Supporting Information for:

Environmental sources, chemistry, fate and transport of per- and polyfluoroalkyl substances: state of the science, key knowledge gaps, and recommendations presented at the August 2019 SETAC focus topic meeting
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Table S1. National-scale U.S. databases that may have information pertinent to potential sources of PFAS release to the environment.

| Database name                                      | Description                                                                 | Pros                                                                 | Cons                                                                 |
|---------------------------------------------------|-----------------------------------------------------------------------------|----------------------------------------------------------------------|----------------------------------------------------------------------|
| **Toxic Release Inventory** (TRI)                  | Tracks use of chemicals that pose a threat to human health and the environment. | Export large datasets; geographic location information available     | PFAS added to the TRI only recently; does not cover all industry sectors; permitted releases only |
| **Hazardous Waste (HW) Generators**                | A search-by-site tool based on information in RCRA Subtitle C Identification Forms. | Nationwide NAICS search and export, geographic location information available | PFAS are not listed waste, registered (HW) generators only           |
| **Enforcement and Compliance History Online** (ECHO)| A single point of access to data from multiple EPA sources including permit, inspection, violation, and enforcement data. Also includes HW generators and the TRI | One stop for multiple US data sources, filter for PFAS, numerous other filter options, geographic information available, numerous tutorials | Data for smaller facilities uncertain                               |
| **Toxic Substances Control Act** (TSCA) Chemical Data Reporting (CDR)** | Data reported by manufacturers (including importers) to EPA regarding production and use of chemicals in commerce | Export nationwide data in multiple formats (e.g., Excel, CSV), geographic location available, | Production > 25,000 lbs/year only; only updated every 4 yrs (current data are from 2016) |
| **Superfund search page**                         | Search for sites associated with the USEPA Superfund National Priorities List (NPL). | Find sites proposed to, on, or deleted from the NPL list. Sites are confirmed sources of PFAS release. Nationwide data; geographic location available. | Searching by contaminant yields incomplete data. Ex: a search for perfluorooctanoic acid did not yield results for site NYD004986741 for which PFOA is a primary contaminant. |
**Table S2.** Summary of PFAS aerobic biotransformation studies. Most studies were in the 22-30 C range. For estimated half-lives ($t_{1/2}$), if $t_{1/2}$ was not achieved within the incubation time, % recovered or transformed for the time period is provided.

| Precursors | Types of microbes or microcosms | Incubation duration | Estimated half-live ($t_{1/2}$) | References |
|------------|---------------------------------|---------------------|---------------------------------|------------|
| **Fluorotelomer Alcohols** |  |  |  |  |
| 8:2 FTOH | Activated sludge – diluted | 28 d | < 28 d | (Wang et al. 2005) |
| Aerobic soils | | 7 months | < 7 d | (Wang et al. 2009) |
| Aerobic soils | | 28 d | < 2 d | (Wang et al. 2009) |
| *Pseudomonas* sp. enriched on octanol | | 67 d | < 7 d | (Liu et al. 2007) |
| *Alkane-oxidizing* | | 28 d | <3 d to < 14 (varied. conditions) | (Kim et al. 2012) |
| *Multiple bacteria strains* | | 28 d | < 1 d to < 7 d | (Kim et al. 2014) |
| Bacterial enrichment culture | | 81 d | 0.2-0.8 d | (Dinglasan et al. 2004) |
| 6:2 FTOH | Aerobic soils | 180 d | < 2 d | (Liu et al. 2010) |
| Aerobic soils | | 84 d | < 2 d | (Liu et al. 2010) |
| Aerobic river sediment | | 100 d | < 2 d | (Zhao et al. 2013) |
| *Aerobic sediment* | | 28 d | < 3 d | (Zhang et al. 2017) |
| *Alkane-oxidizing* | | 28 d | <3 d to < 14 d | (Kim et al. 2014) |
| *Pseudomonas* sp. bacteria | | | |  |
| Mixed bacterial culture | | 90 d | < 2 d | (Liu et al. 2010) |
| *Multiple bacteria strains* | | 28 d | < 0.5 d to < 3 d | (Kim et al. 2014) |
| *Wood-rot fungus* | | 28 d | ~ 2 weeks | (Tseng et al. 2014) |
| Fungi slurries (2 types, 6 isolates) with dispersed C18 | | 28 d | 20-100% transformed within the 28 d | (Merino et al. 2018) |
| **Fluorotelomer Sulfonate** |  |  |  |  |
| 6:2 FTSA | Activated sludge - diluted | 90 d | > 90 d | (Wang et al. 2011) |
| Aerobic river sediment | | 90 d | < 5 d | (Zhang et al. 2016) |
| *Gordonia* sp. | | 120 h | 44% transformed by 120 h | (Van Hamme et al. 2013) |
| *Gordonia* sp. | | 7 d | ~96 h | (Shaw et al. 2019) |
| **Fluorotelomer Derivatives** |  |  |  |  |
| Compound | Environment | Treatment Details | Time (days) | Remarks |
|----------|-------------|-------------------|-------------|---------|
| 8:2 FTS  | Aerobic soils | 80 - 94 d | 5 – 28 d | (Dasu et al. 2012, 2013) |
| 8:2 TBC  | Aerobic soils | 7 months | > 7 months | (Dasu et al. 2013) |
| 4:2, 6:2, 8:2 & 10:2 PAPs | Mixture of raw wastewater & sewage sludge | 92 d | Difficult to discern, artifacts | (Lee et al. 2010) |
| 6:2 diPAP | Aerobic soil | 112 d | 12 d | (Liu and Liu 2016) |
| 6:2 triPAP | FTAC-degrading bacteria and active sludge | 30 d | 1.1% to 22 mol% transformed | (Lewis et al. 2016) |
| 8:2 FTAC | Aerobic soils | 105 d | 3-5 d | (Royer et al. 2015) |
| Microbial cultures inoculated with sludge | 52 d | ~ 2 d | (Dinglasan-Panlilio 2008) |
| 8:2 FTMAC | Aerobic soils | 105 d | 15 d | (Royer et al. 2015) |
| Microbial cultures inoculated with sludge | 42 d | ~ 1 day | (Dinglasan-Panlilio 2008) |
| HMU | Aerobic soils | 180 d | 16-22 months | (Dasu et al. 2013) |
| Microbial cultures inoculated with sludge | 18 d | No degradation | (Dinglasan-Panlilio 2008) |
| FTU | Aerobic soils | 117 d | 3~5 months | (Dasu et al. 2013) |
| FTEOs | WWTP unfiltered effluent | Up to 48 d | ~ 1 day | (Frömel and Knepper 2010) |
| 4:2, 6:2, 8:2 | Aerobic soil slurry | 60 d | 3-5 d | (Harding-Marjanovic et al. 2015) |
| FtTAoS | Aerobic active sludge | 109 d | 53% recovered | (D’Agostino and Mabury 2017) |
| 6:2 FTAA | Aerobic active sludge | 42 d | < 1 d | (Weiner et al. 2013) |
| 6:2 FTAB | Aerobic active sludge | 109 d | 68% recovered | (D’Agostino and Mabury 2017) |
| 6:2 FTAB | Gordonia sp. | 7 d | ~140 h | (Shaw et al. 2019) |

**Perfluoroalkane Sulfonamido Derivatives**

| Compound | Environment | Treatment Details | Time (days) | Remarks |
|----------|-------------|-------------------|-------------|---------|
| N-EtFOSE | Activated sludge | 35 d | ≤ 2-3 d | (Lange 2000) |
| Activated sludge | 4 d | 4.2 d | (Boulanger et al. 2005) |
| Activated sludge | 10 d | 0.7 d | (Rhoads et al. 2008) |
| Marine sediment | 120 d | 44 d (25 °C) | (Benskin et al. 2013) |
| | | 160 d (4 °C) | |
| Aerobic soil | 182 d | 5.23 d | (Mejia-Avendaño and Liu 2015) |
| Aerobic soils (2) | 210 d, 180 d | ~25 to 30 d | (Zhang et al. 2016) |
| Substance        | Environment          | Duration | Breakdown Rate         | Source                        |
|------------------|----------------------|----------|------------------------|-------------------------------|
| N-EtFOSA         | Aerobic soil (from ETFOSE) | 105 d    | 81 d (branch)          | (Liu et al. 2019)            |
| N-EtFOSA         | Aerobic soil         | 182 d    | 13.9~2.1 d             | (Mejia-Avendaño and Liu 2015) |
| SAmPAP           | Marine sediment      | 120 d    | > 380 d (25 °C)        | (Benskin et al. 2013)        |
| PFOSAmS          | Aerobic soil         | 180 d    | >> 180 d               | (Mejia-Avendaño et al. 2016) |
| PFOAAmS          | Aerobic soil         | 180 d    | 142 d                  | (Mejia-Avendaño et al. 2016) |
| PFOSNO           | Aerobic soil         | 90 d     | 15 d                   | (Chen et al. 2020.)          |
| PFOANO           | Aerobic soil         | 90 d     | 3~7 d                  | (Chen et al. 2020.)          |
| Side-chain Fluorinated Polymers |                     |          |                        |                               |
| Polyacrylate polymer | Aerobic soils       | 2 years  | 1200 -1700 years       | (Russell et al. 2008)        |
|                   | Aerobic soils       | 376 d    | 33~112 y               | (Washington et al. 2015)     |
|                   | Rhizobia inoculated soil-plant microcosm | 5.5 m | 8~111 y               | (Rankin et al. 2014)        |
| Polyurethane polymer | Aerobic soils       | 2 years  | 24 - 281 years         | (Russell et al. 2008)        |
Table S3. Summary of PFAS anaerobic biotransformation studies conducted mostly in the 20-37 °C range. When estimated half-lives ($t_{1/2}$) were not available or appropriate, other relevant information is provided.

| Precursor or microcosms | Types of microbes or microcosms | Incubation duration | Estimated half-live ($t_{1/2}$) | References |
|-------------------------|---------------------------------|---------------------|----------------------------------|------------|
| Fluorotelomer Alcohols  | 8:2 FTOH  | Anaerobic sludge | 176 d  | 145 d | (Zhang et al. 2013) |
| Fluorotelomer Alcohols  | 6:2 FTOH  | Anaerobic sediment | 100 d  | ~50 d. | (Zhang et al. 2017) |
| Fluorotelomer Alcohols  | 6:2 FTOH  | Anaerobic sludge | 90 d & 176 d | ~30 d | (Zhang et al. 2013) |
| Fluorotelomer Sulfonate | 6:2 FTSA  | Anaerobic river sediment | 100 d  | 80% remaining at end | (Zhang et al. 2016) |
| Fluorotelomer Sulfonate | 6:2 FtTAoS | Pristine soil and AFFF-impacted soil Sulfate-reducing | 275 d | ~150 d; Primary and stable product 6:2 FtTP (Ft thioether propionate) | (Yi et al. 2018) |
| Fluorotelomer Sulfonate | 6:2 FtTAoS | AFFF-impacted soil Methanogenic | 317 d | ~210-250 d; Primary and stable product 6:2 FtTP | (Field et al. 2017) |
| Fluorotelomer Sulfonate | 6:2 FtTAoS | AFFF-impacted soil Fe-reducing | 317 d | ~240-250 d; Primary and stable product 6:2 FtTP | (Field et al. 2017) |
| Fluorotelomer Sulfonate | 6:2 FtTAoS | AFFF-impacted soil Nitrate-reducing | 317 d | ~90 d; Primary and stable product 6:2 FtTP | (Field et al. 2017) |
| Mixtures                | 2 PFAS mixtures | Anaerobic sludge | 2~3.5 mon | No degradation | (Sáez et al. 2008) |
| Mixtures                | 24 PFAS | Anaerobic municipal landfill microbes | 5 m | 31~44% PFAA precursor to PFASs | (Benskin et al. 2012) |
| Mixtures                | 70 PFAS | Solid wastes reactor with anaerobic methane-producing consortium | 273 d | Total PFAS leaching: 16.7 nmol/kg dry refuse | (Allred et al. 2015) |
| Mixtures                | 70 PFAS | Carpet or clothing reactors with methane-producing consortium | 273~552 d | Total PFAS released: 0.63 to 21.7 nmol/L | (Lang et al. 2016) |
| Mixtures                | 43 PFAS | Anaerobic municipal landfill microbes | Before & after treatment | n.a. | (Busch et al. 2010) |
Table S4: EPA methods for targeted analyses of drinking water (adapted from USEPA 2019b).

| PFAS                                | Acronym  | Chain length | Class  | CAS        | EPA 537 Drinking Water | EPA 537.1 Drinking Water | EPA 533 Drinking Water | EPA 8327 Reagent water, surface water, groundwater, and wastewater effluent |
|-------------------------------------|----------|--------------|--------|------------|------------------------|--------------------------|------------------------|---------------------------------------------------------------|
| Perfluorobutanesulfonic acid        | PFBS     | 4            | PFSA   | 375-73-5   | X                      | X                        | X                      | X                                                              |
| Perfluorodecanoic acid              | PFDA     | 10           | PFCA   | 335-76-2   | X                      | X                        | X                      | X                                                              |
| Perfluorododecanoic acid            | PFDoA    | 12           | PFCA   | 307-55-1   | X                      | X                        | X                      | X                                                              |
| Perfluoroheptanoic acid             | PFHpA    | 7            | PFCA   | 375-85-9   | X                      | X                        | X                      | X                                                              |
| Perfluorohexanesulfonic acid        | PFHxs    | 6            | PFSA   | 355-46-4   | X                      | X                        | X                      | X                                                              |
| Perfluorohexanoic acid              | PFHxA    | 6            | PFCA   | 307-24-4   | X                      | X                        | X                      | X                                                              |
| Perfluorononanoic acid              | PFNA     | 9            | PFCA   | 375-95-1   | X                      | X                        | X                      | X                                                              |
| Perfluorooctanesulfonic acid        | PFOS     | 8            | PFSA   | 1763-23-1  | X                      | X                        | X                      | X                                                              |
| Perfluorooctanoic acid              | PFOA     | 8            | PFCA   | 335-67-1   | X                      | X                        | X                      | X                                                              |
| Perfluorotetradecanoic acid         | PFTeDA   | 14           | PFCA   | 376-06-7   | X                      | X                        | X                      | X                                                              |
| Perfluorotridecanoic acid           | PFTrDA   | 13           | PFCA   | 72629-94-8 | X                      | X                        | X                      | X                                                              |
| Perfluoroundecanoic acid            | PFUnA    | 11           | PFCA   | 2058-94-8  | X                      | X                        | X                      | X                                                              |
| N-ethyl perfluorooctanesulfonamidacetic acid | NEtFOSAA |             | FOSAA  |            | X                      | X                        | X                      | X                                                              |
| N-methyl perfluorooctanesulfonamidacetic acid | NMeFOSAA |             | FOSAA  |            | X                      | X                        | X                      | X                                                              |
| Hexafluoropropylene oxide dimer acid | HFPO-DA  |              | GenX   | 13252-13-6 | X                      | X                        | X                      | X                                                              |
| 11-chlorooxadecafluoro-3-oxaundecane-1-sulfonic acid | 11Cl-PF3OuDS |       |     | 763051-92-9 | X                      | X                        | X                      | X                                                              |
| 9-chlorohexadecafluoro-3-oxanone-1-sulfonic acid | 9Cl-PF3ONS |       |     | 756426-58-1 | X                      | X                        | X                      | X                                                              |
| 4,8-dioxa-3H-perfluorononanoic acid | ADONA     |              | ADONA  | 919005-14-4 | X                      | X                        | X                      | X                                                              |
| Perfluoropentanoic acid             | PFPeA    | 5            | PFCA   | 2706-90-3  | X                      | X                        | X                      | X                                                              |
| Perfluorobutanoic acid              | PFBA     | 4            | PFCA   | 375-22-4   | X                      | X                        | X                      | X                                                              |
| PFAS                        | Acronym | Chain length | Class | CAS     | EPA 537 Drinking Water | EPA 537.1 Drinking Water | EPA 533 Drinking Water | EPA 8327 Reagent water, surface water, groundwater, and wastewater effluent |
|----------------------------|---------|--------------|-------|---------|------------------------|--------------------------|--------------------------|---------------------------------------------------------------------|
| Perfluorodecyl sulfonate   | PFDS    | 10           | PFSA  | 335-77-3 |                        |                          |                          | X                                                                     |
| Perfluorononane sulfonate  | PFNS    | 9            | PFSA  | 17202-41-4 |                        |                          |                          | X                                                                     |
| Perfluoroheptyl sulfonate  | PFHpS   | 7            | PFSA  | 375-92-8 | X                      |                          | X                        | X                                                                     |
| Perfluoropentane sulfonate | PFPeS   | 5            | PFSA  | 68259-08-5 | X                      |                          | X                        | X                                                                     |
| Perfluorooctanesulfonamide | FOSA    | 8            | FOSA  | 754-91-6 |                        |                          |                          | X                                                                     |
| Fluorotelomer sulfonate 8:2| 8:2 FTS | 8            | FTS   | 39108-34-4 | X                      |                          | X                        | X                                                                     |
| Fluorotelomer sulfonate 6:2| 6:2 FTS | 6            | FTS   | 27619-97-2 | X                      |                          | X                        | X                                                                     |
| Fluorotelomer sulfonic acid 4:2 | 4:2 FTS | 4            | FTS   | 757124-72-4 | X                      |                          | X                        | X                                                                     |
| Nonafluoro-3,6-dioxahexanoic acid | NFDHA |                   |       | 151772-58-6 |                        |                          | X                        |                                                                      |
| Perfluoro(2-ethoxyethane)sulfonic acid | PFEESA |                   |       | 113507-82-7 |                        |                          | X                        |                                                                      |
| Perfluoro-3-methoxypropanoic acid | PFMPA |                   |       | 377-73-1     |                        |                          | X                        |                                                                      |
| Perfluoro-4-methoxybutanoic acid | PF MBA |                   |       | 863090-89-5 |                        |                          | X                        |                                                                      |
Table S5: Representative Fragment Ions, Potential Adducts or losses or dimers, trimers identified for both positive and negative ion mode analysis (adapted from Barzen-Hanson et al. 2017).

| Fragments | Mass (Da) | Ionization Mode |
|-----------|-----------|-----------------|
| CF₃       | 68.9952   | ESI Negative    |
| C₂F₅      | 118.992   | ESI Negative    |
| C₃F₇      | 168.9888  | ESI Negative    |
| C₆F₁₃     | 318.9798  | ESI Negative    |
| CF₃O      | 84.9901   | ESI Negative    |
| C₂F₅O     | 134.9869  | ESI Negative    |
| C₃F₇O     | 184.9837  | ESI Negative    |
| SO₃       | 79.9593   | ESI Negative    |
| SO₃H      | 80.9652   | ESI Negative    |
| CO₂       | 43.9893   | ESI Negative    |
| M-COO     | M-43.989830 | ESI Negative |
| M-SO₃     | M-79.9593 | ESI Negative    |
| M-FSO₂    | M-98.9552 | ESI Negative    |
| 2M-H      | 2M-1.007276 | ESI Negative |
| 3M-H      | 3M-1.007276 | ESI Negative |
| C₃H₇O₃S   | 123.0032  | ESI Positive    |
| C₆H₁₀O₂N  | 104.0699  | ESI Positive    |
| C₇H₇NF₁₃  | 348.0052  | ESI Positive    |
| C₇H₇O₃SNF₁₃ | 411.9671 | ESI Positive    |
| C₈H₈O₃SNF₁₃ | 439.9984 | ESI Positive    |
Figure S1. An example of the diversity of non-polymeric PFAS, selected from the list of 150 compounds submitted by USEPA for \textit{in vitro} testing in collaboration with researchers at the National Toxicology Program (USEPA 2020c).
In the main text, an alternative perspective to the 4-Step Process was mentioned. Cousins et al. 2020 reviewed several approaches to PFAS assessments and grouping. They split them into approaches based on intrinsic properties and those estimating cumulative exposure and or effects. They concluded that the most precautionary of all the approaches was the “P-sufficient” approach in which one characteristic, persistence alone, is the driver for grouping of all PFAS. They conclude this approach could be done on an expedited time frame compared to more detailed hazard-based approaches.

However, according to the European Commission Communication on the Precautionary Principle (2000), the complete risk assessment should be performed before making risk management decisions to invoke the precautionary principle and take regulatory actions. This means starting with hazard identification, hazard assessment, exposure assessment, and risk characterization. The Commission stated that “…every decision must be preceded by an examination of all the available scientific data and, if possible, a risk evaluation that is as objective and comprehensive as possible.”

If the scientific data to answer the hazard questions is not available, the 4-Step Process calls for the conservative assumption that the hazard exists. This could potentially result in risk management decisions to act to regulate or restrict the chemical. Those seeking use of the chemical may generate new data to fill the hazard gap, alter their use scenarios, develop stronger control technology, etc. to reduce or eliminate the risk that originally led to the management action in the first place. The Commission Communication includes periodic review of risk measures based on the precautionary principle in light of new scientific data.
Section S2. References Cited

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