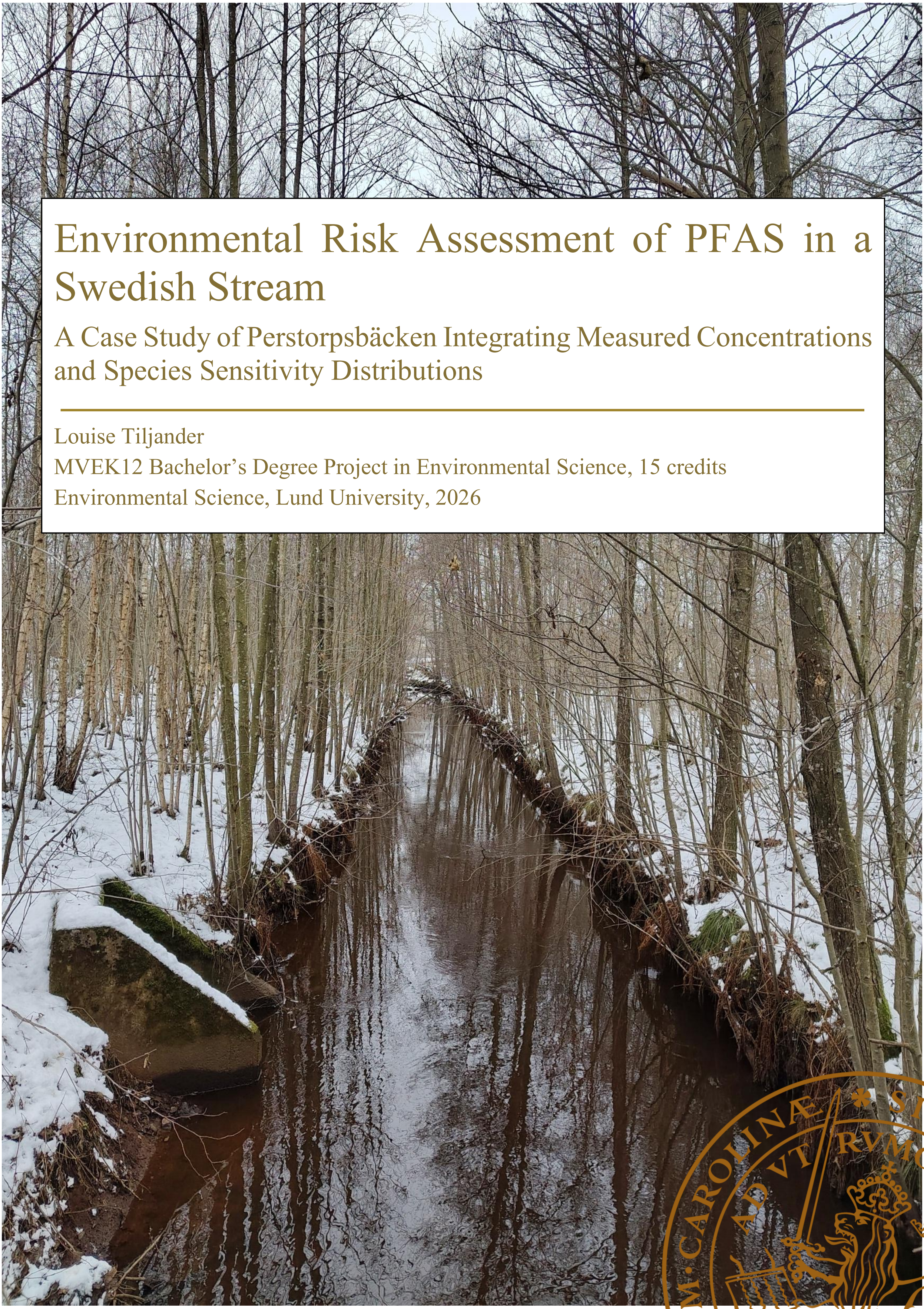

Environmental Risk Assessment of PFAS in a Swedish Stream

A Case Study of Perstorpsbäcken Integrating Measured Concentrations and Species Sensitivity Distributions

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Environmental Science, Lund University, 2026

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Cover image of Perstorpsbäcken by Louise Tiljander

Abstract

Freshwater ecosystems are increasingly threatened by persistent chemical pollutants, including per- and polyfluoroalkyl substances (PFAS), which pose long-term risks to both ecosystems and human health. Small streams downstream of urban and industrial areas are often underrepresented in monitoring programmes, despite their potential vulnerability to PFAS contamination. Furthermore, environmental risk assessments (ERAs) of PFAS in small freshwater systems remain limited, particularly site-specific assessment based measured environmental concentrations (MECs).

This study aimed to assess the occurrence and environmental risk of PFAS in Perstorpsbäcken, a Swedish stream receiving effluents from industrial areas and a wastewater treatment plant. Surface water concentrations of 24 PFAS compounds were measured at four locations along the stream. Using available chronic ecotoxicity data for locally relevant species, predicted no-effect concentrations (PNECs) were derived from species sensitivity distribution (SSD) modelling for the two dominant PFAS compounds in Perstorpsbäcken. Environmental risk was assessed by comparing MECs with the derived PNECs.

The results identified PFOS and PFHxS as the dominant compounds at most sampling sites, and a clear spatial contamination gradient was observed, with concentrations peaking shortly downstream of the wastewater treatment plant. A very low environmental risk was identified at the furthest upstream site, while the remaining locations were classified as having moderate risks. Comparison with previous monitoring data indicated that PFAS-related risks in Perstorpsbäcken may vary over time, suggesting that the stream may periodically be exposed to higher risks under different hydrological conditions.

The findings highlight the importance of site-specific assessments and expanded monitoring and assessment strategies to support ecologically relevant assessments and appropriate water management.

Populärvetenskaplig sammanfattning

PFAS i Perstorpsbäcken – bedömning av faran för bäckens miljö

I ett litet skånskt vattendrag hittades förhöjda halter av så kallade "evighetskemikalier" som kan innebära risker för livet under ytan. Trots att vattnet ser rent ut visar mätningar att påverkan från industri och avloppsvatten är större än vad man tidigare känt till.

PFAS är en stor grupp industrikemikalier med mycket goda vatten-, fett- och smutsavvisande egenskaper samt hög kemisk- och värmestabilitet. PFAS har därför använts i allt från regnkläder och matförpackningar till brandsläckningsskum. Men det som gör dem användbara är också det som gör dem problematiska, att de bryts ned extremt långsamt i naturen. Dessutom sprids de lätt i miljön och kan anrikas i levande organismer. PFAS har kopplats till olika hälsoeffekter hos människor samt till negativa effekter på djur och hela ekosystem. I Sverige och resten av världen upptäcks PFAS allt oftare i sjöar, hav och andra vattendrag. Trots detta vet vi fortfarande relativt lite om hur dessa ämnen påverkar ekosystemen i vattnen.

Vid övervakning och mätning av PFAS faller mindre vattendrag lätt mellan stolarna. Det gör det svårt att bedöma om växt- och djurlivet i dessa miljöer utsätts för risker. I detta examensarbete undersöktes därför förekomsten av PFAS i Perstorpsbäcken, ett mindre vattendrag i Sverige. Bäcken rinner bland annat genom Perstorp och passerar där både industrier och ett reningsverk. Tidigare mätningar visade på förhöjda halter av enstaka PFAS-ämnen, men det saknades kunskap om huruvida fler ämnen kunde förekomma och hur långt föroreningen sträckte sig. Följaktligen hade riskerna av PFAS-föroreningen inte heller kunnat bedömas.

Vattenprover togs på fyra platser längst bäcken, både uppströms och nedströms industrierna och avloppsreningsverket i november 2025. Totalt analyserades 24 olika PFAS-ämnen och nio av dessa påträffades på minst en plats i bäcken. Den sammanlagda halten av PFAS var högre än den gräns som EU just nu håller på att ta fram för ytvatten. Detta innebär att vattnet, utifrån halten av PFAS, inte skulle vara säkert till dricksvattenproduktion.

Risken visade sig dock något lägre för de vattenlevande organismerna vid mättillfället. För de två PFAS ämnen som förekom i högst halter i Perstorpsbäcken, PFOS och PFHxS, bedömes risken som mycket låg på den plats där bäcken rinner in i Perstorp. Däremot ökade risken till måttlig på resterande platser. De högsta halterna av PFAS uppmättes efter att vatten från både industriområdet och avloppsreningsverket hade släppts ut i bäcken. Halterna minskade, men fortsatte att vara förhöjda ungefär två kilometer efter avloppsreningsverket, längre nedströms än vad som tidigare mätts.

En viktig insikt från undersökningen var att risken i Perstorpsbäcken kan variera kraftigt över tid. Vid jämförelse med andra mätningar upptäcktes det att PFAS-halterna kan vara betydligt högre under perioder med låg vattenföring, exempelvis under torra perioder. Under sådana perioder kan förhållandena bli mer påfrestande för det liv som finns i bäcken.

Samtidigt saknas fortfarande kunskap om alla effekter som PFAS kan ha på organismer och ekosystem. För att kunna göra säkrare bedömningar krävs därför mer forskning och utökad övervakning. Undersökningen visade på förekomst och potentiell risk för miljön och att små vattendrag periodvis kan påverkas betydligt av kemikalieutsläpp. Sådana miljöer behöver kartläggas och därefter inkluderas i arbetet med att skydda vatten och biologisk mångfald.

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Acronyms and abbreviations

AF – Assessment factor

CCME – Canadian Council of Ministers of the Environment

EEA – European Environment Agency

ECHA – European Chemicals Agency

ERA – Ecological/Environmental risk assessment

EQS – Environmental quality standard

HC5 – Hazardous concentration for 5% of species

LOQ – Limit of quantification

MEC – Measured environmental concentration

PBT – Persistent, bioaccumulative, toxic

PEC – Predicted environmental concentration

PFAS – Per- and polyfluoroalkyl substances

PNEC – Predicted no-effect concentration

RSD – Relative standard deviation

RQ – Risk quotient

SGU – Sveriges geologiska undersökning (The geological survey of Sweden)

SMHI – Sveriges meteorologiska och hydrologiska institut (The Swedish meterologicical and hyrological institute)

SPE – Solid-phase extraction

SSD – Species sensitivity distribution

EPA – U.S Environmental Protection Agency

VISS – Vatteninformationssystem Sverige (The Swedish water information system)

WWTP – Wastewater treatment plant

1 Introduction

Freshwater ecosystems are increasingly threatened by multiple interacting stressors that impact water quality, destabilize biodiversity, and reduce the provision of essential ecosystem services. The majority of these stressors affecting the chemical status of freshwater ecosystems are anthropogenic, with chemical pollution representing one of the most significant pressures (Bănăduc et al., 2024; European Environment Agency [EEA], 2024). According to EEA, approximately 70 % of reported surface water bodies in the EU did not achieve good chemical status in 2021 (EEA, 2024). This failure was largely attributed to concentrations of persistent, bioaccumulative, and toxic substances (PBTs) exceeding established environmental quality standards (EQS). Among these substances, perfluorooctane sulfonate (PFOS) exceeded its EQS in approximately 2% of reported surface water bodies (EEA, 2024).

PFOS belongs to a large group called per- and polyfluoroalkyl substances (PFAS), often referred to as "forever chemicals" or "forever pollutants" due to their persistence, mobility, toxicity, and bioaccumulative potential. These properties, combined with PFAS being found widely in aquatic environments, have caused increasing global concern from both environmental and health perspectives (EEA, 2024; Giesy & Kannan, 2001; Zareitalabad et al., 2013; Abunda et al., 2020; Buck et al., 2011; Henry & Timmer, 2025; Brunn et al., 2023). As a result, the need for comprehensive regulation and systematic monitoring of PFAS in the environment has increased substantially in recent years (European Chemicals Agency [ECHA], 2023; Abunda et al., 2020; Henry & Timmer, 2025).

PFAS-contaminated aquatic environments pose a particular challenge for water resource management due to PFAS representing a complex group of compounds with diverse physicochemical properties, multiple emission sources, and varying biological effects (Abunda et al., 2020, Barber et al., 2025; Henry & Timmer, 2025; Buck et al., 2011; Evich et al., 2022). While research on human health effects of PFAS has advanced rapidly, knowledge regarding ecological and environmental risks remains comparatively limited (Gkika et al., 2023; Ruffle et al., 2023; Ankley et al., 2020). A few PFAS compounds have been shown to cause reproductive, developmental, neurotoxic, immunotoxic, and metabolic effects in aquatic organisms (Zhang et al., 2025; Brunn et al., 2023). However, for the majority of PFAS substances, ecotoxicity data are sparse or absent, resulting in considerable uncertainty in establishing EQS for freshwater ecosystems (Ruffle et al., 2023; Ankley et al., 2020).

Environmental and ecological risk assessments (ERAs) are used to estimate the likelihood that exposure to chemical stressors will cause adverse effects in ecosystems (U.S Environmental Protection Agency [EPA], 1998). In such assessments, the Predicted Environmental Concentration (PEC) of a chemical is compared to a threshold concentration below which adverse effects are not expected to occur (EPA, 2008; ECHA, 2016; ECHA, 2008). Due to the cost and time-consuming nature of sampling and chemical analyses, ERAs frequently rely on modelled PECs. These concentrations are often estimated using emission inventories, usage data, or consumption-based models (ECHA, 2016). However, a recent study by Barber et al. (2025) shows that modelled PECs frequently underestimate measured environmental concentrations (MECs) of PFAS compounds, leading to underestimated environmental risks. Consequently, risk assessments based on measured concentrations are essential, especially in smaller freshwater sources where monitoring data is sparse.

The threshold concentration used in ERAs is referred to as the Predicted No-Effect Concentration (PNEC) (ECHA, 2008; EPA, 1998). There are two standardized approaches for deriving PNECs: an approach dividing the toxicity value of the most sensitive species by an assessment factor (AF), and a statistical approach called species sensitivity distribution (SSD) (ECHA, 2008; Gredelj et al., 2018; Fox et al, 2020). The SSD approach is generally considered more robust and transparent, as it incorporates toxicity data from multiple species and explicitly accounts for uncertainty through confidence intervals (Ruffle et al., 2023; Gredelj et al., 2018; Fox et al, 2020). In an SSD, several statistical distributions are fitted to a dataset of chronic toxicity values across species, and a hazardous concentration protecting a predefined proportion of species is derived. This value is subsequently divided by an AF to account for remaining uncertainties (ECHA, 2008).

Perstorpsbäcken is a small freshwater stream located in southern Sweden that has previously been identified as potentially impacted by PFAS contamination. In 2017, a stormwater monitoring study detected elevated concentrations of PFOS at a single sampling location shortly downstream of a wastewater treatment plant (WWTP), exceeding the EQS (Vatteninformationssystem Sverige [VISS], n.d.1; VISS, n.d.2). As the study was part of a broader monitoring programme, no additional PFAS compounds were included in the analysis (VISS n.d.2). Another study was conducted during 2021 – 2022 reported even higher concentrations of PFOS, as well as elevated concentrations of perfluorooctanoic acid (PFOA). Similar to the earlier study, the screening was part of a larger project limited to only these two PFAS compounds (Lindbäck et al., 2023). Neither study measured PFAS concentrations further than approximately 100 meters downstream from the WWTP (VISS, n.d.2; Lindbäck et al., 2023). The Swedish Water Information System (VISS) considers the available measurement data insufficient for status- and risk classification of PFAS in Perstorpsbäcken (VISS, n.d.1).

Since the previous investigations, analytical methods for PFAS have improved, enabling measurement of a broader range of PFAS and at substantially lower limits of quantifications (LOQs). Given the environmental concern associated with PFAS, the limited spatial and chemical coverage of previous studies, the time elapsed since the last measurements, and the absence of a risk status, there is a clear need for a more comprehensive assessment of PFAS contamination in Perstorpsbäcken, including an environmental risk evaluation.

1.1 Aim and research questions

The aim of this study is to assess the environmental risk posed by the dominant PFAS compounds in Perstorpsbäcken. MECs are obtained through the analysis of water samples collected at four locations along an extended section of the stream compared to previous studies. The analytical screening includes 24 PFAS compounds, the majority of them listed in the suggested EU directive 2008/105/EC on environmental quality standards. The SSD approach is used to derive PNECs for the PFAS compounds detected at the highest concentrations. By conducting an ERA by integrating measured concentrations with SSD-based PNECs, the goal is to provide new insights into the environmental risk and management of PFAS contamination in Perstorpsbäcken.

The research questions are:

1. Which PFAS compounds occur at the highest concentrations in Perstorpsbäcken?

2. Do the measured concentrations of the dominant PFAS compounds cause a risk to the aquatic ecosystem in Perstorpsbäcken?
3. How do the measured concentrations and the estimated risk differ between upstream and downstream samples relative to the wastewater treatment plant?

1.2 Scope and limitations

This study focuses exclusively on PFAS concentrations in surface water from Perstorpsbäcken. Only the two most dominant PFAS compounds detected in the screening are included in the subsequent risk assessment, while the other detected compounds are discussed. Sampling is limited to four locations and was conducted on a single occasion, which does not capture seasonal variation or short-term fluctuations in PFAS concentrations. The ecotoxicological data used for the SSDs were restricted to freshwater species relevant to Swedish ecosystems, excluding marine and terrestrial organisms. Consequently, the reliability of the SSD results depends on the availability and quality of existing toxicity data. Potential mixture effects, including synergistic, additive, or antagonistic interactions among PFAS compounds or with other contaminants, are not accounted for in the risk calculations. Furthermore, the measured PFAS concentrations represent conditions at the time of sampling and do not account for historical contamination, sediment-associated PFAS, or bioaccumulation processes. As a result, actual organism exposure may be higher than indicated by measured water concentrations.

2 Methodology

2.1 Study area

Perstorpsbäcken is a small stream located in Southern Sweden (Figure 1). It flows from the north-east of, and through, the town Perstorp, and continues to the west. The stream is of natural origin and has a total length of approximately 20 kilometres (VISS, n.d.1). Upstream parts of the stream are hydrologically connected to a porous Quaternary groundwater aquifer. Besides this connection, no additional groundwater exchanges have been documented (VISS, n.d.1; VISS, n.d.3). Perstorpsbäcken discharges into Bäljane å, which subsequently flows into Rönne å, before reaching the Kattegat via the town Ängelholm.

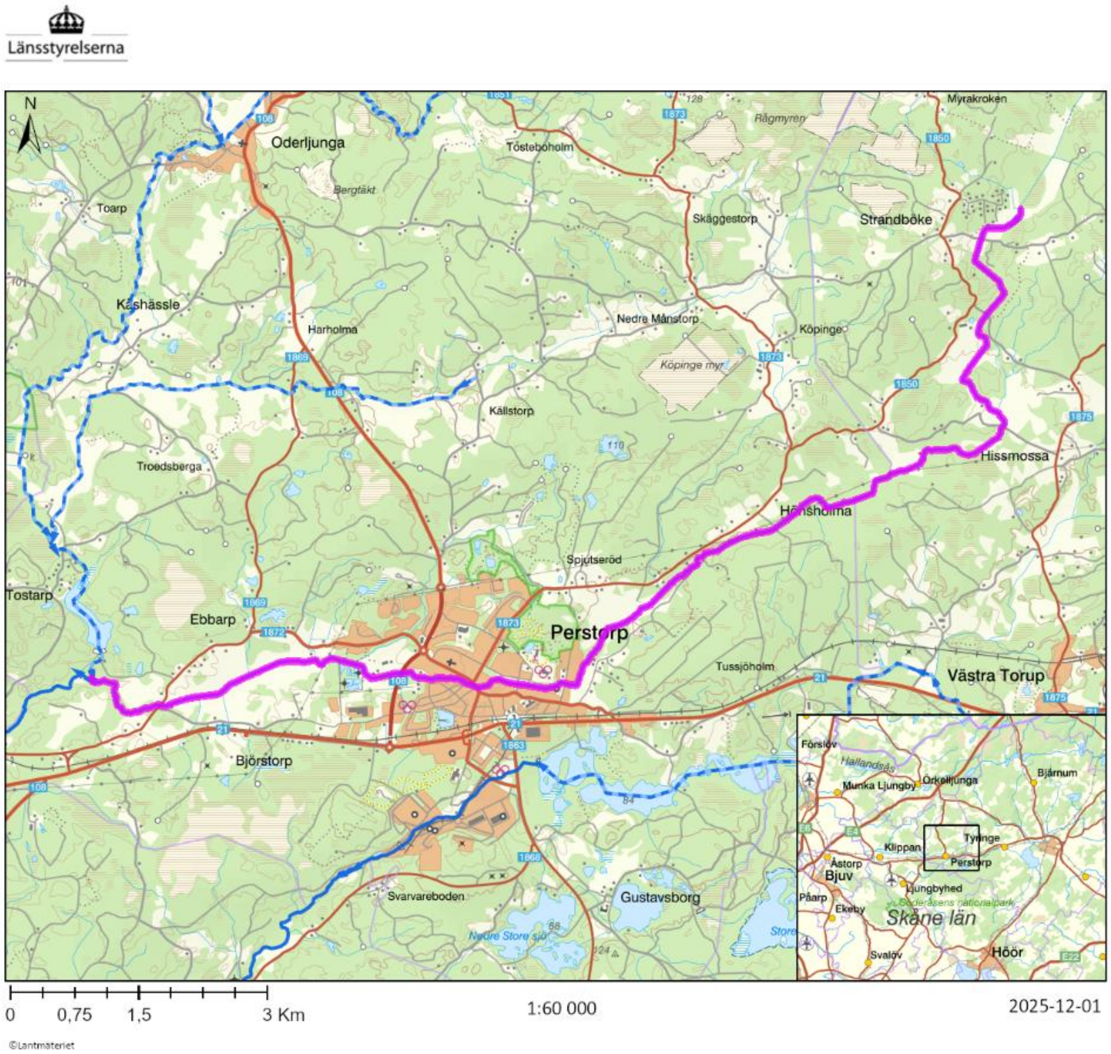


Figure 1. *Map of Perstorpsbäcken. The main map shows the full course of the stream (highlighted in purple) as it flows through the municipality of Perstorp. The inset map indicates the location of the main map in a broader regional area. The map was obtained from the Water Information System Sweden (VISS) water map tool, and Perstorpsbäcken was manually highlighted for visual clarity.*

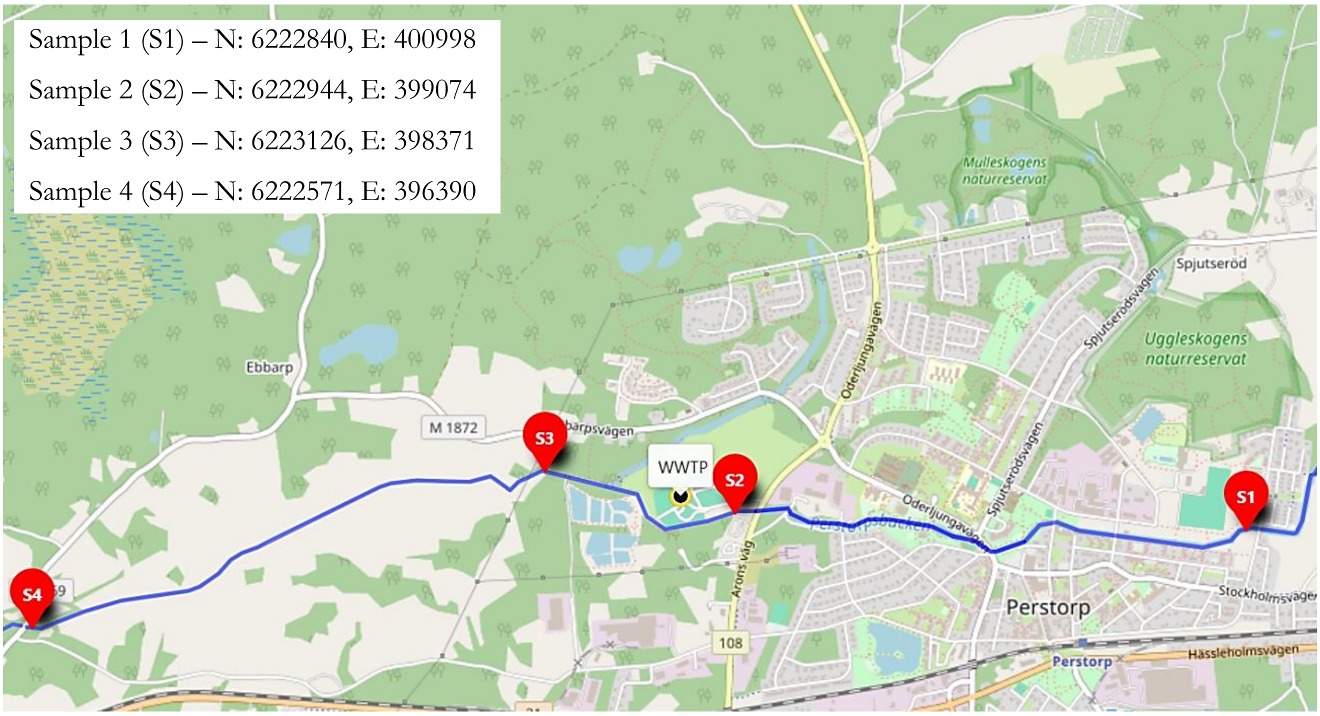
According to the current water management cycle (2021-2027), Perstorpsbäcken is classified as having moderate ecological status and poor chemical status (VISS, n.d.1). The poor chemical status is due to elevated concentrations of polybrominated diphenyl ethers (PBDEs) and mercury, both exceeding their respective EQS. In addition, tetrachloroethylene, trichloroethylene, benzo(a)pyrene, and PFOS are listed as priority substances in the water body. However, none of them have been assessed for chemical status or risk (VISS, n.d.1).

Previous measurements of PFAS in Perstorpsbäcken are limited. A single stormwater sample collected by The Geological Survey of Sweden (Sveriges Geologiska Undersökning, SGU) in 2017 near the WWTP in Perstorp reported a PFOS concentration of 3.9 ng/L, exceeding the EQS of 0.65 ng/L (Directive 2008/105/EC; Directive 2013/39/EU; VISS, n.d.1). Based on these results, the WWTP was identified as a potential point source of PFOS (VISS, n.d.1; VISS, n.d.2).

A more extensive monitoring effort was carried out in 2021-2022 through a collaboration between Kristianstad University, Länsstyrelsen Skåne, and Region Skåne (Lindbäck et al., 2023). In this study, five water samples were collected at five locations of Perstorpsbäcken: three upstream of the WWTP, one sample of the WWTP effluent, and one sample approximately 100 meters downstream. However, since the study primarily focused on pharmaceuticals in relation to water treatment, only two PFAS compounds, PFOS and Perfluorooctanoic acid (PFOA), were included (Lindbäck et al., 2023). Elevated concentrations of both compounds were reported, and PFOS concentrations ranged between 34 and 97 ng/L, significantly higher than in the previous study (VISS, n.d.1; Lindbäck et al., 2023).

2.2 Sampling

The local WWTP connected to Perstorpsbäcken served as the central reference point for sampling design. Sampling locations were selected based on accessibility to the stream, with the aim of collecting two samples upstream of the WWTP and two samples downstream. The exact sampling points and their coordinates are shown in Figure 2. Sample 1 (S1) was taken in the west part of Perstorp, upstream of both the WWTP and the industrial areas, to obtain a sample unaffected by either the industrial effluents or wastewater. Sample 2 (S2) was collected between a water inflow from an industrial area in the eastern part of Perstorp and the WWTP, to get a sample potentially affected by industrial effluents but not by wastewater. Sample 3 was collected approximately 0.1 kilometres downstream of the WWTP discharge point, to obtain a sample potentially affected by both the industrial effluents and the wastewater. Sample 4 (S4) was collected approximately 2.2 kilometres downstream from the WWTP discharge point, to get a sample of concentrations further downstream than previous studies (Figure 2).



Sample 1 (S1) – N: 6222840, E: 400998
Sample 2 (S2) – N: 6222944, E: 399074
Sample 3 (S3) – N: 6223126, E: 398371
Sample 4 (S4) – N: 6222571, E: 396390

Figure 2. *Map of the sampling section of Perstorpsbäcken, showing the four sampling points (S1-S4) and their coordinates together with the wastewater treatment plant (WWTP). The sampling section (dark blue) and the locations are displayed in a custom layer, and the underlying map base is generated in uMap (© OpenStreetMap contributors).*

Surface water samples were collected using 250 mL high-density polyethylene (HDPE) bottles mounted on a sampling pole. Each bottle was rinsed once with stream water at the sampling point before collecting the final sample. The samples were collected at a depth of approximately 0.2 metres and as close to the middle of the stream as possible. Nitrile gloves were worn throughout the sampling procedure to minimize contamination risks. After collection, the samples were transported and stored in a Styrofoam box with ice packs until laboratory analysis. Laboratory analysis was conducted the following day.

The sampling took place 24th of November 2025, between 9:00 and 13:00. The temperature during sampling was approximately 0-1°C with occasional low-amount snowfall. The water flow in all sample points was assessed to be normal based on the season. Further visual observations at the sampling sites included the presence of litter at S1 and signs of anthropogenic modification at S3 and S4.

2.3 Chemical analysis

All chemical analyses were performed at MoLab, Kristianstad University, using solid-phase extraction (SPE) followed by ultra-high-performance liquid chromatography coupled to tandem mass spectrometry (UHPLC-MS/MS). The analysis of the 24 PFAS compounds were conducted using a newly developed and validated PFAS method on an UPLC-MS/MS systems from waters (USA). The multi PFAS method originates from the PFOS method developed by Svahn & Björklund (2016; 2019).

The analysis was carried out on whole-water samples, in accordance with recommendations from the Swedish Agency for Marine and Water Management (HVMFS 2019:25) and the EU Watch List (Commission Implementing Decision 2025/439), as PFAS compounds may occur both dissolved and associated with particle matter. A procedural blank sample of 250 ml MilliQ water was included from the beginning of the analytical workflow for method validation.

Prior to the laboratory work, a safety briefing was provided by MoLab personnel, and a risk assessment covering all chemicals handled during the analysis was completed.

2.3.1 Sample preparation and SPE loading

Before extraction, all samples were spiked with 100 µL formic acid (FoA; 10%), 100 µL ethylenediaminetetraacetic acid (EDT; saturated solution), and an internal standard mixture of eight isotopically labelled PFAS compounds for dilution calibration (Svahn & Björklund, 2019).

Solid-phase extraction was performed using Oasis HLB SPE columns (200 mg) in which approximately 2 g of finely ground Fischer sand had been added, functioning as an in-line filter. This design prevents clogging of the inlet frit and enables efficient whole-water analysis without prefiltration (Svahn & Björklund, 2019). Samples were loaded onto the SPE columns using compressed air, and the pressure was adjusted as needed to maintain a stable flow rate. After sample loading, the columns were dried under positive pressure at 2 bar for 20 minutes.

Analytes were eluted into glass tubes using 6 mL of methanol and 0.5 mL ammonia (NH_3: 5%; aq). The eluates were evaporated at 40°C for approximately 20 minutes using a TurboVap evaporator. The evaporated residues were transferred into autosampler vials for instrumental analysis (Svahn & Björklund, 2019). Internal standard solutions were also added to the vials used for calibration and instrument control.

2.3.2 Instrumental analysis

A total of 24 PFAS compounds were included in the screening. LOQs and relative standard deviation (RSD) for each compound are provided in Table 1.

All 24 PFAS compounds were analysed using the chromatographic method of the UPCL-MS/MS system (Svahn & Björklund, 2019). Target compounds were separated chromatographically before ionized and detected in multiple reaction monitoring mode, providing high sensitivity and selectivity for trace-level analysis (Svahn & Björklund, 2016). Quantification was performed using isotope dilution with internal standards.

Samples were analysed beginning with those expected to have the lowest PFAS concentrations to minimize potential carry-over effects.

Table 1. *The 24 PFAS compounds analysed by UPLC–MS/MS, including abbreviations, full names, chemical formulas, limits of quantification (LOQs), and relative standard deviations (RSDs).*

Abbreviation	Full name	Chemical Formula	LOQ (ng/L)	RSD (%)
PFPeA	Perfluoropentanoic acid	C_4F_9COOH	3	4.2
PFHxA	Perfluorohexanoic acid	$C_5F_{11}COOH$	1	0.5
PFHpA	Perfluoroheptanoic acid	$C_6F_{13}COOH$	1	3.6
PFOA	Perfluorooctanoic acid	$C_7F_{15}COOH$	0.5	3.9
PFNA	Perfluorononanoic acid	$C_8F_{17}COOH$	0.5	1.5
PFDA	Perfluorodecanoic acid	$C_9F_{19}COOH$	0.5	3.5
PFUnA	Perfluoroundecanoic acid	$C_{10}F_{21}COOH$	1	3.1
PFDoDA	Perfluorododecanoic acid	$C_{11}F_{23}COOH$	0.5	9.1
PFTrDA	Perfluorotridecanoic acid	$C_{12}F_{25}COOH$	1	3.2
PFTeDA	Perfluorotetradecanoic acid	$C_{13}F_{27}COOH$	1	2.7
PFBS	Perfluorobutane sulfonic acid	$C_4F_9SO_3H$	0.5	5.1
PFPeS	Perfluoropentane sulfonic acid	$C_5F_{11}SO_3H$	1	6.3
PFHxS	Perfluorohexane sulfonic acid	$C_6F_{13}SO_3H$	1	2
PFHpS	Perfluoroheptane sulfonic acid	$C_7F_{15}SO_3H$	1	4.3
PFOS	Perfluorooctane sulfonic acid	$C_8F_{17}SO_3H$	0.5	4.9
PFNS	Perfluoro-1-nonanesulfonate	$C_9F_{19}SO_3H$	2	7.8
PFDS	Perfluorodecane sulfonic acid	$C_{10}F_{21}SO_3H$	2	15
PFDoS	Perfluoro-1-dodecanesulfonate	$C_{12}F_{25}SO_3H$	2	7.2
PFOSA	Perfluorooctanesulfonamide	$C_8F_{17}SO_2NH_2$	5	13.2
N-MeFOSAA	N-methylperfluorooctanesulfonamidoacetic acid	$C_8F_{17}SOON(CH_3)CH_2CO_2H$	2	6.2
N-EtFOSAA	N-ethylperfluorooctanesulfonamidoacetic acid	$C_8F_{17}SOON(C_2H_5)CH_2CO_2H$	2	1.4
4:2FTS	1H,1H, 2H, 2H-Perfluorohexane sulfonic acid	$C_4F_9(CH_2)_2SO_3H$	0.5	3.7
6:2FTS	1H,1H, 2H, 2H-Perfluorooctane sulfonic acid	$C_6F_{13}(CH_2)_2SO_3H$	1	2.7
8:2FTS	1H,1H, 2H, 2H-Perfluorodecane sulfonic acid	$C_8F_{17}(CH_2)_2SO_3H$	1	2.5

2.4 Ecotoxicity modelling

To assess whether the measured PFAS concentrations in Perstorpsbäcken pose a potential risk to the aquatic ecosystem, effect-based thresholds were required. Therefore, PNECs were derived for the two PFAS compounds detected at the highest concentrations in the water samples. The PNECs were derived using the SSD approach based on chronic ecotoxicity data from multiple freshwater species to represent long-term exposure scenarios in a freshwater ecosystem (ECHA, 2008; EPA, 1998; Fox et al, 2020).

The SSD approach was selected because when there is sufficient ecotoxicity data it provides a more statistically robust method than single-species approaches, as it accounts for variability in sensitivity, enables extrapolation beyond the tested species, and provides uncertainty estimates through confidence intervals (Gredelj et al., 2018; Fox et al, 2020; ECHA, 2008). The full R script used in the modelling is provided in Appendix C.

2.4.1 Data collection

To model the SSDs, ecotoxicity data for the two dominant PFAS compounds identified in Perstorpsbäcken were collected from the U.S. EPA ECOTOX Knowledgebase, which includes only peer-reviewed studies. To ensure ecological relevance for Perstorpsbäcken, only freshwater species were included. Priority was given to standard test species and locally occurring species. When these were unavailable, surrogate species were selected based on ecological similarity or by representation of functional groups present in Perstorpsbäcken.

Two strict criteria were applied to determine whether an SSD could be constructed: (1) a minimum of 10 species (preferably at least 15), and (2) coverage of at least three trophic levels. When possible, datasets were also evaluated against extended criteria to identify limitations in data (ECHA, 2008; Canadian Council of Ministers of the Environment [CCME], 2007):

- at least 8 taxonomic groups,
- at least 3 fish species,
- at least 3 aquatic or semi-aquatic invertebrates (including at least one planktonic crustacean),
- at least 1 algae species,
- at least 1 species of higher plants,
- at least 1 amphibian,
- at least 1 insect, and
- at least 1 non-chordate, non-arthropod species (not otherwise represented).

For each species, only one toxicity value was included in the SSD. Only chronic effects were considered, and the accepted endpoints were EC10, EC20 (effect concentrations causing a 10% and 20 % response), NOEC (no observed effect concentration), and LOEC (lowest observed effect concentration) (ECHA, 2008; CCME, 2007). When multiple endpoints were available for a species, the most sensitive (lowest) effect concentration was selected to avoid underestimation of risk (CCME, 2007). Preference was given to effects on growth, development, and reproduction, as these are the recommended endpoints when conducting a risk assessment. If preferred effects were unavailable, effects on behaviour, physiology, and population were used, in accordance with ERA guidelines (ECHA, 2008; CCME, 2007).

2.4.2 SSD modelling and PNEC derivation

An SSD was constructed for each PFAS compound using the *shinyssdtools* package in RStudio. Several statistical distributions (gamma, lgumbel, llogis, lnorm, lnorm_lnorm, weibull) were fitted to the data. The best-fit distribution was selected based on the lowest Akaike Information Criterion (AIC/AICc). When no single distribution clearly outperformed the others, model averaging was applied to account for model uncertainty (Fox et al., 2020).

From each SSD, the hazardous concentrations for 5 % of species ($HC5_{50}$) and its 95% confidence intervals ($HC5_{lcl}$ and $HC5_{ucl}$) were derived. The $HC5_{50}$ represents a concentration at which 95% of species are expected to be protected and the percentage is commonly applied in ERAS as a balance between ecological protectiveness and statistical robustness (ECHA, 2008; Posthuma et al., 2002). To account for residual uncertainty, PNECs were calculated by dividing each $HC5_{50}$ value by an AF (Equation 1).

$$PNEC = \frac{HC5_{50}}{AF}$$

Equation 1

AFs were selected based on the dataset criteria. When both strict and extended criteria were met, an AF of 5 was applied, in accordance with ECHA guidelines (ECHA, 2008). When only the strict criteria were met, an AF of 10 was chosen to account for the data limitations.

2.5 Risk calculations

The environmental risk posed by the two dominant PFAS compounds in Perstorpsbäcken was evaluated by using a deterministic risk quotient (RQ). RQs were calculated for each compound at all sampling sites. The RQ approach is commonly applied and recommended in ERA frameworks for aquatic ecosystems (EPA, 1998; ECHA, 2008; ECHA, 2016).

The RQs was defined as the ratio between the MEC in Perstorpsbäcken and the PNECs derived from the SSD modelling (Equation 2). The ratio indicated whether measured concentrations approached or exceeded the effect thresholds and thus provided an estimate of the likelihood of adverse ecological effects (EPA, 1998; ECHA, 2008; ECHA, 2016).

$$RQ = \frac{MEC}{PNEC}$$

Equation 2

Risk levels were interpreted according to established thresholds commonly applied in ERA, where $RQ > 1$ indicates a high risk of adverse environmental effects (ECHA, 2008; EPA, 1998; ECHA, 2016). To allow for a more nuanced interpretation of potential risk, additional RQ categories frequently used in aquatic risk assessments were applied. Accordingly, RQ values < 0.01 were classified as very low risk, values between 0.01 and 0.1 as low risk, and values between 0.1 and 1 as moderate risk (Hernando et al., 2006; Razak et al., 2025; Guo et al., 2020; Molnar et al., 2021).

3 Results

3.1 Measured PFAS concentrations in Perstorpsbäcken

A total of 24 PFAS compounds were analysed in surface water samples collected at the four locations along Perstorspbäcken. Out of these, nine compounds were detected in at least one sample, and four compounds exceeded their respective LOQs (Table 2). PFOS and PFHxS occurred at the highest concentrations in three samples (samples 2, 3, and 4) and were therefore identified as the two dominant PFAS compounds in Perstorpsbäcken (Table 2). PFOS and PFHxS occurred at the highest concentrations in three samples (samples 2, 3 and 4) and were therefore identified as the two dominant PFAS compounds in the stream. Out of the two, PFOS consistently occurred at higher concentrations than PFHxS (Table 2).

Table 2. *Measured environmental concentrations (ng/L) of the 24 analysed PFAS compounds in four water samples from Perstorpsbäcken. The two dominant compounds are highlighted. Compounds not detected in a given sample are marked "nd". Sample locations are shown in Figure 2, and the full chemical names along with LOQs for each compound are provided in Table 1.*

PFAS compound	**Concentration (ng/L)**			
	Sample 1	**Sample 2**	**Sample 3**	**Sample 4**
PFPeA	<LOQ	<LOQ	<LOQ	<LOQ
PFHxA	nd	nd	nd	nd
PFHpA	nd	nd	nd	nd
PFOA	<LOQ	<LOQ	0.5	<LOQ
PFNA	<LOQ	nd	nd	<LOQ
PFDA	nd	<LOQ	<LOQ	<LOQ
PFUnA	nd	nd	nd	<LOQ
PFDoDA	nd	nd	nd	nd
PFTrDA	nd	nd	nd	nd
PFTeDA	nd	nd	nd	nd
PFBS	0.7	1.0	0.9	<LOQ
PFPeS	nd	<LOQ	<LOQ	<LOQ
PFHxS	nd	1.5	2.5	1.8
PFHpS	nd	nd	nd	nd
PFOS	nd	6.5	7.5	6.0
PFNS	nd	nd	nd	nd
PFDS	nd	nd	nd	nd
PFDoS	nd	nd	nd	nd
PFOSA	nd	nd	nd	nd
N-MeFOSAA	nd	nd	nd	nd
N-EtFOSAA	nd	nd	nd	nd
4:2FTS	nd	nd	nd	nd
6:2FTS	nd	nd	nd	nd
8:2FTS	nd	nd	nd	nd
Total PFAS	>0.7	>9	>11.4	>7.8

The furthest upstream site (Sample 1), located before both the industrial water release and the WWTP, showed the lowest total PFAS concentration (>0.7 ng/L). At this site, only PFBS exceeded its LOQ, while PFPeA, PFOA, and PFNA were detected below their respective LOQs (Table 2). At sample location 2, located downstream of industrial effluents but upstream of the WWTP, the total PFAS concentration increased to >9 ng/L. Seven PFAS compounds were detected in the sample, with PFBS (1.0 ng/L), PFHxS (1.5 ng/L), and PFOS (6.5 ng/L) exceeding their LOQs (Table 2).

The highest total PFAS concentration (>11.4) was observed at Sample 3, located approximately 100 meters downstream of the WWTP discharge point. At this site, PFOS (7.5 ng/L) and PFHxS (2.5 ng/L) reached their maximum MECs in the stream (Table 2). At this location, PFOA (0.5 ng/L) could be quantified, whereas in Sample 2 where it was detected below its LOQ (Table 2). PFOS (6.0 ng/L) declined compared to Samples 2 and 3, while the PFHxS concentration (1.8 ng/L) was lower than in sample 3 but slightly higher than in sample 2 (Table 2).

Further downstream at Sample 4, approximately 2.2 kilometres downstream the WWTP, nine PFAS compounds were detected, representing the location with most compounds detected. However, total PFAS concentrations declined to >7.8 ng/L, lower than the two previous sample locations but remained elevated compared to Sample 1 (Table 2).

Overall, both PFOS and PFHxS, as well as total PFAS increased markedly between the two upstream sites located before and after the industrial effluent location. The concentrations peaked immediately downstream of the WWTP and declined further downstream (Table 2).

3.2 Ecotoxicity modelling

SSDs were constructed for PFOS and PFHxS based on their dominance in Perstorpsbäcken. The data collection for the SSD modelling resulted in 27 species across 9 groups and 8 phyla for PFOS, and 10 species across 5 groups and 3 phyla for PFHxS (Appendix A).

The resulting model average SSDs for PFOS and PFHxS are shown in Figure 3 and Figure 4, respectively, as a cumulative proportion of species affected as a function of concentration together with the estimated $HC5_{50}$ values. For both compounds model averaging was applied to derive the final HC5 values, as no single fitted distribution provided a clearly superior fit (Appendix B).

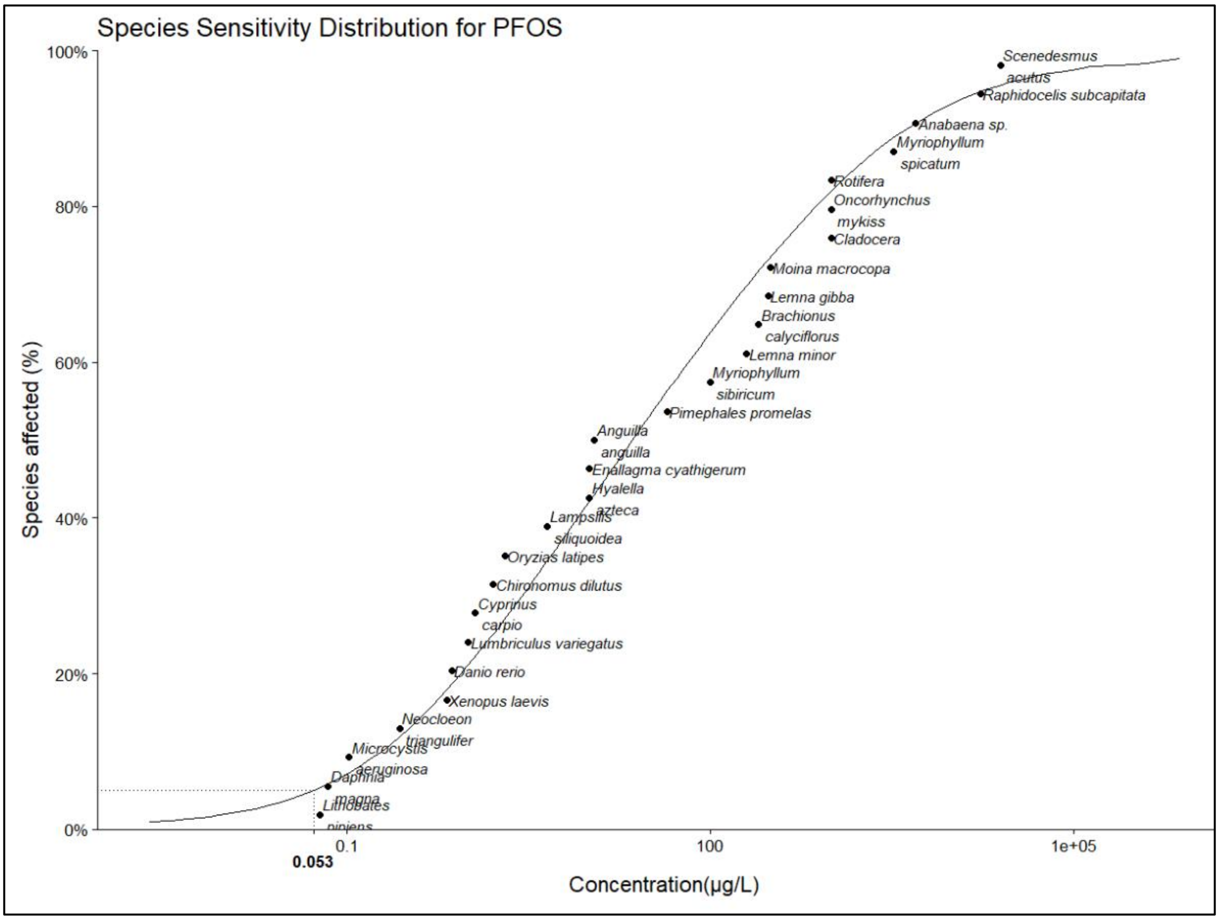


Figure 3. *Species Sensitivity distribution (SSD) for PFOS based on chronic freshwater ecotoxicity data. The SSD shows the cumulative proportion of species affected (%) as a function of effect concentration. The dashed line indicates the HC5 (0.053 µg/L) derived by model averaging and represents the concentration expected to protect 95% of freshwater species. Individual data points represent species-specific effect concentrations and are labelled with scientific species names.*

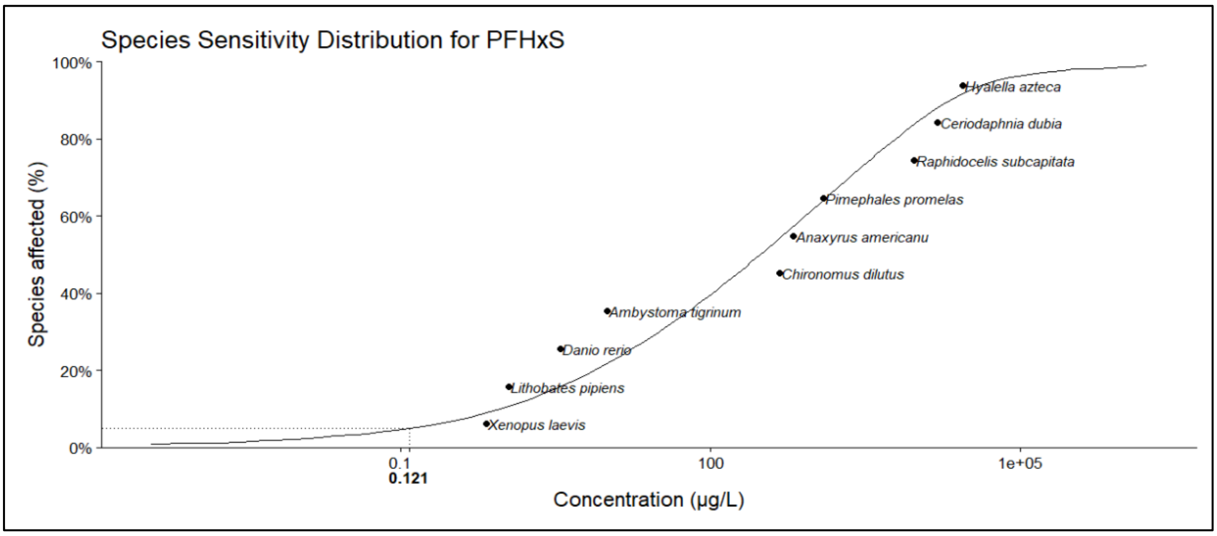


Figure 4. *Species Sensitivity distribution (SSD) for PFHxS based on chronic freshwater ecotoxicity data. The SSD shows the cumulative proportion of species affected (%) as a function of effect concentration. The dashed line indicates the HC5 (0.121 µg/L) derived by model averaging and represents the concentration expected to protect 95% of freshwater species. Individual data points represent species-specific effect concentrations and are labelled with scientific species names.*

For PFOS, the model-averaged $HC5_{50}$ was 53 ng/L, with a lower confidence limit ($HC5_{lcl}$) of 1.1 ng/L and an upper confidence limit ($HC5_{ucl}$) of 455 ng/L (Figure 3, Table 3). The extracted ecotoxicity dataset for PFOS was considered robust in terms of fulfilling the criteria of species coverage. Consequently, an AF of 5 was applied, resulting in a PNEC of 10.6 ng/L (Table 3).

For PFHxS, the model-averaged $HC5_{50}$ was higher, at 121 ng/L, but had a substantially wider confidence interval ranging from 0.03 ng/L to 22 800 ng/L (Figure 4, Table 3). The extracted ecotoxicity dataset for PFOS fulfilled the strict criteria of species coverage but not the extended criteria. Therefore, an AF of 10 was applied, yielding a PNEC of 12.1 ng/L (Table 3).

Table 3. *SSD-derived $HC5_{50}$ values (ng/L), associated lower and upper confidence levels ($HC5_{lcl}$ and $HC5_{ucl}$), selected assessment factors (AFs), and resulting predicted no-effect concentrations (PNECs) for PFOS and PFHxS. PNECs were calculated with Equation 1. Details on fitted distributions and model averaging are provided in Appendix B.*

PFAS compound	$HC5_{50}$ (ng/L)	$HC5_{lcl}$ (ng/L)	$HC5_{ucl}$ (ng/L)	AF	PNEC (ng/L)
PFOS	53	1.1	455	5	10.6
PFHxS	121	0.03	22800	10	12.1

3.3 Risk calculations

RQs for PFOS and PFHxS were calculated for each sampling location by comparing the MECs with the SSD derived PNECs. The MECs, PNECs, RQs, and corresponding qualitative risk categories at each sampling site are presented in Table 4.

Table 4. *Measured environmental concentrations (MECs), predicted no-effect concentrations (PNECs), calculated risk quotients (RQs), and corresponding qualitative risk classifications for PFOS and PFHxS at the four sampling locations in Perstorpsbäcken. RQs were calculated as the ratio between MEC and PNEC (Equation 2), MECs are from Table 2, and PNECs are from Table 3.*

Sample location	PFAS compound	MEC (ng/L)	PNEC (ng/L)	RQ	Risk classification
Sample 1: Upstream Perstorp	PFOS	nd	10.6	<0.01	Very low
	PFHxS	nd	12.1	<0.01	Very low
Sample 2: Upstream WWTP	PFOS	6.5	10.6	0.61	Moderate
	PFHxS	1.5	12.1	0.12	Moderate
Sample 3: Downstream WWTP	PFOS	7.5	10.6	0.71	Moderate
	PFHxS	2.5	12.1	0.21	Moderate
Sample 4: Downstream Perstorp	PFOS	6.0	10.6	0.57	Moderate
	PFHxS	1.8	12.1	0.15	Moderate

At the most upstream site (S1), PFOS and PFHxS were not detected. Consequently, RQs for both compounds were <0.01, indicating a very low environmental risk at this site (Table 4, Figure 5). At the second sample upstream the WWTP (S2), but located downstream of the industrial effluent discharge point, MECs increased for both compounds, and hence the RQs increased. While the MECs did not exceed their respective PNECs, both RQs corresponded to a moderate risk category (Table 4, Figure 5).

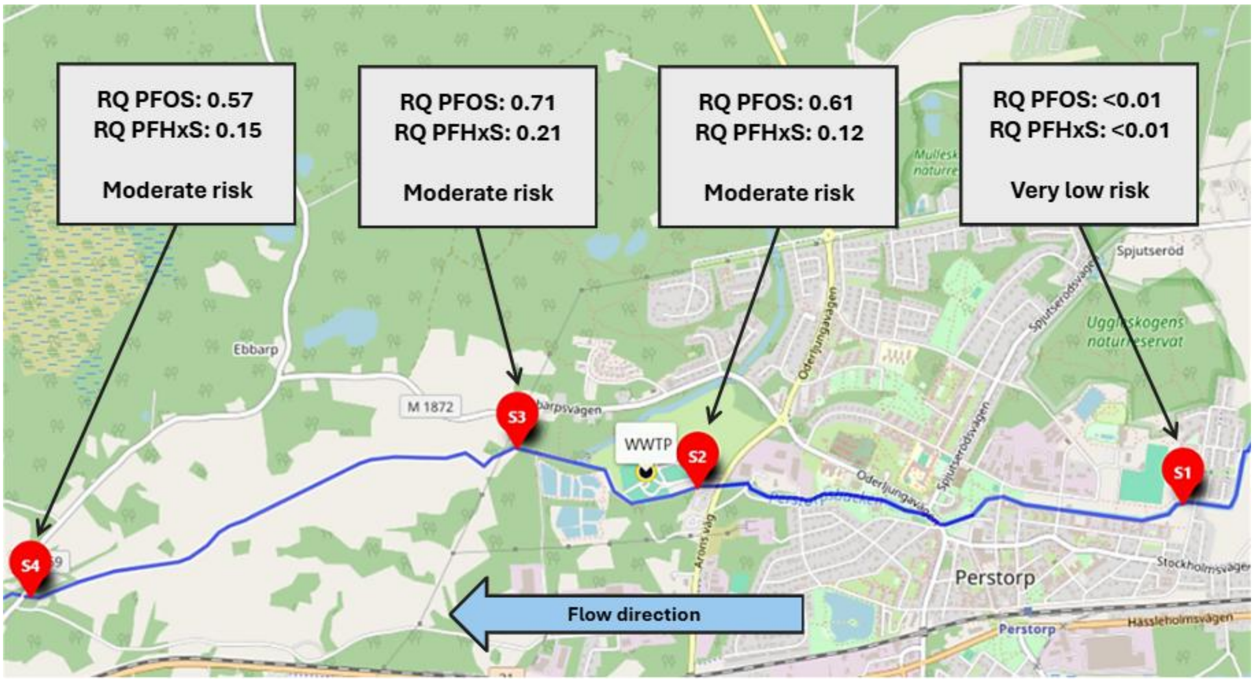


Figure 5. *Spatial distribution of environmental risk in Perstorpsbäcken based on risk quotients (RQs) for PFOS and PFHxS at the four sampling locations (S1 – S4). RQs are displayed for each sampling location together with the corresponding qualitative risk classification. The underlying map base is generated in uMap (© OpenStreetMap contributors).*

The highest RQs for both compounds were observed at sample site 3 (S3), approximately 100 metres downstream the WWTP discharge point (Figure 5). At this location PFOS reached an RQ of 0.71, while PFHxS had an RQ of 0.21. Although PFOS concentrations approached the PNEC, it did not exceed it. Both compounds were classified as posing a moderate ecological risk at the site (Table 4, Figure 5). At the most downstream sampling location (S4), RQs were slightly lower than at the previous sampling site but remained within the moderate risk category (Table 4, Figure 5).

Spatially, the largest increase in quantitative risk for both compounds was between S1 and S2, where also the only change in qualitative risk occurred. While the quantitative risk changed between the following sampling sites, the RQs indicated no change in qualitative risk (Table 4, Figure 5).

4 Discussion

4.1 Occurrence and spatial distribution of PFAS in Perstorpsbäcken

Out of the 24 PFAS compounds included in the analytical screening, nine were detected in at least one water sample from Perstorpsbäcken (Table 2). This detection frequency is somewhat lower than that reported in a Swedish monitoring study by Nguyen et al. (2017), where 13 out of 26 PFAS compounds were detected in river waters. However, the monitoring study included several rivers across Sweden, most of which were substantially larger than Perstorpsbäcken, which may partly explain the higher number of detected compounds (Nguyen et al., 2017). Moreover, only 18 of the PFAS compounds analysed were common to both studies, which could also contribute to the observed differences in detection frequency (Nguyen et al., 2017).

In the monitoring study by Nguyen et al. (2017), PFBS and PFHxS were reported as the most dominant PFAS compounds in the rivers, and while not dominant, PFOS showed a detection frequency of 98% (Nguyen et al., 2017). In the present study, PFOS and PFHxS dominated the PFAS profile at the majority of sampling locations in Perstorpsbäcken (Table 2). The third most dominant compound was PFBS, making the compound domination in Perstorpsbäcken largely consistent with the monitored rivers (Nguyen et al., 2017). The dominance of PFOS observed in the present study, as well as the high detection frequency in the river study, further aligns with its frequently documented occurrence in urban freshwater environments and it being one of the most prevalent PFAS compounds in surface waters in general (Nguyen et al., 2017; EEA, 2024; Dasu et al., 2022; Sun & Li, 2024).

The monitoring study by Nguyen et al. (2017) generally reported lower concentrations of PFOS, PFBS, and PFHxS in Swedish rivers than those observed in Perstorpsbäcken, with only a few exceptions. In the present study, both sampling locations S2 and S3 exhibited higher total PFAS concentrations than the average total PFAS levels reported for the rivers included in the monitoring (Nguyen et al., 2017). This indicates that PFAS contamination in Perstorpsbäcken both slightly upstream and downstream of the WWTP is elevated relative to background concentrations observed in the larger Swedish river systems.

A clear spatial gradient in PFAS concentrations was observed along the sampling transect. Substantially lower concentrations were measured at the upstream reference site (S1) compared following locations (Table 2), indicating limited background contamination. The largest increase in PFAS concentrations occurred between S1 and S2, suggesting that industrial effluents and diffuse urban sources constitute the primary contributors of PFAS inputs in the stream. The highest concentrations of PFOS, PFHxS, and total PFAS were measured shortly downstream of the WWTP (S3), strongly implicating the treatment plant as an additional point source (Table 2). This finding is consistent with previous studies showing that WWTPs are well-established sources of PFAS to aquatic environments, as conventional treatment processes are largely ineffective at removing these substances (Ankley et al., 2020; Krlovic, 2024). Consequently, PFAS originating from households, industry, and commercial products are being released into water bodies via WWTP effluents (Ankley, 2020; Krlovic 2024). However, the relatively smaller increase in concentrations between S2 and S3 indicates that, although the WWTP acts point source, PFAS contamination in Perstorpsbäcken is predominantly influenced by upstream inputs. This underscores the importance of an extended sampling transect, as sampling only at S1 and S3 would have led to the incorrect conclusion that the WWTP is the dominant source of PFAS.

Further downstream, approximately 2.2 kilometres from the WWTP (S4), PFAS concentrations declined but remained elevated compared to the upstream reference site (S1) (Table 2). This limited reduction could suggest that dilution, sorption to sediments, and other attenuation processes are insufficient to substantially reduce the concentrations over this distance, highlighting the high mobility and environmental persistence of PFAS compounds (ERA, 2024; Brunn et al., 2023). Although, the contribution of additional pollution sources between S3 and S4 cannot be excluded, the MECs demonstrate that PFAS contaminations extends further downstream than previously documented in Perstorpsbäcken.

Smaller steams are often underrepresented in monitoring programmes, and PEC-based approaches have been shown to frequently underestimate PFAS concentrations (Barber et al., 2025). The elevated MECs observed downstream in Perstorpsbäcken, despite it being a relatively small stream, therefore underscores the importance of site-specific measurements that account for both longitudinal transports as well as lateral inputs in order to capture the true spatial extent of PFAS contamination.

4.2 Comparison with EQS and previous monitoring data

PFOS concentrations exceeded the current EQS for inland surface waters (0.65 ng/L) by a wide margin at sampling locations S2–S4 (Table 2). This EQS is primarily based on the protection of human health via fish consumption (Directive 2008/105/EC; Directive 2013/39/EU; SGU, 2024). Although no EQS has yet been established for PFHxS as an individual substance, its inclusion on the EU Directive 2008/105/EC reflects growing regulatory concern regarding its environmental and health impacts (Commission Implementing Decision 2025/439).

Furthermore, the Water Framework Directive is currently under revision, and the European Council and Parliament have recently reached a provisional agreement to update the list of priority substances in surface and groundwater, including the introduction of an EQS for the sum of 25 PFAS compounds (SCHEER, 2025; Council of the European Union, 2025). The proposed standard is 4.4 ng/L, expressed as PFOA equivalents and based on relative potency factors derived from human health assessments (RIVM, 2018; Council of the European Union, 2025). When applying this approach, the proposed EQS is exceeded in S2 (~13.9 ng/L), S3 (~17.5 ng/L), and S4 (~13.1 ng/L). While these EQSs are primarily intended to protect human health, their exceedance underscores the broader significance of the PFAS contamination in Perstorpsbäcken.

While VISS (n.d.1) states that the previously available PFAS data for Perstorpsbäcken is insufficient for chemical status classification, the present study substantially expands both the chemical and spatial scope by including multiple PFAS compounds along a larger section of the stream. The observed exceedance of the proposed EQS for the sum of PFAS at most sampling sites indicates that Perstorpsbäcken would be at risk of failing good chemical status with respect to PFAS under the revised Water Framework Directive (SCHEER, 2025; Council of the European Union, 2025; EEA, 2024).

However, the interpretation of chemical status based on threshold exceedances is influenced by temporal variability in concentrations. At sampling location S3, the measured PFOS concentration in the present study (7.5 ng/L) was higher than the concentration reported at the same location in 2017 (3.9 ng/L) (VISS n.d.1; VISS n.d.2). This may suggest that the PFOS contamination has persisted and potentially intensified over time. However, hydrological data from the Swedish Meteorological and Hydrological Institute (SMHI) shows that water flows in Scania were generally higher during 2017 than during the sampling period for the present study (SMHI, 2024; SMHI, 2025). Higher flow conditions are likely to result in dilution of dissolved contaminants, and further dispersion of pollutants, which may partly explain the lower concentrations observed in 2017 (Chashechkin & Rozental, 2019).

Substantially higher PFAS concentrations were reported in measurements conducted between 2021 and 2022 at approximately the same location as S3. During this period, PFOS concentrations ranged from 34 to 97 ng/L, and PFOA was measured at 3.1 ng/L in 2022, compared to 7.5 ng/L and 0.5 ng/L, in the present study (Lindbäck et al., 2023). Hydrological data indicate that both water flow and precipitation during the sampling months in 2021–2022 were considerably lower than during the sampling for the present study (SMHI, 2024; SMHI, 2025). Notably, the highest PFOS concentrations measured in 2021-2022 were during periods of lowest flow, while lower concentrations coincided with higher flow conditions (Lindbäck et al., 2023; SMHI, 2024). This further supports the interpretation that hydrological conditions, particularly flow rates, are a key factor influencing observed PFAS concentrations in Perstorpsbäcken. This observation is in accordance with a study by Chashechkin & Rozental (2019) which demonstrated that dispersion of chemicals is supported and sometimes initiated by hydrodynamic factors such as water flow.

4.3 Environmental risk implications

The ERA based on MECs and SSD indicated very low environmental risk at the upstream reference site (S1), while moderate risk was identified at the rest of the locations (S2 – S4) for both PFOS and PFHxS (Table 4). PFOS consistently exhibited higher RQs than PFHxS and approached an RQ of 1 at the site immediately downstream of the WWTP (S3), indicating concentrations close to levels associated with ecological effects in sensitive aquatic species (Table 4).

Although none of the calculated RQs exceeded unity in the present study, an RQ below 1 does not imply the absence of environmental effects. Moderate risk levels may still negatively affect sensitive species, particularly under conditions of long-term exposure. PFOS has been present in elevated concentrations in Perstorpsbäcken since at least 2017, suggesting chronic exposure to aquatic organisms over several years (VISS, n.d.1). Such exposure durations are rarely captured by standard toxicity tests, which are often limited in temporal scope (Ankley et al., 2020, Gkika et al., 2023). In addition, the bioaccumulative nature of many PFAS compounds implies that internal concentrations in the aquatic organisms may be substantially higher than those inferred from water concentrations alone (Brunn et al., 2023; Ankley et al., 2020; ERA, 2024).

Further insight into potential risk levels can be gained by comparing the present results with the previous monitoring data from 2021–2022, with PFOS concentrations ranging from 34 to 97 ng/L during lower flow rates (Lindbäck et al., 2023). When comparing these concentrations with the PNEC derived in the present study, the resulting RQs ranges approximately between 3 and 9, indicating high environmental risk. This highlights the importance of considering the hydrological variability when conducting ERAs.

Subsequently, while the present assessment indicates moderate environmental risk, substantially higher risks may occur during other hydrological scenarios in locations both up- and downstream the WWTP. The aquatic ecosystem is therefore likely subject to episodic or seasonal periods of high risk in addition to long term exposure. Projected changes in precipitations and intensified extreme weather events associated with climate change may further amplify the frequency and magnitude of such risk fluctuations (Rosso et al., 2025; Tan et al., 2023).

4.4 Uncertainty and limitations of the ERA

Given that PFAS contamination and associated risk assessments are sensitive subjects, it is important to openly address uncertainties and limitations of the method to avoid overestimating the certainty of the results. All data inputs, coding script, and additional outputs from the SSD-modelling are provided in Appendices A, B and C to ensure transparency and allow independent review. This transparency is particularly important for PFAS, as public perception of these contaminants can easily generate concern or alarm (Liu & Yang, 2025).

There are several sources of uncertainty and methodological limitations that should be considered when interpreting the results of the ERA for PFAS in Perstorpsbäcken. First, the assessment is based on a single sampling occasion conducted under relatively high-flow conditions. As demonstrated by the comparisons with previous monitoring, PFAS concentrations in the stream influenced by hydrological variability. Consequently, the MECs presented here may underestimate concentrations and associated risks during periods of lower flow.

Second, the risk assessment does not account for PFAS partitioning to sediments or accumulation in aquatic biota. The absence of sediment and biota data therefore introduces uncertainty and likely leads to an underestimation of long-term ecological risks, particularly for higher trophic levels.

Additional uncertainty arises from the derivation of PNECs using the SSD approach. Although SSDs are widely regarded as statistically robust and transparent, their reliability depends on the availability, quality, and taxonomic representativeness of ecotoxicological data (ECHA, 2008; De Laender et al., 2007, Gredejl et al., 2018; Fox et al., 2020; Belanger et al., 2017). For PFAS, toxicity data are biased toward a small number of compounds and species, as shown by the sparse dataset for PFHxS, resulting in particularly wide confidence intervals (Gredejl et al., 2018; Gkika et al., 2023; Ruffle et al., 2023). Such limitations increase uncertainty in the derived PNEC and, consequently in the resulting risk estimates.

The SSD approach assumes that protecting the most sensitive species is sufficient to protect ecosystem structure and function. However, SSDs are based on single-species toxicity tests and do not capture ecological interactions, indirect effects, or the influence of abiotic factors, which may limit the ecological realism (De Laender et al., 2007; Gredejl et al., 2018; Fox et al., 2020; Belanger et al., 2017). While the present assessment restricted toxicity data to freshwater species relevant to the local ecosystem, surrogate test species do not fully represent the sensitivity of the actual species present in Perstorpsbäcken, causing either over- or underestimation of risks (Ankley et al., 2020; Belanger et al., 2017).

Chemical mixture effects are another important source of uncertainty. The risk assessment evaluated PFOS and PFHxS individually, whereas aquatic ecosystems are typically exposed to complex mixtures of PFAS and other contaminants, particularly downstream of WWTPs (Ankley at al., 2020; Houtz et al., 2016; Hu et al., 2016). Additive, synergistic, or antagonistic interactions among PFAS compounds, as well as with other contaminants, could not be considered. Because PFAS commonly occur as mixtures in the environment, this represents a key limitation of the present assessment and ERAs in general (Ankley et al., 2020; Houtz et al., 2016).

Finally, methodological challenges also arise from the rapidly decreasing EQSs for PFAS within the EU regulatory framework. Many analytical methods currently applied in routine monitoring have LOQs that exceed current or proposed EQSs, limiting their usefulness for exposure assessments (SCHEER, 2025; Ruffle et al., 2023). The present study further demonstrates the importance of using analytical methods with sufficiently low LOQs and good precision (low RSD) to detect and quantify environmentally relevant PFAS concentrations and allow meaningful comparison with new regulatory thresholds where sums of PFAS compounds are used (SCHEER, 2025).

5 Conclusions

In Perstorpsbäcken a clear spatial gradient was identified along the sampling transect, demonstrating a strong influence from anthropogenic sources. PFAS concentrations and associated environmental risks increased substantially downstream of the industrial effluent discharge point and peaked shortly downstream of the WWTP. This indicates that industrial discharges are the dominant source if PFAS to the stream, with the WWTP acting as a secondary but distinct point source.

Among the detected compounds, PFOS and PFHxS dominated the PFAS profile, with PFOS consistently exhibiting the highest concentrations and RQs. Although none of the calculated RQs exceeded unity during the sampling period, moderate environmental risks to the aquatic ecosystems were identified at three of the four sampling locations.

The SSD derived PNECs enabled further risk characterization by allowing comparison with PFOS concentrations measured under other hydrological conditions. This indicated that periods of lower flow rates are likely to result in substantially higher PFOS concentrations and associated environmental risks than those observed during the high-flow conditions under which the present study was conducted.

Although the ERA focused on individual compounds and did not account for mixture toxicity, sediment partitioning, or bioaccumulations, the persistence of PFAS compounds and evidence form previous monitoring suggests that aquatic organisms in Perstorpsbäcken are subject to long-term chemical stress. The exceedance of applicable EQSs, even during high-flow conditions, further underscores the relevance of the contamination from both ecological and human health perspectives.

Overall, the findings highlight the need for continued and more comprehensive monitoring of PFAS in Perstorpsbäcken. Future efforts should include repeated sampling under varying hydrological conditions, extended spatial coverage to assess downstream transport toward receiving waters, and the inclusion of sediments and biota. Improved consideration of PFAS mixtures and the generation of additional ecotoxicological data are also essential to refine future ERAs and to support effective management and mitigation strategies for PFAS-contaminated freshwater systems. As scientific knowledge and methodological approaches continue to advance, updated ERAs will be necessary to ensure robust and ecologically relevant risk evaluations and appropriate management strategies.

6 Acknowledgements

I would like to express my sincere gratitude to my supervisor, Maria Hansson, for her valuable guidance and constructive feedback throughout the entire project. I would also like to extend a special thank you to my external supervisor, Ola Svahn, for giving me the special opportunity to use his laboratory and for generously sharing his methods, knowledge, and experience in analytical chemistry. This support made the study both possible and truly enjoyable.

The chemical analysis was funded by Interreg South Baltic (EU) Project no. STHB.02.02-IP.01-0001/23: LIMIT - Innovative concepts for sustainable water treatment targeting PFAS and other critical micropollutants from point sources in the South Baltic Sea area.

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8 Appendix

Appendix A. Ecotoxicity data

Table A1. *Ecotoxicity data for PFHxS used in the SSD, including species group, scientific and common species names, effect, endpoint, effect concentration (µg/L) and duration (days) derived from U.S EPA ECOTOX Knowledgebase. Phylum is included for further taxonomic division.*

Species group	Phylum	Species scientific name	Species common name	Effect	Endpoint	Effect concentration (µg/L)	Duration (days)
Algae	Chlorophyta	Raphidocelis subcapitata	Green algae	Population	NOEC	9 333	1
Amphibians	Chordata	Xenopus laevis	African clawed frog	Growth	NOEC	0.676	8
Amphibians	Chordata	Lithobates pipiens	Leopard frog	Growth	NOEC	1.118	31
Amphibians	Chordata	Ambystoma tigrinum	Tiger salamander	Growth	LOEC	10	31
Amphibians	Chordata	Anaxyrus americanus	American toad	Growth	NOEC	634	26
Crustaceans	Arthropoda	Ceriodaphnia dubia	Water flea	Growth	EC20	15 800	7
Crustaceans	Arthropoda	Hyalella azteca	Scud	Growth	EC20	27 300	7
Fish	Chordata	Pimephales promelas	Fathead minnow	Growth	NOEC	1 238	42
Fish	Chordata	Danio rerio	Zebra danio	Growth	NOEC	3.5	5
Insects	Arthropoda	Chironomus dilutus	Midge	Growth	EC10	466	19

Table A2. *Ecotoxicity data for PFOS used in the SSD, including species group, scientific and common species names, effect, endpoint, effect concentration (µg/L) and duration (days) derived from U.S EPA ECOTOX Knowledgebase. Phylum is included for further taxonomic division.*

Species group	Phylum	Species scientific name	Species common name	Effect	Endpoint	Effect concentration (µg/L)	Duration (days)
Algae	Cyanobacteria	Anabaena sp.	Blue-green algae	Population	NOEC	5 000	3
Algae	Chlorophyta	Scenedesmus acutus	Green algae	Population	NOEC	25 000	4
Algae	Chlorophyta	Raphidocelis subcapitata	Green algae	Population	EC10	17 000	2
Algae	Cyanobacteria	Microcystis aeruginosa	Blue-green algae	Population	NOEC	0.104	7
Amphibians	Chordata	Xenopus laevis	African clawed frog	Growth	NOEC	0.666	8
Amphibians	Chordata	Lithobates pipiens	Leopard frog	Development	LOEC	0.06	30
Crustaceans	Arthropoda	Cladocera	Water flea	Population	NOEC	1 000	7
Crustaceans	Arthropoda	Daphnia magna	Water flea	Development	LOEC	0.0693	12
Crustaceans	Arthropoda	Moina macrocopa	Water flea	Reproduction	LOEC	312	7
Crustaceans	Arthropoda	Hyalella azteca	Scud	Growth	EC20	10	7
Fish	Chordata	Danio rerio	Zebra danio	Growth	NOEC	0.734	180
Fish	Chordata	Oncorhynchus mykiss	Rainbow trout	Growth	NOEC	1 000	14
Fish	Chordata	Pimephales promelas	Fathead minnow	Growth	NOEC	44	42
Fish	Chordata	Cyprinus carpio	Common carp	Growth	NOEC	1.15	76
Fish	Chordata	Oryzias latipes	Japanese medka	Growth	LOEC	2	16
Fish	Chordata	Anguilla anguilla	Common eel	Growth	NOEC	11	28
Plants	Embryophyta	Lemna minor	Common duckweed	Growth	LOEC	200	14
Plants	Embryophyta	Myriophyllum spicatum	Eurasian Watermilfoil	Growth	EC10	3 300	28
Plants	Embryophyta	Lemna gibba	Inflated duckweed	Growth	NOEC	300	42
Plants	Embryophyta	Myriophyllum sibiricum	Water Milfoil	Growth	EC10	100	42
Insects	Arthropoda	Chironomus dilutus	Midge	Growth	EC10	1.62	19
Insects	Arthropoda	Neocloeon triangulifer	Mayfly	Growth	EC10	0.272	14
Insects	Arthropoda	Enallagma cyathigerum	Damselfly	Development	NOEC	10	300
Invertebrates	Rotifera	Brachionus calyciflorus	Freshwater rotifer	Reproduction	LOEC	250	4
Invertebrates	Rotifera	Rotifera	Rotifer	Population	NOEC	1 000	35
Molluscs	Mollusca	Lampsilis siliquoidea	Lamp-mussel	Development	NOEC	4.52	44
Worms	Annelida	Lumbriculus variegatus	Oligochaete, Worm	Growth	NOEC	1	28

Appendix B. Species sensitivity distribution modelling

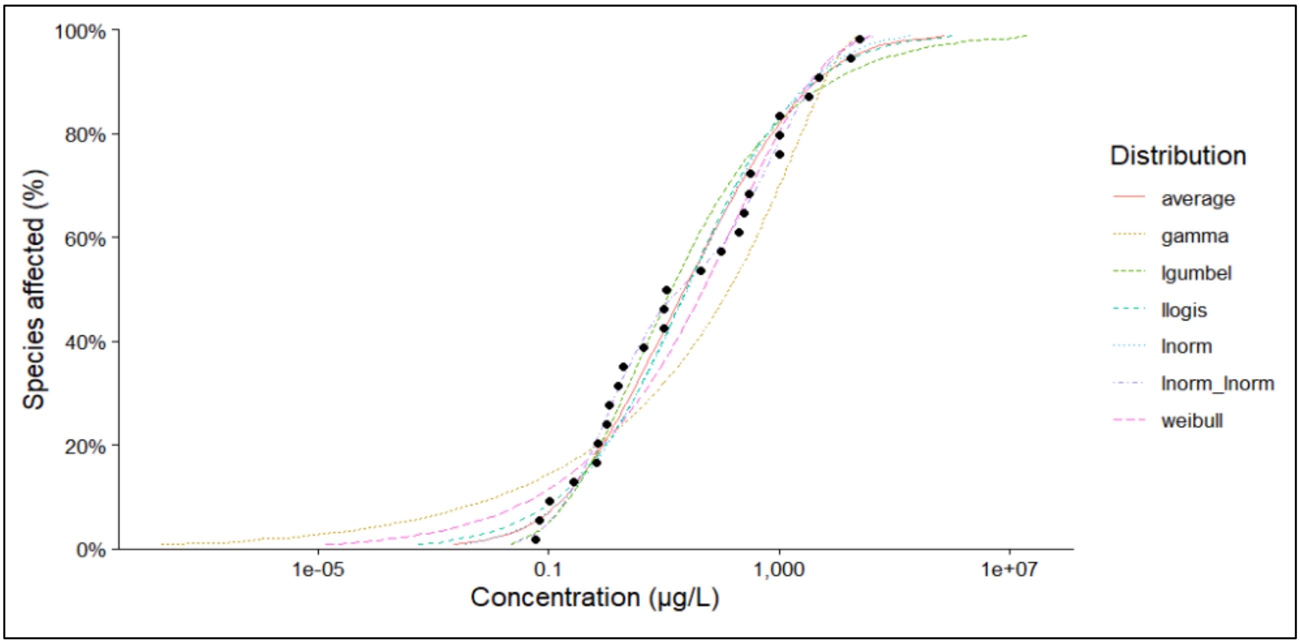

Figure B1. *Fitted distributions to PFOS ecotoxicity data. Each point represents effect concentrations (µg/L) for the different species in Table A2, and curves represents different probability distributions.*

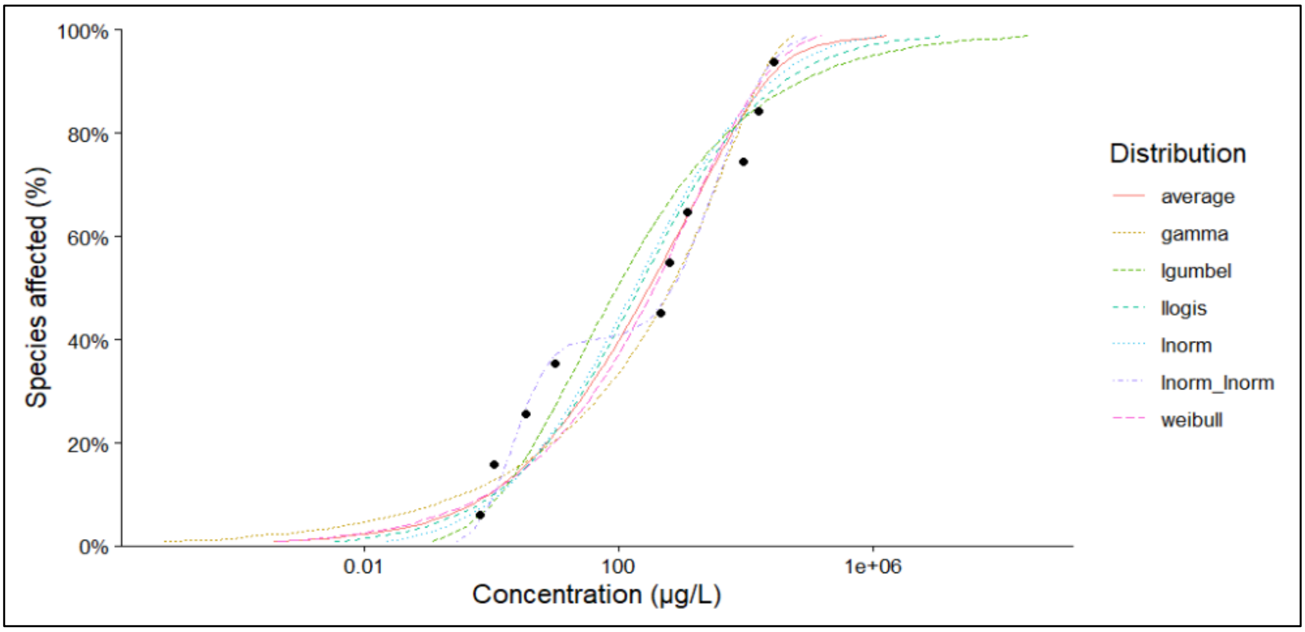

Figure B2. *Fitted distributions to PFHxS ecotoxicity data. Each point represents effect concentrations (µg/L) for the different species in Table A1, and curves represents different probability distributions.*

Table B1. *Goodness-of-fit statistics and model selection criteria for candidate probability distributions fitted to PFOS ecotoxicity data. Metrics include likelihood-based information criteria and goodness-of-fit tests used to evaluate model performance. The fitted data is found in Table A2, and the visual fits of the distributions are shown in Figure B1.*

dist	npars	nobs	log_lik	aic	aicc	delta	weight	bic	ad	ks	cvm	at_bound	computable
<chr>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<lgl>	<lgl>
gamma	2	27	-166	337	337	8.030	0.007	339	1.300	0.195	0.2370	FALSE	TRUE
lgumbel	2	27	-163	330	330	0.798	0.269	332	0.458	0.139	0.0726	FALSE	TRUE
llogis	2	27	-164	331	332	2.410	0.120	334	0.477	0.119	0.0791	FALSE	TRUE
lnorm	2	27	-162	329	329	0.000	0.400	331	0.439	0.119	0.0756	FALSE	TRUE
lnorm_lnorm	5	27	-160	329	332	2.780	0.100	336	0.161	0.070	0.0185	FALSE	TRUE
weibull	2	27	-164	332	332	2.700	0.104	334	0.545	0.151	0.0857	FALSE	TRUE

Table B2. *Goodness-of-fit statistics and model selection criteria for candidate probability distributions fitted to PFHxS ecotoxicity data. Metrics include likelihood-based information criteria and goodness-of-fit tests used to evaluate model performance. The fitted data is found in Table A1, and the visual fits of the distributions are shown in Figure B2.*

dist	npars	nobs	log_lik	aic	aicc	delta	weight	bic	ad	ks	cvm	at_bound	computable
<chr>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<lgl>	<lgl>
gamma	2	10	-79.3	163	164	0.000	0.307	163	0.396	0.196	0.0604	FALSE	TRUE
lgumbel	2	10	-80.1	164	166	1.720	0.130	165	0.537	0.244	0.0934	FALSE	TRUE
llogis	2	10	-80.2	164	166	1.950	0.116	165	0.456	0.182	0.0718	FALSE	TRUE
lnorm	2	10	-79.7	163	165	0.810	0.205	164	0.482	0.197	0.0787	FALSE	TRUE
lnorm_lnorm	5	10	-76.0	162	177	12.600	0.001	163	0.233	0.142	0.0341	FALSE	TRUE
weibull	2	10	-79.5	163	165	0.473	0.242	164	0.422	0.197	0.0623	FALSE	TRUE

Table B3. *Distribution-specific and model averaged HC5 for PFOS derived from the SSD analysis. HC5 estimates (est) are shown for each fitted statistical distribution (dist) together with standard errors (se), confidence intervals (lcl, ucl) and model weights (wt). The visual fit of the model average is shown in Figure 3.*

dist	proportion	est	se	lcl	ucl	wt	level	est_method	ci_method	boot_method	nboot	pboot	dists	samples
<chr>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<chr>	<chr>	<chr>	<int>	<dbl>	<list>	<list>
average	0.05	0.0530329768	0.14883371	1.084932e-03	0.4672932	1.000000000	0.95	multi	weighted_samples	parametric	10000	1.0000	<chr [6]>	<dbl [0]>
gamma	0.05	0.0002221804	0.17088577	2.448732e-07	0.1274199	0.007236896	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>
lgumbel	0.05	0.0977727994	0.14115341	2.763744e-02	0.5104882	0.268665483	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>
llogis	0.05	0.0264699819	0.11654788	1.914977e-03	0.3557778	0.120191324	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>
lnorm	0.05	0.0486669589	0.16275824	5.929396e-03	0.5202618	0.400351721	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>
lnorm_lnorm	0.05	0.0977127827	0.13969291	2.898796e-02	0.4869049	0.099790677	0.95	cdf	percentile	parametric	10000	0.9998	<chr [1]>	<dbl [0]>
weibull	0.05	0.0045422318	0.09184087	1.056256e-04	0.1887033	0.103763899	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>

Table B4. *Distribution-specific and model averaged HC5 for PFHxS derived from the SSD analysis. HC5 estimates (est) are shown for each fitted statistical distribution (dist) together with standard errors (se), confidence intervals (lcl, ucl) and model weights (wt). The visual fit of the model average is shown in Figure 4.*

dist	proportion	est	se	lcl	ucl	wt	level	est_method	ci_method	boot_method	nboot	pboot	dists	samples
<chr>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<chr>	<chr>	<chr>	<int>	<dbl>	<list>	<list>
average	0.05	0.12122237	14.674415	3.185719e-05	23.08631	1.0000000	0.95	multi	weighted_samples	parametric	10000	0.9998	<chr [5]>	<dbl [0]>
gamma	0.05	0.01383861	39.369862	9.723687e-07	41.06743	0.3071042	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>
lgumbel	0.05	0.54357221	5.999198	7.326595e-02	13.84986	0.1297335	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>
llogis	0.05	0.18569302	7.414357	2.203543e-03	14.80675	0.1159358	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>
lnorm	0.05	0.32476696	13.411294	1.303611e-02	19.54385	0.2048537	0.95	cdf	percentile	parametric	10000	1.0000	<chr [1]>	<dbl [0]>
weibull	0.05	0.08484429	15.986136	3.406737e-04	21.96773	0.2423728	0.95	cdf	percentile	parametric	10000	0.9999	<chr [1]>	<dbl [0]>

Appendix C. R script used for SSD modelling

~~~
##Replicable version of SSD in RStudio
#The code is derived from the website version of shinyssdtools, and adapted to work in Rstudio)

#Installation of needed packages for SSD (version 0.54 is needed for "xfun")
```{r}
install.packages(c("ssdtools", "ggplot2", "dplyr", "xfun"))
```
#Opening packages
```{r}
library(ssdtools)
library(ggplot2)
library(dplyr)
```

##SSD for PFOS
#Input data (Appendix A, Table A2)
```{r}
data <- structure(list(
  Conc = c(5000, 25000, 17000, 0.104, 0.666, 0.06, 1000, 0.0693, 312, 10, 0.734, 1000, 44, 1.15, 2, 11, 200, 3300, 300, 100, 1.62, 0.272, 10, 250, 1000, 4.52, 1),
  Species = c("Anabaena sp.", "Scenedesmus\n acutus ", "Raphidocelis subcapitata", "Microcystis\n aeruginosa", "Xenopus laevis", "Lithobates\n pipiens", "Cladocera ", "Daphnia\n magna", "Moina macrocopa", "Hyalella\n azteca", "Danio rerio", "Oncorhynchus\n mykiss", "Pimephales promelas", "Cyprinus\n carpio", "Oryzias latipes", "Anguilla\n anguilla", "Lemna minor", "Myriophyllum\n spicatum", "Lemna gibba", "Myriophyllum\n sibiricum", "Chironomus dilutus", "Neocloeon\n triangulifer", "Enallagma cyathigerum", "Brachionus\n calyciflorus", "Rotifera ", "Lampsilis\n siliquoidea", "Lumbriculus variegatus"),
  Group = c("Algae", "Algae", "Algae", "Algae", "Amphibians", "Amphibians", "Crustaceans", "Crustaceans", "Crustaceans", "Crustaceans", "Fish", "Fish", "Fish", "Fish", "Fish", "Fish", "Plants", "Plants", "Plants", "Plants", "Insects", "Insects", "Insects", "Invertebrates ", "Invertebrates ", "Molluscs", "Worms")
), row.names = c(NA, 27L), class = "data.frame")
colnames(data) <- make.names(colnames(data))
```
#Visual comparison of the fit of multiple distributions (Appendix B, Figure B1)
~~~

~~~
```{r}
dist <- ssd_fit_dists(
  data,
  left = 'Conc',
  dists = c('gamma', 'lgumbel', 'llogis', 'lnorm', 'lnorm_lnorm', 'weibull'),
  silent = TRUE,
  reweight = FALSE,
  rescale = FALSE
)
ssd_plot_cdf(
  dist,
  ylab = 'Species affected (%)',
  xlab = 'Concentration (µg/L)',
  delta = Inf,
  average = NA,
  theme_classic = TRUE,
  text_size = 12
)
```
#Numeric comparison of the fit of distributions (Appendix B, Table B1)
```{r}
ssd_gof(dist) %>% dplyr::mutate_if(is.numeric, ~ signif(., 3))
pred <- predict(dist, proportion = unique(c(1:99, 5)/100))
```
#Species Sensitivity Distribution plot with HC5 for the model average (Appendix B, Figure B3)
```{r}
ssd_plot(
  data, pred,
  left = 'Conc',
  label = 'Species',
  shape = NULL, color = NULL,
  label_size = 3,
  ylab = 'Species affected (%)',
  xlab = 'Concentration(µg/L)',
~~~

~~~
  ci = FALSE,
  shift_x = 1.05,
  hc = 0.05,
  big.mark = ',',
  trans = 'log10',
  xlimits = NULL,
  xbreaks = c(0.1, 100, 1e+05),
  text_size = 12,
  theme_classic = TRUE
) +
ggtitle('Species Sensitivity Distribution for PFOS') +
scale_color_brewer(palette = 'Dark2', name = NULL) +
scale_shape(name = NULL)
```
#HC5 with confidence levels (10 000 iterations) for all fitted distributions (Appendix B, Table B3)
```{r}
dplyr::bind_rows(
  ssd_hc(dist, proportion = 0.05, ci = TRUE, nboot = 10000L, min_pboot = 0.8),
  ssd_hc(
    dist,
    proportion = 0.05,
    ci = TRUE,
    average = FALSE,
    nboot = 10000L,
    min_pboot = 0.8)
)
```



##SSD for PFHxS


#Input data (Appendix A, Table A1)
~~~

~~~
```{r}
data <- structure(list(Conc = c(1238, 27300, 15800, 0.676, 9333, 1.118, 10, 634, 3.5, 466), Species = c("Pimephales promelas", "Hyalella azteca", "Ceriodaphnia dubia", "Xenopus laevis", "Raphidocelis subcapitata", "Lithobates pipiens", "Ambystoma tigrinum", "Anaxyrus americanu", "Danio rerio", "Chironomus dilutus"), Group = c("Fish", "Crustaecans", "Crustaecans", "Amphibians", "Algae", "Amphibians", "Amphibians", "Amphibians", "Fish", "Insects")), row.names = c(NA, 10L), class = "data.frame")
colnames(data) <- make.names(colnames(data))
```
#Visual comparison of the fit of multiple distributions (Appendix B, Figure B2)
```{r}
dist <- ssd_fit_dists(
  data,
  left = 'Conc',
  dists = c('gamma', 'lgumbel', 'llogis', 'lnorm', 'lnorm_lnorm', 'weibull'),
  silent = TRUE,
  reweight = FALSE, rescale = FALSE
  )
ssd_plot_cdf(
  dist,
  ylab = 'Species affected (%)',
  xlab = 'Concentration (µg/L)',
  delta = Inf,
  average = NA,
  theme_classic = TRUE,
  text_size = 12)
```
#Numeric comparison of the fit of distributions (Appendix B, Table B2)
```{r}
ssd_gof(dist) %>% dplyr::mutate_if(is.numeric, ~ signif(., 3))
pred <- predict(dist, proportion = unique(c(1:99, 5)/100))
```
#Species Sensitivity Distribution plot with HC5 for the model average (Appendix B, Figure B4)
```{r}
ssd_plot(
  data,
  pred,
~~~

~~~~
  left = 'Conc',
  label = 'Species',
  shape = NULL,
  color = NULL,
  label_size = 3,
  ylab = 'Species affected (%)',
  xlab = 'Concentration (µg/L)',
  ci = FALSE,
  shift_x = 1.05,
  hc = 0.05,
  big.mark = ',',
  trans = 'log10',
  xlimits = NULL,
  xbreaks = c(0.1, 100, 1e+05),
  text_size = 12,
  theme_classic = TRUE) +
  ggtitle('Species Sensitivity Distribution for PFHxS') +
  scale_color_brewer(palette = 'Dark2',
  name = NULL) +
  scale_shape(name = NULL)
```
#HC5 with confidence levels (10 000 iterations) for all fitted distributions (Appendix B, Table B4)
```{r}
dplyr::bind_rows(ssd_hc(dist, proportion = 0.05, ci = TRUE, nboot = 10000L, min_pboot = 0.8),
ssd_hc(dist, proportion = 0.05, ci = TRUE, average = FALSE, nboot = 10000L, min_pboot = 0.8))
```
~~~~

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