Name	Abbr.				
		(PAPs)				
40143-76-8	Perfluorohexyl phosphonic acid	PFHxPA (PAPs)	Fluorosurfactant	commercial product	Paper and packaging [A,B],	3
	1-chloro-perfluorohexyl phosphonic acid	Cl-PFHxPA (PAPs)	Fluorosurfactant	commercial product	Paper and packaging [A,B]	3
40143-77-9	Sodium bis(perfluorohexyl) phosphinate	6:6 PFPi (PAPs)	Fluorosurfactant	commercial product	Paper and packaging [A,B],	3
577-11-7	Di-2-ethylhexyl sulfosuccinate, sodium salt		Waxes and resins	commercial product	Carpets, leather and apparel textiles and upholstery [B],	3
4261-72-7	Stearamidomethyl pyridine chloride		Waxes and resins	commercial product	Carpets, leather and apparel, textiles and upholstery [A,B],	3
556-67-2	Octamethyl cyclotetrasiloxane	D4	Manufacturing intermediate for the production of silicone polymers[43]	manufacturing intermediate	Carpets, leather and apparel, textiles and upholstery, coating and coating additives [A,B].	1
541-02-6	Decamethyl cyclopentasiloxane	D5	Manufacturing intermediate for the production of silicone polymers[44]	manufacturing intermediate	Carpets, leather and apparel, textiles and upholstery, coating and coating additives [A,B].	3
540-97-6	Dodecamethyl cyclohexasiloxane	D6	Manufacturing intermediate for the production of silicone polymers[45]	manufacturing intermediate	Carpets, leather and apparel, textiles and upholstery, coating and coating additives [A,B].	4
107-46-0	Hexamethyl disiloxane	MM (or		manufacturing	Carpets, leather and	4

[43] Wang, De-Gao, et al. "Review of recent advances in research on the toxicity, detection, occurrence and fate of cyclic volatile methyl siloxanes in the environment." *Chemosphere* Vol. 93, Issue 5, October 2013: 711–725
URL: http://www.sciencedirect.com/science/article/pii/S0045653512012805

[44] Wang, De-Gao, et al. "Review of recent advances in research on the toxicity, detection, occurrence and fate of cyclic volatile methyl siloxanes in the environment." *Chemosphere* Vol. 93, Issue 5, October 2013: 711–725
URL: http://www.sciencedirect.com/science/article/pii/S0045653512012805

[45] Wang, De-Gao, et al. "Review of recent advances in research on the toxicity, detection, occurrence and fate of cyclic volatile methyl siloxanes in the environment." *Chemosphere* Vol. 93, Issue 5, October 2013: 711–725
URL: http://www.sciencedirect.com/science/article/pii/S0045653512012805

Compound			Functionality	Occurrence	Applications[37]	Class (results of the assessment)
CAS no	Name	Abbr.				
		HMDS)	Manufacturing intermediate for the production of silicone polymers[46]	intermediate	apparel, textiles and upholstery, coating and coating additives [A,B].	
107-51-7	Octamethyl trisiloxane	MDM	Manufacturing intermediate for the production of silicone polymers.	manufacturing intermediate	Carpets, leather and apparel, textiles and upholstery, coating and coating additives [A,B].	4
141-62-8	Decamethyl tetrasiloxane	MD2M	Manufacturing intermediate for the production of silicone polymers.[47]	manufacturing intermediate	Carpets, leather and apparel, textiles and upholstery, coating and coating additives [A,B].	4
141-63-9	Dodecamethyl pentasiloxane	MD3M	Manufacturing intermediate for the production of silicone polymers.[48]	manufacturing intermediate	Carpets, leather and apparel, textiles and upholstery, coating and coating additives [A,B].	4
38640-62-9	Diisoproplynaftalene		Waxes and resins	commercial product	Coating and coating additives [A,B].	4
35860-37-8	Triisopropylnaftalene		Waxes and resins	commercial product	Coating and coating additives [A,B]	4
69009-90-1	Diisopropyl-1,1'-biphenyl		Waxes and resins	commercial product	Coating and coating additives [A,B]	4
25640-78-2	1-Isopropyl-2-phenyl-benzene		Waxes and resins	commercial product	Coating and coating	4

[46] http://echa.europa.eu/documents/10162/c98c53e1-7228-4985-8f87-6e202788106f

[47] http://echa.europa.eu/documents/10162/c98c53e1-7228-4985-8f87-6e202788106f

[48] https://echa.europa.eu/documents/10162/13632/intentions_2013_en.pdf

Compound			Functionality	Occurrence	Applications[37]	Class (results of the assessment)
CAS no	Name	Abbr.				
					additives [A,B]	
67674-67-3	(Hydroxyl) Terminated polydimethylsiloxane		Non ionic surfactant[49]	commercial product	Coating and coating additives [A,B]	3
Pesticides						
120068-37-3	Fipronil		Pesticides	commercial product	Insecticides for control of red imported fire ants and termites. Insect bait for control of leaf-cutting ants from *Atta sppand Acromyrmex spp* [B]	4
71751-41-2	Abamectin		Pesticides	commercial product	Insecticides for control of red imported fire ants and termites	4
95737-68-1	Pyriproxyfen		Pesticides	commercial product	Insecticides for control of red imported fire ants and termites [B]	4
122-14-5	Fenitrothion[50]		Pesticides	commercial product	Insecticides for control of red imported fire ants and termites. Insect bait for control of leaf-cutting ants from *Atta spp and Acromyrmex spp* [B]	4
138261-41-3, 105827-78-9	Imidacloprid		Pesticides	commercial product	Insecticides for control of red imported fire ants and termites [B]	4
52315-07-8	Cypermethrin		Pesticides	commercial product	Insecticides for control of red imported fire ants and termites[A]	4
52918-63-5	Deltamethrin		Pesticides	commercial product	Insecticides for control of	4

[49] http://www.cdms.net/ldat/mp9fi001.pdf
http://www.siltech.com/msds/P2002.2.pdf
http://www.hitochem.com/uploadfile/20120411191716530.pdf

[50] According to ABRAISCA, this substance is not an insect bait.

Compound			Functionality	Occurrence	Applications[37]	Class (results of the assessment)
CAS no	Name	Abbr.				
					red imported fire ants and termites. Insect bait for control of leaf-cutting ants from *Atta spp and Acromyrmex spp* [B]	
2921-88-2	Chlorpyrifos		Pesticides	commercial product	Insecticides for control of red imported fire ants and termites [B]	2
67485-29-4	Hydramethylnon[50]		Pesticides	commercial product	Insecticides for control of red imported fire ants and termites. Insect bait for control of leaf-cutting ants from *Atta spp and Acromyrmex spp* [A51]	4
Commercial brands						
	Polyfox®		Polymer coating	commercial product	Coating and coating additives [A,B]	3
	Emulphor® FAS		Polymer coating	commercial product	Coating and coating additives [A,B] Metal plating [A,B]	3
	Enthone®		Polymer coating	commercial product	Coating and coating additives [A,B] Metal plating [A,B]	3
	Zonyl®		Polymer coating	commercial product	Carpets, leather and apparel, textiles and upholstery [A,B]	3
	Capstone®		Polymer coating	commercial product	Coating and coating additives , carpets, leather and apparel, textiles and upholstery, and metal plating [A,B]	3

[51] Submission by Ecuador, http://chm.pops.int/TheConvention/POPsReviewCommittee/Meetings/tabid/2266/Default.aspx

Compound			Functionality	Occurrence	Applications[37]	Class (results of the assessment)
CAS no	Name	Abbr.				
	Nuva®		Polymer coating	commercial product	Carpets, leather and apparel, textiles and upholstery [A,B]	3
	Unidyne®		Polymer coating	commercial product	Carpets, leather and apparel, textiles and upholstery [A,B]	3
	Rucoguard®		Polymer coating	commercial product	Carpets, leather and apparel, textiles and upholstery [A,B]	3
	Oleophobol®		Polymer coating	commercial product	Carpets, leather and apparel, textiles and upholstery [A,B],	3
	Asahiguard®		Polymer coating	commercial product	Carpets, leather and apparel, textiles and upholstery [A,B]	3
	Solvera®		Polymer coating	commercial product	Paper and packaging [A,B]	3

Appendix 2: Results of the prioritization of alternatives to PFOS

Substance			Molecular weight [g/mol][54]	Functionality & occurrence	POP indicators									Category (result of prioritisation step)
					Bioaccumulation[52]			Persistence[53]			RIVM modelled			
CAS no	Name	Abbr.			log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	
29420-49-3	Perfluorobutane sulfonate potassium salt	PFBSK	338.19	Fluorosurfactant	EPI: -0.33		32 – 126[55]	180	360	1620	1.00	1.00	0.00	III
3871-99-6	Perfluorohexanesulfonate potassium salt	PFHxSK	438	Fluorosurfactant	EPI: 1.01		68[56], 100[57]	180	360	1620	1.01	1.00	0.01	III
756-13-8	Dodecafluoro-2-methylpentan-3-one		316.04	Fluoro surfactant	2.79[58] EPI: 2.79						1.05	1.00	0.05	III
	Perfluorohexane ethyl sulfonyl betaine			Fluoro surfactant										III
34455-29-3	Carboxymethyldimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]propylammonium hydroxide		537.415	Fluoro surfactant	EPI: 2.9			180	360	1620	1.06	0.99	0.07	III
163702-07-6	Methyl nonafluorobutyl ether		250.06	Fluoro surfactant	EPI: 3.34			180	360	1620	1.14	0.93	0.11	III

[52] No data on BMF or TMF were available from the sources consulted.

[53] Epi Suite, level III fugacity model if nothing else is stated.

[54] If molecular weight is not available a short description from the producer is described.

[55] http://www.usask.ca/toxicology/jgiesy/pdf/publications/JA-689.pdf

[56] http://www.chemspider.com/Chemical-Structure.10654380.html

[57] http://webnet.oecd.org/CCRWEB/ChemicalDetails.aspx?ChemicalID=69fd4915-cbb4-4c6e-bb35-ee20e61ec8fc

[58] http://www.chemspider.com/Chemical-Structure.2062563.html

Substance			Molecular weight [g/mol][54]	Functionality & occurrence	POP indicators									Category (result of prioritisation step)
					Bioaccumulation[52]			Persistence[53]			RIVM modelled			
CAS no	Name	Abbr.			log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	
163702-08-7	Methyl nonafluoro isobutyl ether		250.06	Fluoro surfactant	EPI: 3.23			180	360	1620	1.13	0.93	0.10	III
27619-97-2	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctane-1-sulphonate	6:2 FTS		Fluoro surfactant	EPI: 2.66		< 50[59]				0.47	0.43	0.04	III
59587-38-1	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctane-1-sulphonate potassium salt	6:2 FTS K		Fluoro surfactant	EPI: -0.11						0.42	0.42	0.003	III
	1,1,2,2,-tetrafluoro-2-(perfluorohexyloxy)-ethane sulfonate	F-53	516.13	Fluoro surfactant	EPI: 2.78			180	360	1620	1.06	1.00	0.06	III
	2-(6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyloxy)-1,1,2,2-tetrafluoroethane sulfonate	F-53B	532.58	Fluoro surfactant	EPI: 3.1			180	360	1620	1.09	1.00	0.09	III
355-86-2	Tris(octafluoropentyl) phosphate	POFPP	702.07	Fluoro surfactant	EPI: 7.21			180	360	1620	1.27	0.64	0.63	III
563-09-7	Tris(heptafluorobutyl) phosphate	PHFBP	644.12	Fluoro surfactant	EPI:7.02			180	360	1620	1.30	0.59	0.71	III
358-63-4	Tris(trifluoroethyl) phosphate	PTEHP	344.07	Fluoro surfactant	EPI:2.12			180	360	1620	0.42	0.40	0.02	III
40143-76-8	Perfluorohexyl phosphonic acid	PFHxPA	400	Fluoro surfactant	EPI:3.06	3.55[60]		180	360	1620	1.28	0.99	0.29	III

[59] Dr. Stephen Korzeniowski,"Fluortelomer products in the Environment – an update", oral presentation DuPont (2008). http://www2.dupont.com/Forafac/en_US/assets/downloads/fluorotelomer_in_environment_nfpa2008_02june_shk.pdf

[60] Quinete, N., et al., Degradation studies of new substitutes for perfluorinated surfactants. Arch. Environ. Contam. Toxicol., 2010. 59: p. 20-30.

Substance			Molecular weight [g/mol][54]	Functionality & occurrence	POP indicators									Category (result of prioritisation step)
					Bioaccumulation[52]			Persistence[53]			RIVM modelled			
CAS no	Name	Abbr.			log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	
	1-chloro-perfluorohexyl phosphonic acid	Cl-PFHxPA	416.49	Fluoro surfactant	EPI:3.37	4.01[61]		180	360	1620	1.37	0.99	0.38	II
	Sodium bis(perfluorohexyl) phosphinate							180	360	1620	1.58	0.77	0.81	III
Non fluorinated alternatives (13 substances)														
577-11-7	Di-2-ethylhexyl sulfosuccinate, sodium salt		444.56	Waxes and resins Sulfosuccinate	EPI:3.95			9	17	78	0.04	0.03	0.01	III
4261-72-7	Stearamidomethyl pyridine chloride		411.08	Waxes and resins Stearamide	EPI: 5.16			38	75	338	0.49	0.25	0.24	III
38640-62-9	Diisoproplynaftalene		212.34	Waxes and resins Aromatics	EPI:6.08		2630[62]	38	75	338	1.08	0.27	0.81	II
35860-37-8	Triisopropylnaftalene		254.42	Waxes and resins Aromatics	EPI:7.54		138038[63]	38	75	338	1.20	0.39	0.81	II
69009-90-1	Diisopropyl-1,1'-biphenyl		238.38	Waxes and resins Aromatics	EPI:6.67		104712[64]	38	75	338	1.24	0.31	0.93	II

[61] Quinete, N., et al., Degradation studies of new substitutes for perfluorinated surfactants. Arch. Environ. Contam. Toxicol., 2010. 59: p. 20-30.

[62] http://webnet.oecd.org/CCRWEB/ChemicalDetails.aspx?ChemicalID=5bbb30fa-beb8-4c8a-941c-1e8f8bb1c8c3

[63] http://www.chemspider.com/Chemical-Structure.106232.html

[64] http://www.chemspider.com/Chemical-Structure.157882.html

Substance			Molecular weight [g/mol][54]	Functionality & occurrence	POP indicators									Category (result of prioritisation step)
					Bioaccumulation[52]			Persistence[53]			RIVM modelled			
CAS no	Name	Abbr.			log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	
25640-78-2	1-Isopropyl-2-phenyl-benzene		196.29	Waxes and resins Aromatics	5,21[65]	5,21[66]		38	75	338	0.97	0.19	0.78	II
67674-67-3	(Hydroxyl) Terminated polydimethylsiloxane		550 - 650	Non ionic surfactant										III
Pesticides (9 substances)[67]														
120068-37-3	Fipronil		437.15	Pesticides		3,75	321	Exper: 68.0	field. 65,0 Lab: 142.0	Exper: 68.0	1.40	1.00	0.40	IV
71751-41-2	Abamectin		866.60	Pesticides		4,40	69	Exper. 89.0	Field: 1,0 Lab:28,7	Exper: 89	1.36	0.97	0.38	IV
95737-68-1	Pyriproxyfen		321.37	Pesticides		5,37	1379	Exper: 4.2	Field . 6.5 Lab: 6.7	Exper: 4.2	0.82	0.63	0.19	IV
122-14-5	Fenitrothion		277.23	Pesticides		3,32	29	Exper: 1,6	Lab: 2.7	Exper: 1,6	0.60	0.31	0.29	IV
138261-41-3, 10582	Imidacloprid		255.66	Pesticides		0,57	1	Exper: 129	Field: 174 Lab: 187	Exper: 129	0.33	0.33	0.00	IV

[65] http://www.chemspider.com/Chemical-Structure.21974.html

[66] VU University Amsterdam, J Weiss 2012

[67] All P and B data for the pesticides, except for hydramethylnon, are taken from document UNEP/POPS/POPRC.8/INF/28. For these 8 pesticides data of DT50water/sediment for the whole water/sediment system [days] is listed

Substance			Molecular weight [g/mol][54]	Functionality & occurrence	POP indicators									Category (result of prioritisation step)
					Bioaccumulation[52]			Persistence[53]			RIVM modelled			
CAS no	Name	Abbr.			log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	
7-78-9														
52315-07-8	Cypermethrin		416.31	Pesticides		6.60	356	Exper: 2	Field: 10 Lab: 60	Exper: 2	1.26	0.86	0.36	II
52918-63-5	Deltamethrin		505.20	Pesticides		4.60	1400	Exper: 65	Field:21 Lab: 26	Exper: 65	1.06	0.75	0.31	II
2921-88-2	Chlorpyrifos		350.89	Pesticides		5.00	1374	Exper: 36.5	Field: 21 Lab: 76	Exper: 36,5	1.41	0.85	0.56	II
67485-29-4	Hydramethylnon		494.5	Pesticides	7.54[68]	2.31[69] [70]	36[71]	<0.04[72] [73]	5[74] 7-391[75]	7-28[76] (sandy loam)	1.67	0.95	0.72	IV

[68] http://www.chemspider.com/Chemical-Structure.4445168.html, Since Hydramethylnon is a fluorinated substance, log Kow may not reflect the bioaccumulation potential.

[69] http://www.cdpr.ca.gov/docs/emon/pubs/fatememo/hydmthn.pdf

[70] http://www.fluoridealert.org/wp-content/pesticides/hydramethylnon.toxnet.hsdb.htm

[71] http://www.fluoridealert.org/wp-content/pesticides/hydramethylnon.toxnet.hsdb.htm

[72] http://www.cdpr.ca.gov/docs/emon/pubs/fatememo/hydmthn.pdf

[73] http://npic.orst.edu/factsheets/hydragen.pdf

[74] http://www.cdpr.ca.gov/docs/emon/pubs/fatememo/hydmthn.pdf

[75] http://npic.orst.edu/factsheets/hydragen.pdf

[76] http://www.fluoridealert.org/wp-content/pesticides/hydramethylnon.toxnet.hsdb.htm

Substance			Molecular weight [g/mol][54]	Functionality & occurrence	POP indicators									Category (result of prioritisation step)
					Bioaccumulation[52]			Persistence[53]			RIVM modelled			
CAS no	Name	Abbr.			log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	
Commercial brands (11 brands) Error! Bookmark not defined.														
	Polyfox®		1150-4480[77] Reactive intermediates in the formulation of acrylic, ester and urethane polymers and copolymers[78]	Polymers when applied										III
	Emulphor® FAS		High-molecular fatty alcohol polyglycol ether sulphate, sodium salt[79]	Polymers										III
	Enthone®		nanofinish technology[80]	Polymers										III
	Zonyl®		Fluoropolymers[81]	Polymers										III

[77] http://www.omnova.com/products/chemicals/documents/PolyFoxReactivePolymerIntermediates09March30.pdf

[78] http://www.omnova.com/products/chemicals/PolyFox.aspx

[79] http://www.formulation-technologies.basf.com/productdetails?prd=30061192

[80] http://www.enthone.com/New_Technology_Development/ORMECON_Acquisition.aspx

[81] http://www2.dupont.com/Teflon_Industrial/en_US/products/product_by_type/additives/index.html

Substance			Molecular weight [g/mol][54]	Functionality & occurrence	POP indicators									Category (result of prioritisation step)
					Bioaccumulation[52]			Persistence[53]			RIVM modelled			
CAS no	Name	Abbr.			log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	
	Capstone®		> 40 000 (acrylate polymer 3000-5000 (urethane polymer)	Polymers										III
	Nuva®		C6 side chain fluoropolymers[82].	Polymers when applied.										III
	Unidyne®		Side chain fluoropolymers[83]	Polymers when applied										III
	Rucoguard®		Aqueous C_6-based Fluorocarbon Polymeric Dispersions[84]	Polymers										III

[82] http://newsroom.clariant.com/clariant-expands-as-its-c6-chemistry-nuva%C2%AE-n-increasingly-gets-the-textile-industry%E2%80%99s-approval/

[83] http://daikin-america.com/unidyne-repellants-and-surfactants/

[84] http://www.rudolf.de/en/products/co-producer-b2b/10-water-oil-and-soil-repellent-agents/11-c6-based-fluorocarbon-polymers.html

Substance			Molecular weight [g/mol][54]	Functionality & occurrence	POP indicators									
					Bioaccumulation[52]			Persistence[53]			RIVM modelled			
CAS no	Name	Abbr.			log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	Category (result of prioritisation step)
	Oleophobol®		Dispersion of a polymer, perfluorinated compound[85]	Polymers										III
	Asahiguard®		C6 fluorinated polymer technology[86]	Polymers when applied										III
	Solvera®		Perfluoropolyether[87]	Polymers										III

[85] http://www.relish.co.in/oleophobolzsr.pdf

[86] http://www.textileworld.com/Articles/2013/June/Textile_News/AGC_Chemicals_Americas_Releases_PFOA-Free_AsahiGuard_AG-E550D_Water-Oil_Repellent

[87] TDS_Solvera_PT_5045_PG.pdf

Appendix 3: Results of the prioritization of manufacturing intermediates for alternatives to PFOS

Substance					POP indicators									
					Bioaccumulation[88]			Persistence[89]			RIVM modelled			
CAS no	Name	Abbr.	Molecular weight [g/mol][90]	Functionality & occurrence	log Kow (modelled)	log Kow (exp)	BCF (exp)	Half life Water (days)	Half life Soil (days)	Half life Sediment (days)	PB-score	P-score	B-score	Category (result of prioritisation step)
2043-47-2	1*H*,1*H*,2*H*,2*H*-Perfluorohexanol or 3,3,4,4,5,5,6,6,6-nonafluorobutyl ethanol	4:2 FTOH	264.02	Raw material for surfactant and surface protection products	Epi: 3.66	3.30[91]		180	360	1620	0.36	0.27	0.09	III
647-42-7	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanol	6:2 FTOH	364.1	Raw material for surfactant and surface protection products	Epi: 4.41	4.54[92]	34-99[93]		Exper: < 2[94]	Exper: < 2	0.66	0.36	0.30	III
2144-53-8	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl ester	6:2 FMA	432.18	Raw material for surfactant and surface protection products[95]	Epi: 6.32	5.2[96]		180	360	1620	0.79	0,39	0.40	I

[88] No data on BMF or TMF were available from the sources consulted.

[89] Epi Suite, level III fugacity model if nothing else is stated.

[90] If molecular weight is not available a short description from the producer is described.

[91] http://www.publish.csiro.au/?act=view_file&file_id=EN10143_AC.pdf

[92] ENVIRON "Assessment of POP Criteria for Specific Short-Chain Perfluorinated Alkyl Substances", project number; 0134304A, (2014)

[93] ENVIRON "Assessment of POP Criteria for Specific Short-Chain Perfluorinated Alkyl Substances", project number; 0134304A, (2014)

[94] ENVIRON "Assessment of POP Criteria for Specific Short-Chain Perfluorinated Alkyl Substances", project number; 0134304A, (2014)

[95] Buck et al. "Perfluoroalkyl and polyfluoroalkyl Substances in the Environment: Terminology, Classification and Origins", Integrated Environmental Assessment and Management, Vol 7, Number 4 – pp 513-541 (2011)

[96] ENVIRON "Assessment of POP Criteria for Specific Short-Chain Perfluorinated Alkyl Substances", project number; 0134304A, (2014)

556-67-2	Octamethyl cyclotetrasiloxane	D4	296.2	Siloxanes. intermediate for the production of silicone polymers	EPI: 6.74	4.34 to 6.49[97]		Exper. < 6.5 Not persistent[98]	Exper. < 5.2 Not persistent[99]	Exper. 288-588 estimated. > 365 Persistent[100]	1.16	0.26	0.88	II
541-02-6	Decamethyl cyclopentasiloxane	D5	370.8	Siloxanes intermediate for the production of silicone polymers	EPI: 8.03	4.76 to 7.61[101]		Estimated > 182 Persistent[102]	Estimated < 182 Not persistent[103]	Estimated: > 365 Persistent[104]	1.30	0.40	0.89	II
540-97-6	Dodecamethyl cyclohexasiloxane	D6	444.93	Siloxanes intermediate for the production of silicone polymers	EPI:9.06	5,86 to 9.06[105][106]		Exper. >411 Persistent[107]	Estimated < 182 No exper. data	Estimated >365 Persistent[108]	1.26	0.55	0.71	II

[97] Wang, De-Gao, et al. "Review of recent advances in research on the toxicity, detection, occurrence and fate of cyclic volatile methyl siloxanes in the environment."Chemosphere Vol. 93, Issue 5, October 2013: 711–725; URL: http://www.sciencedirect.com/science/article/pii/S0045653512012805

[98] https://www.ec.gc.ca/ese-ees/2481B508-1760-4878-9B8A-270EEE8B7DA4/batch2_556-67-2_en.pdf

[99] https://www.ec.gc.ca/ese-ees/2481B508-1760-4878-9B8A-270EEE8B7DA4/batch2_556-67-2_en.pdf

[100] https://www.ec.gc.ca/ese-ees/2481B508-1760-4878-9B8A-270EEE8B7DA4/batch2_556-67-2_en.pdf

[101] Wang, De-Gao, et al. "Review of recent advances in research on the toxicity, detection, occurrence and fate of cyclic volatile methyl siloxanes in the environment." Chemosphere Vol. 93, Issue 5, October 2013: 711–725

[102] http://www.ec.gc.ca/ese-ees/13CC261E-5FB0-4D33-8000-EA6C6440758A/batch2_541-02-6_en.pdf

[103] http://www.ec.gc.ca/ese-ees/13CC261E-5FB0-4D33-8000-EA6C6440758A/batch2_541-02-6_en.pdf

[104] http://www.ec.gc.ca/ese-ees/13CC261E-5FB0-4D33-8000-EA6C6440758A/batch2_541-02-6_en.pdf

[105] Wang, De-Gao, et al. "Review of recent advances in research on the toxicity, detection, occurrence and fate of cyclic volatile methyl siloxanes in the environment." *Chemosphere* Vol. 93, Issue 5, October 2013: 711–725

[106] http://www.ec.gc.ca/ese-ees/FC0D11E7-DB34-41AA-B1B3-E66EFD8813F1/batch2_540-97-6_en.pdf

[107] http://www.ec.gc.ca/ese-ees/FC0D11E7-DB34-41AA-B1B3-E66EFD8813F1/batch2_540-97-6_en.pdf

[108] http://www.ec.gc.ca/ese-ees/FC0D11E7-DB34-41AA-B1B3-E66EFD8813F1/batch2_540-97-6_en.pdf

107-46-0	Hexamethyl disiloxane	MM (or HMDS)	162.38	Siloxanes intermediate for the production of silicone polymers	EPI:5.25			15	30	135	0.54	0.09	0.45	III
107-51-7	Octamethyl trisiloxane	MDM	236.54	Siloxanes intermediate for the production of silicone polymers.	EPI:6.6	6.60 [109]	3610 - 7730[110]	38 Estimated[111] >182	75 Estimated[112] 120	338 Estimated[113] 480 No experimental data available	0.76	0.06	0.71	II
141-62-8	Decamethyl tetrasiloxane	MD2M	310.69	Siloxanes intermediate for the production of silicone polymers	EPI:8.21	8.21 [114]		38	75	338	0.91	0.20	0.71	II
141-63-9	Dodecamethyl pentasiloxane	MD3M	384.85	Siloxanes intermediate for the production of silicone polymers	EPI:9.61 7,8[115]			38	75	338	0.93	0.44	0.49	III

[109] https://www.ec.gc.ca/ese-ees/19584F14-D972-46A1-B71C-FA9A36FFB0FE/batch12_107-51-7_en.pdf

[110]https://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=19584F14-1#toc30

[111] http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=19584F14-1

[112] http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=19584F14-1

[113] http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=19584F14-1

[114] VU University Amsterdam, J Weiss 2012
https://www.ec.gc.ca/ese-ees/19584F14-D972-46A1-B71C-FA9A36FFB0FE/batch12_107-51-7_en.pdf

[115] http://webnet.oecd.org/hpv/UI/handler.axd?id=1A45D30D-D373-4696-8753-2FDF04A4B536

Appendix 4: Results of the screening assessment for 9 alternatives to PFOS

Substance	**Persistence Annex D 1 (b)**	**Bioaccumulation Annex D 1 (c)**	**LRT Annex D 1 (d)**	**Adverse effects: ecotoxicity Annex D 1 (e)**	**Adverse effects to human health Annex D 1 (e)**
Decamethyl cyclopentasiloxane (D5)	Yes	Yes	Yes	Insufficient data	Insufficient data
Dodecamethyl cyclohexasiloxane (D6)	Yes	No	Yes	No	No
Decamethyl tetrasiloxane (MD2M)	Equivocal data	No	Yes	No	No
Diisoproplynaftalene (DIPN)	Yes	Yes	No	Yes	No
Diisopropyl-1,1'-biphenyl	Insufficient data	Insufficient data	No	Insufficient data	Insufficient data
1-Isopropyl-2-phenyl-benzene	No	Yes	No	Yes	No
Octamethyl cyclotetrasiloxane (D4)	Yes	Yes	Yes	Yes	Yes
Octamethyl trisiloxane (MDM)	Equivocal data	Yes	Yes	No	No
Triisopropylnaftalene (TIPN)	Yes	Yes	No	Insufficient data	Insufficient data

Appendix 5: Summary of information on non-chemical alternatives to PFOS submitted during the intersessional period between POPRC-9 and POPRC-10

Applications[116]	**Alternatives**[117]
Hard chrome plating	Physical covers (netting, balls) for metal plating baths (Cr VI) to diminish hydrogen burst and reduce misting need to be further investigated (A)
Photolitography	Non-chemical alternatives to PFOS include shifting to digital photography(A)
Insect baits for control methods for leaf-cutting ants from *Atta spp.* and *Acromyrnex spp*.	• The entomopathogenic Metarrhizium anisopliae can cause the decline and ultimate death of small colonies and recent research indicates that the entomopathogenic fungi Beauveria bassiana and Aspergillus ochraceus can cause 50% mortality within 4-5 days in laboratory conditions(A). • Natural products that can be effective under certain conditions include limonoids extracted from the roots of the South Brazilian endemic plant Raulinoa echinata (A).
Insecticides for control of red imported fire ants and termites	• The general consensus of entomologists and myrmecologists is that permanent, sustainable control of these ants in the USA will likely depend on self-sustaining biological control agents. At least 30 natural enemies have been identified in South America (B). • Biological controls for red imported fire ant (RIFA) include a group of decapitating phorid flies (*Pseudacteon* spp) which parasitize the ants. The microsporidian protozoan *Thelohania solenopsae* and the fungus *Beauveria bassiana* are also promising controls for RIFA. *B. bassiana* has been shown to control RIFA under field conditions in Taiwan. Three viruses, SINV-1, SINV-2, SINV-3, have been found infecting fire ants in the field, and two of these, SINV1 and 3 appear to be associated with significant mortality, indicating their potential as biological control agents. Other potential biological controls include the endoparasitic fungi *Myrmecomyces annellisae* and *Myrmicinosporidium durum*, and the parasite *Mattesia* sp (B).
Carpets, leather and apparel, textiles and upholstery and coating and coating additives	Hyperbranched hydrophobic polymers (dendritic, i.e., highly branched polymers) and specifically adjusted comb polymers as active components is one example of nonfluorinated alternative technologies that can provide superhydrophobic surfaces (but not provide oil repellency, soil and stain release), meaning contact angles larger than 150° that can be applied in coatings, textile, leather etc. Dendrimers may be in the region of nano sized materials meaning features with an average diameter between 1 to 100 nm (B).
Paper and packaging	The Norwegian paper producer Nordic Paper is using mechanical processes to produce, without using any persistent chemical, extra-dense paper that inhibits leakage of grease through the paper (B).

[116] Applications listed in part I of Annex B to the Convention for which the alternative is relevant

[117] Available information is extracted from (A) Guidance on alternatives to PFOS, its salts and PFOSF and their related chemicals (UNEP/POPS/POPRC.9/INF/11/rev1) or (B) Information from the technical paper on the identification and assessment of alternatives to the use of PFOS, its salts and PFOSF and their related chemicals in open applications UNEP/POPS/POPRC.8/INF/17.