



Sveriges lantbruksuniversitet  
Swedish University of Agricultural Sciences

Department of Aquatic Sciences and  
Assessment

# Environmental monitoring of organic micropollutants and PFAS in river outlets

Oksana Golovko, Aleksandra Skrobonja, Lutz Ahrens, Karin Wiberg

Department of Aquatic Sciences and Assessment, Swedish University of Agricultural Sciences (SLU), Uppsala, Sweden.

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## 1. Introduction

Swedish Agency for Marine and Water Management (Havs- och vattenmyndigheten) sees a need to increase knowledge about the presence of organic micropollutants (OMPs) in the water environment. The need for monitoring applies particularly to the presence of per- and polyfluoroalkyl substances (PFAS), but also other persistent substances such as drug residues, pesticides and industrial chemicals.

A range of potentially harmful OMPs, such as pharmaceuticals, personal care products, industrial chemicals and pesticides, have been detected in surface water [1, 2]. OMPs detected in the surface water can lead to a variety of concerns for human and ecosystem health, including endocrine disruption, antibiotic resistance, and developmental disorders [2-4].

In Sweden, there are several water bodies where concentrations of PFOS or the sum of 11 PFAS are exceeding current guideline values or environmental quality standards (EQS) (according to HVMFS 2019:25). Therefore, there is a need to perform monitoring of PFAS in Swedish aquatic environment.

The purpose of the current project was to monitor rivers for extended chemical analyzes in order to:

- increase knowledge about the presence of OMPs in the water environment, and
- strengthen monitoring resulting from the water management regulation.

## **2. Material and methods**

### **2.1 Target analytes and chemicals**

#### *2.1.1 OMPs*

All analytical standards used for analysis were of high purity grade (>95%). Native standards were acquired from Sigma-Aldrich (Sweden). Isotopically labeled standards (IS) for the target compounds were obtained from Wellington Laboratories (Canada), Teknolab AB (Kungsbacka, Sweden), Sigma-Aldrich, and Toronto Research Chemicals (Toronto, Canada). Detailed information about internal standards (IS) and native standards can be found elsewhere [5]. A list of the OMPs included in the study, is given in Appendix Table A1.

#### *2.1.2 PFAS*

All analytical standards used for analysis were of high purity grade (>98%). Native and IS were acquired from Wellington Laboratories (Canada) (for details see elsewhere [6]). A list of the PFAS included in the study, is given in Appendix Table A2.

#### *2.1.3 Other chemicals*

Ultrapure water was generated by a Milli-Q (MQ) Advantage Ultrapure Water purification system and filtered through a 0.22 µm Millipak Express membrane and an LC-Pak polishing unit (Merk Millipore, Billerica, MA). Methanol, acetonitrile, formic acid and ammonia of high analytical grade were acquired from Sigma-Aldrich (Sweden).

### **2.2 Sampling**

In November 2022, a sampling campaign was carried out to collect 32 surface water samples at River Outlets sites, Table A3. The monitoring programme River Outlet is part of the Freshwater programme of the Swedish Agency for Marine and Water Management (Havs- och vattenmyndigheten) within the national environmental monitoring, and includes the outlets of our major rivers to the Sea. The sampling for the current study was an extension of the regular sampling and was conducted by contracted sampling staff. Pre-cleaned high-density polyethylene bottles, disposable gloves and ethanol/water cleaning liquid to rinse any sample equipment needed was sent to the contracted staff. The grab samples, 1 L each, were collected and sent to SLU. For quality control, 2 triplicates were taken for evaluation the repeatability of the study. Three empty bottles were opened but not filled but were thereafter handled in the same way as the real samples to serve as field blanks. No target analytes were detected in field blanks.

### **2.3 Sample preparation**

#### *2.3.1 OMPs*

Procedures for preparation of water samples for instrument analysis were done as described previously by Söregård et al. [7]. Briefly, water samples (200 mL) and laboratory method blanks

( $n = 3$ ) were extracted by solid-phase extraction (SPE) using Oasis HLB-cartridges (6 mL, 200 mg, 30  $\mu\text{m}$ ).

### 2.3.2 PFAS

Procedures for preparation of water samples for instrument analysis were done as described previously [8]. Briefly, water samples (500 mL) and laboratory method blanks ( $n = 3$ ) were extracted by solid-phase extraction (SPE) using Oasis WAX-cartridges (6 mL, 150 mg, 30  $\mu\text{m}$ ).

## 2.4 Instrumental analysis and quality control

### 2.4.1 OMPs

The water samples were analyzed by a DIONEX UltiMate 3000 ultra-high pressure liquid chromatography (UPLC) system (Thermo Scientific, Waltham, MA, USA) coupled to a triple quadrupole mass spectrometer (MS/MS) (TSQ QUANTIVA, Thermo Scientific, Waltham, MA, USA).

The data obtained were evaluated using TraceFinder™ 3.3. software (Thermo Fisher). Quality assurance and quality controls for the water samples included analysis of method blanks, two triplicates and calculation of limit of quantification (LOQ). The concentration ranges of the calibration curves for the target analytes were 0.01-1000 ng/L. The method blanks were prepared and extracted in the same way as the samples. No target analytes were detected in method blanks.

For calculating the sum of the concentration, the concentrations below LOQ was taken as 0.

### 2.4.2 PFAS

Chemical analysis was performed using a Sciex Triple Quad 3500 UPLC–MS/MS system (Sciex, USA). The data obtained were evaluated using the SCIEX OS-MQ software 3.0 software (Sciex, USA). Quality assurance and quality controls for the water samples included analysis of method blanks, two triplicates and calculation of limit of quantification (LOQ). The concentration ranges of the calibration curves for the target analytes were 0.01-100 ng/L. The method blanks were prepared and extracted in the same way as the samples. Linear and branched PFHxS (LPFHxS, BPFHxS) and PFOS (LPFOS, BPFOS) were quantified separately. For calculating the sum of the concentration, the concentrations below LOQ was taken as 0.

### 3. Results and discussion

#### 3.1 OMPs

In total 85 OMPs and 29 PFAS were analyzed. Out of 85 OMPs, 43 compounds were found at least one sample (Table 1). Compound composition and concentration ranges varied largely between sampling locations.

For individual OMPs, the highest concentrations were found for valsartan, tramadol and caffeine (Figure 1). Caffeine was detected in every sample with a concentration range 6.5–79 ng/L. It has been suggested that caffeine is a suitable wastewater indicator for surface water, with presence of this compound being a strong indication of wastewater contamination [9, 10].

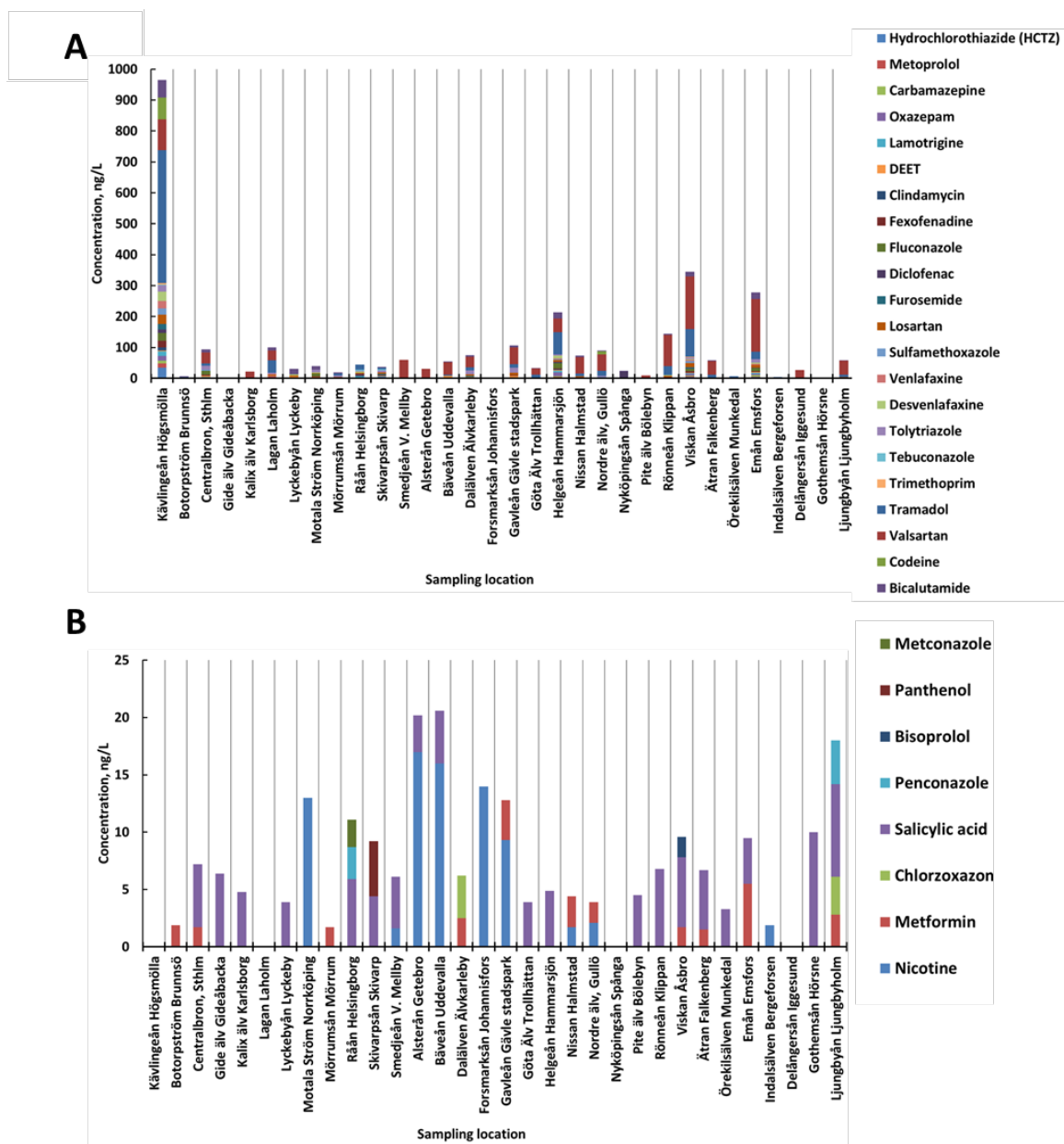
Most of the studied OMPs were found in the sample from Kävlingeån Högsmölla, with a wide range of concentrations, from 1.5 ng/L for roxithromycin to 430 ng/L for tramadol (Figure 1A). Several OMPs were detected only at this sampling site, e.g., citalopram, mirtazapine, clarithromycin, memantine, propranolol, roxithromycin, amitriptyline, sertraline and irbesartan.

In contrast, nicotine, metformin, chlorzoxazone, salicylic acid, penconazole, bisoprolol, panthenol and metconazole were detected in different sampling locations, but not in Kävlingeån Högsmölla (Figure 1B). Erythromycin was found only in Emån Emsfors at a concentration level of 61 ng/L.

The EQSs for diclofenac (0,1 µg/L expressed as annual average) and ciprofloxacin (0,1 µg/L expressed as maximum allowable concentration according to HVMFS 2019:25) were not exceeded at any site. In the proposal for a revised Environmental Quality Standards Directive (EQSD) there are annual average (AA) EQSs for inland surface waters for azithromycin (0,019 µg/L), carbamazepine (2.5 µg/L), clarithromycin (0.13 µg/L), diclofenac (0.04 µg/L) and erythromycin (0.5 µg/L). The measured environmental concentrations were significantly below the proposed EQSs.

For example, the proposed annual average (AA) EQSs for inland surface waters are for:

- azithromycin 0,019 µg/L but all the studied locations had concentrations below 3.1 ng/l (< LOQ),
- carbamazepine 2.5 µg/L but in the studied location the highest concentration was 8.9 ng/L in Kävlingeån Högsmölla,
- clarithromycin 0.13 µg/L but in the studied location this compound was found only in Kävlingeån Högsmölla at concentration level 1.8 ng/l,
- diclofenac 0.04 µg/L but in the studied location the highest concentration was 11 ng/L in Kävlingeån Högsmölla,
- erythromycin 0.5 µg/L but in the present study it was found only in Emån Emsfors at concentration level 61 ng/l.



**Figure 1. Concentrations of detected OMPs in water samples collected during November 2022.**

### 3. 2 PFAS

In total, 15 different PFAS were detected in the water samples including both linear and branched PFHxS and PFOS, respectively (Figure 2). At least one PFAS was detected at all sites with an average concentration of 12 ng/L for  $\sum$ PFAS (median 8.7 ng/L for  $\sum$ PFAS). The highest sum of 17 PFAS were detected in Centralbron and Botorpström Brunnsö and with 66 and 62 ng/L for  $\sum$ PFAS. The highest detection frequency (DF) had LPFOS and BPFOS (DF = 100%), followed

by PFBA (97%), BPFHxS (97%), PFHxA (91%), LPFHxS (91%), PFHpA (88%), PFBS (82%), and PFOA (72%). Highest average concentrations were found for PFBA with 5.6 ng/L followed by PFPeA (1.4 ng/L) and PFHxA (1.2 ng/L). The annual average (AA) EQS for inland surface waters for PFOS (0.65 ng/L) was exceeded at 18 out of 32 sites (56% of the sites).

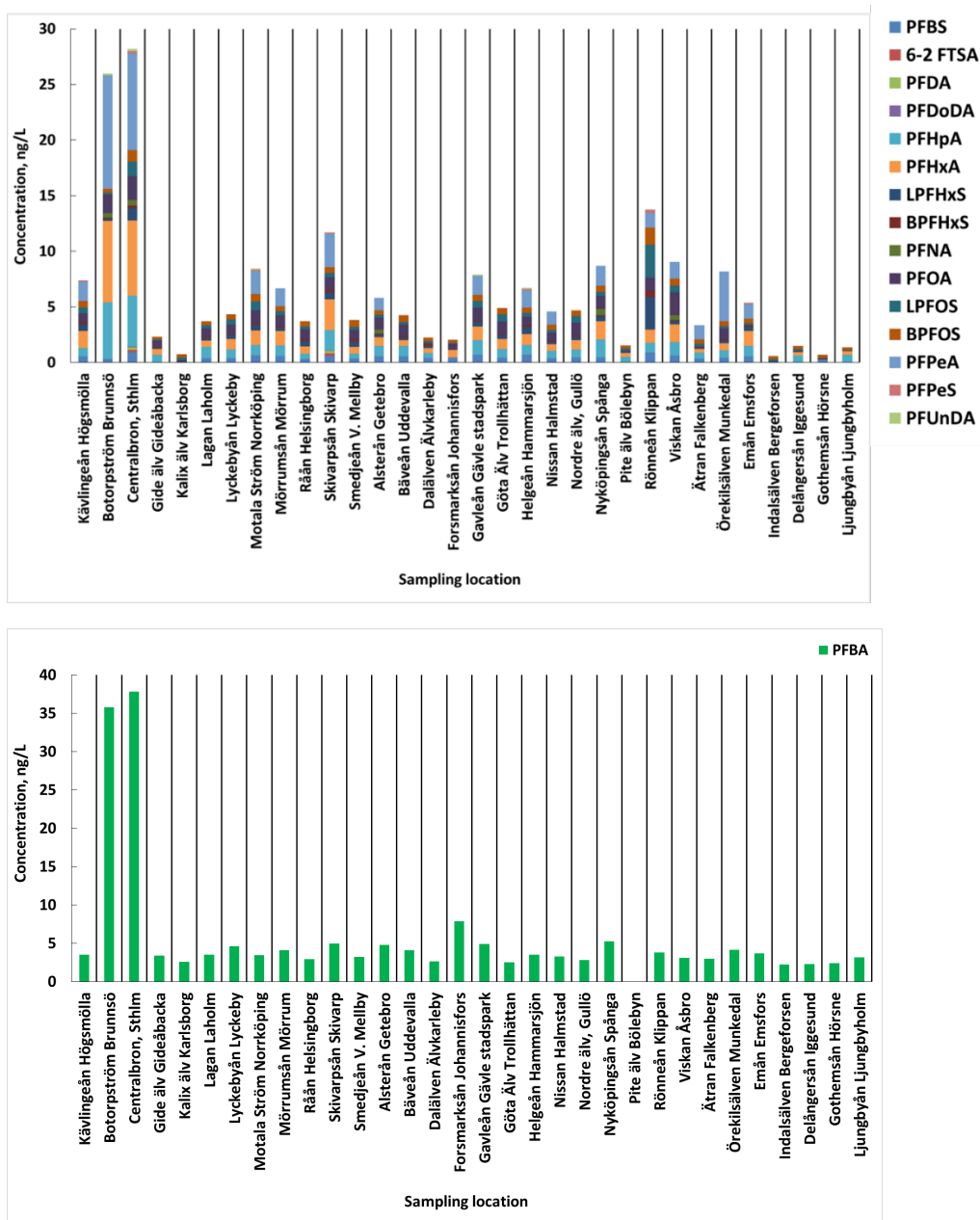


Figure 2. Concentrations of detected PFAS in water sampled during November 2022.

#### **4. Conclusions**

A total of 60 contaminants were detected in at least one sample. It is important to understand and quantify the impacts of OMPs on aquatic environments as it can be used for prioritization of measures. The annual average (AA) EQS for inland surface waters for PFOS (0.65 ng/L) was exceeded at 18 out of 32 sites (56% of the sites). The proposed annual average (AA) EQSs for azithromycin (0,019 µg/L), carbamazepine (2.5 µg/L), clarithromycin (0.13 µg/L), diclofenac (0.04 µg/L) and erythromycin were not exceeded at any site.

To better manage and sustain future water resources, it is essential to develop scientific knowledge that can be used to support environmental authorities in their decision and guidance processes.



## Acknowledgements

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## References

1. Martínez-Piernas, A.B., et al., *Validation and application of a multiresidue method based on liquid chromatography-tandem mass spectrometry for evaluating the plant uptake of 74 microcontaminants in crops irrigated with treated municipal wastewater*. Journal of Chromatography A, 2018. **1534**: p. 10-21.
2. Christou, A., et al., *Long-term wastewater irrigation of vegetables in real agricultural systems: Concentration of pharmaceuticals in soil, uptake and bioaccumulation in tomato fruits and human health risk assessment*. Water Research, 2017. **109**: p. 24-34.
3. Rivera-Utrilla, J., et al., *Pharmaceuticals as emerging contaminants and their removal from water. A review*. Chemosphere, 2013. **93**(7): p. 1268-1287.
4. Rizzo, L., et al., *Urban wastewater treatment plants as hotspots for antibiotic resistant bacteria and genes spread into the environment: A review*. Science of The Total Environment, 2013. **447**: p. 345-360.
5. Rostvall, A., et al., *Removal of pharmaceuticals, perfluoroalkyl substances and other micropollutants from wastewater using lignite, Xylit, sand, granular activated carbon (GAC) and GAC+Polonite® in column tests – Role of physicochemical properties*. Water Research, 2018. **137**: p. 97-106.
6. Nassazzi, W., F.Y. Lai, and L. Ahrens, *A novel method for extraction, clean-up and analysis of per- and polyfluoroalkyl substances (PFAS) in different plant matrices using LC-MS/MS*. Journal of Chromatography B, 2022. **1212**: p. 123514.
7. Söregård, M., et al., *Mass loads, source apportionment, and risk estimation of organic micropollutants from hospital and municipal wastewater in recipient catchments*. Chemosphere, 2019. **234**: p. 931-941.
8. Kothawala, D.N., et al., *Influence of dissolved organic matter concentration and composition on the removal efficiency of perfluoroalkyl substances (PFASs) during drinking water treatment*. Water Res, 2017. **121**: p. 320-328.
9. Glassmeyer, S.T., et al., *Transport of Chemical and Microbial Compounds from Known Wastewater Discharges: Potential for Use as Indicators of Human Fecal Contamination*. Environmental Science & Technology, 2005. **39**(14): p. 5157-5169.
10. Buerge, I.J., et al., *Caffeine, an Anthropogenic Marker for Wastewater Contamination of Surface Waters*. Environmental Science & Technology, 2003. **37**(4): p. 691-700.

**Appendix. Table A1. List of included OMPs in the study**

Compound	Category	Type	CAS number	Molecular formula	Monoisotopic mass (Da)	Log K <sub>owc</sub>
Albuterol (Salbutamol)	Pharmaceutical	Beta blocker	18559-94-9	C <sub>13</sub> H <sub>21</sub> NO <sub>3</sub>	239,1	0,64
Amitriptyline	Pharmaceutical	Antidepressant	50-48-6	C <sub>20</sub> H <sub>23</sub> N	277,1	4,95
Amoxicillin	Pharmaceutical	Antibiotic	26787-78-0	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S	365,104542	0,87
Atenolol	Pharmaceutical	Beta blocker	29122-68-7	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	266	0,16
Atorvastatin	Pharmaceutical	Antilipidemic Agents	134523-00-5	C <sub>33</sub> H <sub>35</sub> FN <sub>2</sub> O <sub>5</sub>	558,2	-
Azithromycin	Pharmaceutical	Antibiotic	83905-01-5	C <sub>38</sub> H <sub>72</sub> N <sub>2</sub> O <sub>12</sub>	748,5	4,02
BAM (Dichlorobenzamide)	Pesticide	Metabolite of dichlobenil	2008-58-4	C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> NO	189	1,29
Bezafibrate	Pharmaceutical	Antilipemic drug	41859-67-0	C <sub>19</sub> H <sub>20</sub> ClNO <sub>4</sub>	361,1	4,25
Bicalutamide	Pharmaceutical	Antineoplastic agent	90357-06-5	C <sub>18</sub> H <sub>14</sub> F <sub>4</sub> N <sub>2</sub> O <sub>4</sub> S	430,373	2,3
Bisoprolol	Pharmaceutical	Antihypertensive	6722-44-9	C <sub>18</sub> H <sub>31</sub> NO <sub>4</sub>	325,225308	1,87
Caffeine	Stimulant		58-08-02	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>	194,1	-0,07
Carbamazepine	Pharmaceutical	Antiepileptic	298-46-4	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O	236	2,25
Cetirizine	Pharmaceutical	Antihistamine	83881-51-0	C <sub>21</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>	388,89	<b>1,7</b>
Chloramphenicol	Pharmaceutical	Antibiotic	56-75-7	C <sub>11</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub>	322	1,14
Chlorzoxazone	Pharmaceutical	Muscle relaxant?	95-25-0	C <sub>7</sub> H <sub>4</sub> ClNO <sub>2</sub>	168,993056	1,31
Ciprofloxacin	Pharmaceutical	Antibiotic (quinolone)	85721-33-1	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>	331,13322	0,28
Citalopram	Pharmaceutical	Antidepressant	59729-33-8	C <sub>20</sub> H <sub>21</sub> FN <sub>2</sub> O	324,1	3,74
Clarithromycin	Pharmaceutical	Antibiotic	81103-11-9	C <sub>38</sub> H <sub>69</sub> NO <sub>13</sub>	747,4	3,16
Climbazole	Pharmaceutical	Antifungal	38083-17-9	C <sub>15</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>	292	3,76
Clindamycin	Pharmaceutical	Antibiotic	21462-39-5	C <sub>18</sub> H <sub>33</sub> ClN <sub>2</sub> O <sub>5</sub> S	424,981	2,16
Clotrimazole	Pesticide	Antifungal agent	23593-75-1	C <sub>22</sub> H <sub>17</sub> ClN <sub>2</sub>	344,1	6,26
Clozapine	Pharmaceutical	Antipsychotic	5786-21-0	C <sub>18</sub> H <sub>19</sub> ClN <sub>4</sub>	326,1	3,35
Codeine	Pharmaceutical	Opiates, opioids and metabolites	76-57-3	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>	299,1	1,28
DEET (diethyltoluamide)	Pesticide	Insect repellent	134-62-3	C <sub>12</sub> H <sub>17</sub> NO	191,1	2,26
Desvenlafaxine (O-desmethylvenlafaxine)	Pharmaceutical	Antidepressant	93413-62-8	C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub>	263,1	2,72
Diazepam	Pharmaceutical	Sedative	439-14-5	C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O	284	2,70
Diclofenac	Pharmaceutical	NSAID (nonsteroidal anti-inflammatory drug)	15307-86-5	C <sub>14</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>	295	4,02
Diltiazem	Pharmaceutical	Antihypertensive	42399-41-7	C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> S	414,1	2,79
Erythromycin	Pharmaceutical	Antibiotic	114-07-8	C <sub>37</sub> H <sub>67</sub> NO <sub>13</sub>	733,4	-
Ethylparaben	Paraben	Antifungal preservative	120-47-8	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	166	2,49
Fexofenadine	Pharmaceutical	Antihistamine	153439-40-8	C <sub>32</sub> H <sub>39</sub> NO <sub>4</sub>	501,656	2,81
Fluconazole	Pharmaceutical	Antifungal	86386-73-4	C <sub>13</sub> H <sub>12</sub> F <sub>2</sub> N <sub>6</sub> O	306,1	0,25
Fluoxetine	Pharmaceutical	Antidepressant	54910-89-3	C <sub>17</sub> H <sub>18</sub> F <sub>3</sub> NO	309,134049	4,09
FOSA (perfluoro-octane sulfonamide)	PFAS		754-91-6	C <sub>8</sub> H <sub>2</sub> F <sub>17</sub> NO <sub>2</sub> S	498,9	7,58
Furosemide	Pharmaceutical	Diuretics	54-31-9	C <sub>12</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>5</sub> S	330	2,32
Gemfibrozil	Pharmaceutical	Antilipidemic Agents	25812-30-0	C <sub>15</sub> H <sub>22</sub> O <sub>3</sub>	250,1	4,77
Hydrochlorothiazide	Pharmaceutical	Diuretics	58-93-5	C <sub>7</sub> H <sub>8</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>	296,9	-0,10
Ifosfamide	Pharmaceutical	Anticancer	3778-73-2	C <sub>7</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> P	260,02482	0,86
Enilconazole (Imazalil)	Pesticide	Fungicide	35554-44-0	C <sub>14</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O	296,18	4,10
Ipconazole	Pesticide	Fungicide	125225-28-7	C <sub>18</sub> H <sub>24</sub> ClN <sub>3</sub> O	333,16	4,65

Irbesartan	Pharmaceutical	Antihypertensive	138402-11-6	C <sub>25</sub> H <sub>28</sub> N <sub>6</sub> O	428,2	5,31
Lamotrigine	Pharmaceutical	Antiepileptic	84057-84-1	C <sub>9</sub> H <sub>7</sub> Cl <sub>2</sub> N <sub>5</sub>	255	0,99
Lidocaine	Pharmaceutical	Anesthetic	137-58-6	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O	234,1	1,66
Loperamide	Pharmaceutical	Antidiarrhoeal	53179-11-6	C <sub>29</sub> H <sub>33</sub> ClN <sub>2</sub> O <sub>2</sub>	476,223056	5,5
Losartan	Pharmaceutical	Antihypertensive	114798-26-4	C <sub>22</sub> H <sub>23</sub> ClN <sub>6</sub> O	422,1	4,01
Memantine	Pharmaceutical	Alzheimer	41100-52-1	C <sub>21</sub> H <sub>21</sub> N	179,307	3,28
Metconazole	Pesticide	Fungicide	125116-23-6	C <sub>17</sub> H <sub>22</sub> ClN <sub>3</sub> O	319,829	4,19
Metformin	Pharmaceutical	Biguanide hypoglycemic agent (non-insulin-dependent diabetes mellitus)	657-24-9	C <sub>4</sub> H <sub>11</sub> N <sub>5</sub>	129,101445	-2,64
Methylparaben	Paraben	Antifungal preservative	99-76-3	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	152	2,00
Metoprolol	Pharmaceutical	Beta blocker	51384-51-1	C <sub>15</sub> H <sub>25</sub> NO <sub>3</sub>	267,1	1,69
Metronidazole	Pharmaceutical	Antibiotic	443-48-1	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>3</sub>	171	0,00
Miconazole	Pesticide	Antifungal agent	22916-47-8	C <sub>18</sub> H <sub>14</sub> Cl <sub>4</sub> N <sub>2</sub> O	413,986	6,25
Mirtazapine	Pharmaceutical	Antidepressant	85650-52-8	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub>	265,1	3,03
Nicotine	Stimulant		54-11,5	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>	162,1	1,00
Oxazepam	Pharmaceutical	Sedative	604-75-1	C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>	286	3,34
Oxycodone	Pharmaceutical	Opiates, opioids and metabolites	76-42-6	C <sub>18</sub> H <sub>21</sub> NO <sub>4</sub>	315,1	0,66
Panthenol	Pharmaceutical	Moisturizer	16485-10-2	C <sub>9</sub> H <sub>19</sub> NO <sub>4</sub>	205,131408	-1,92
Penconazole	Pesticide	Fungicide	66246-88-6	C <sub>13</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>3</sub>	283,064	4,67
Primidone	Pharmaceutical	Antiepileptic	125-33-7	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	218,1	0,73
Prochloraz	Pesticide	Fungicide	67747-09-05	C <sub>15</sub> H <sub>16</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	375,665	4,13
Propranolol	Pharmaceutical	Beta blocker	525-66-6	C <sub>16</sub> H <sub>21</sub> NO <sub>2</sub>	259,1	2,60
Propylparaben	Paraben	Antifungal preservative	94-13-3	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>	180	2,98
Ramipril	Pharmaceutical	Antihypertensive	87333-19-5	C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>	416,231122	3,32
Ranitidine	Pharmaceutical	Antisecretory Agent	66357-35-5	C <sub>13</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub> S	314,1	0,29
Roxithromycin	Pharmaceutical	Antibiotic	80214-83-1	C <sub>41</sub> H <sub>76</sub> N <sub>2</sub> O <sub>15</sub>	836,5	-
Salicylic acid	Pharmaceutical	NSAID (nonsteroidal anti-inflammatory drug)	69-72-7	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	138	2,24
Sertraline	Pharmaceutical	Antidepressant	79617-96-2	C <sub>17</sub> H <sub>17</sub> Cl <sub>2</sub> N	305	5,29
Simvastatin	Pharmaceutical	Statins (HMG CoA reductase inhibitors)	79902-63-9	C <sub>25</sub> H <sub>38</sub> O <sub>5</sub>	418,271924	4,68
Sotalol	Pharmaceutical	Beta blocker	3930-20-9	C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S	272,1	0,37
Sulfamethoxazole	Pharmaceutical	Antibiotic	723-46-6	C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S	253	0,48
Tebuconazole	Pesticide	Fungicide	107534-96-3	C <sub>16</sub> H <sub>22</sub> ClN <sub>3</sub> O	307,818	3,89
Terbutaline	Pharmaceutical	Beta adrenergic receptor agonists	23031-25-6	C <sub>12</sub> H <sub>19</sub> NO <sub>3</sub>	225,136493	0,9
Tetraconazole	Pesticide	Fungicide	112281-77-3	C <sub>13</sub> H <sub>11</sub> Cl <sub>2</sub> F <sub>4</sub> N <sub>3</sub> O	372,146	4,25
Thiabendazole	Pharmaceutical	Anthelmintic	148-79-8	C <sub>10</sub> H <sub>7</sub> N <sub>3</sub> S	201,036068	2,47
Tolytriazole	Industrial chemical		13351-73-0	C <sub>7</sub> H <sub>7</sub> N <sub>3</sub>	133,063997	-
Tramadol	Pharmaceutical	Analgesics (painkiller)	27203-92-5	C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub>	263,1	3,01
Trimethoprim	Pharmaceutical	Antibiotic	738-70-5	C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>	290,1	0,73
Valsartan	Pharmaceutical	Antihypertensive	137862-53-4	C <sub>24</sub> H <sub>29</sub> N <sub>5</sub> O <sub>3</sub>	435,2	3,65
Venlafaxine	Pharmaceutical	Antidepressant	93413-69-5	C <sub>17</sub> H <sub>27</sub> NO <sub>2</sub>	277,2	3,28
Guanylurea	Pharmaceutical	Metabolite of metformin		C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> O	102,1	-3,57
Butyl methoxy-dibenzoyl-methane	Ultraviolet filter			C <sub>37</sub> H <sub>40</sub> O <sub>4</sub>	548,7	4,51
Octocrylene	Ultraviolet filter			C <sub>24</sub> H <sub>27</sub> NO <sub>2</sub>	361,5	6,88

Benzophenone-3	Ultraviolet filter			C14H12O3	228,24	3,79
Fipronil	Pesticide	insecticide		C12H4Cl2F6N4OS	437,1	4,00

**Table A2. List of PFASs included in the study**

Name	Abbreviation	Group
Perfluorobutanoic acid	PFBA	PFCAs
Perfluoropentanoic acid	PFPeA	
Perfluorohexanoic acid	PFHxA	
Perfluoroheptanoic acid	PFHpA	
Perfluorooctanoic acid	PFOA	
Perfluorononanoic acid	PFNA	
Perfluorodecanoic acid	PFDA	
Perfluoroundecanoic acid	PFUnDA	
Perfluorododecanoic acid	PFDoDA	
Perfluorotridecanoic acid	PFTriDA	
Perfluorotetradecanoic acid	PFTeDA	
Perfluorobutane sulfonic acid	PFBS	PFSAs
Perfluoropentane sulfonic acid	PFPeS	
Perfluorohexane sulfonic acid (linear)	L-PFHxS	
Perfluorohexane sulfonic acid (branched)	B-PFHxS	
Perfluoroheptane sulfonic acid	PFHpS	
Perfluorooctane sulfonic acid (linear)	L-PFOS	
Perfluorooctane sulfonic acid (branched)	B-PFOS	
Perfluorononane sulfonic acid	PFNS	
Perfluorodecane sulfonic acid	PFDS	FOSAs
Perfluorooctane sulfonamide	FOSA	
Methylperfluorooctanesulfonamidoacetic acid	MeFOSAA	FOSAAs
Ethylperfluorooctanesulfonamidoacetic acid	EtFOSAA	
4:2 Fluorotelomer sulfonat	4:2 FTSA	FTSAs
6:2 Fluorotelomer sulfonat	6:2 FTSA	
8:2 Fluorotelomer sulfonat	8:2 FTSA	
Ammonium perfluoro (2-methyl-3-oxahexanoate)	HFPO-DA (GenX)	
Propanoic Acid / Ammonium 2,2,3-trifluoro-3-(1,1,2,2,3,3-hexafluoro-3-(trifluoromethoxy)propoxy)propanoate	NaDONA (ADONA)	
6:2 chlorinated polyfluorinated ether sulfonate	6:2 Cl-PFESA (9Cl-PF3ONS) (F-53B)	
8:2 chlorinated polyfluorinated ether sulfonate	8:2 Cl-PFESA (11Cl-PF3OUdS)	

**Table A3. List of locations included in the study**

Station name	SWEREF_N	SWEREF_E	X_Id	Y_Id	Län	Läns- bokstav	Nivå (m)
Botorpström Brunnsö	6392208	589249	6393390	1541220	8	H	0.5
Centralbron, Sthlm	6580488	674315	6580650	1628410	1	AB	0.5
Gide älv Gideåbacka	7031457	705271	7030550	1665720	22	Y	0.5
Kalix älv Karlsborg	7326323	872437	7324070	1836040	25	BD	0.5
Kävlingeån Högsmölla	6183240	379372	6186780	1328810	12	M	0.5
Lagan Laholm	6265128	380076	6268750	1330510	13	N	0.1
Lyckebyån Lyckeby	6228238	540991	6230060	1491190	10	K	0.5
Motala Ström Norrköping	6495264	565175	6496730	1518380	5	E	0.5
Mörrumsån Mörrum	6227369	484539	6229500	1434500	10	K	0.5
Råån Helsingborg	6208257	361524	6212050	1311220	12	M	0.5
Skivarpsån Skivarp	6145730	411067	6148860	1360020	12	M	0.5
Smedjeån V. Mellby	6264652	375369	6268270	1325770	13	N	0.1
Alsterån Getebro	6318968	570581	6320330	1521670	8	H	0.5
Bäveån Uddevalla	6471414	321035	6475820	1273690	14	O	0.3
Dalälven Älvkarleby	6716428	633862	6717420	1589740	3	C	0.5
Forsmarksån Johannisfors	6694697	676984	6695000	1632460	3	C	0.1
Gavleån Gävle stadspark	6728334	616191	6729240	1572240	21	X	0.5
Göta Älv Trollhättan	6463558	340767	6467710	1293300	14	O	0.5
Helgeån Hammarsjön	6199820	451131	6202770	1400910	12	M	0.5
Nissan Halmstad	6285017	369787	6288770	1320400	13	N	0.1
Nordre älv, Gullö	6415408	317213	6419809	1269355	14	O	0.5
Nyköpingsån Spånga	6520892	611899	6523700	1564420	4	D	0.3
Pite älv Bölebyn	7265405	792380	7264100	1755250	25	BD	0.5
Rönneån Klippan	6221174	384636	6224670	1334580	12	M	0.5
Viskan Åsbro	6347240	337607	6351360	1288950	13	N	0.5
Ätran Falkenberg	6309352	347407	6313380	1298330	13	N	0.1
Örekilsälven Munkedal	6484891	306641	6489300	1259640	14	O	0.5
Emån Emsfors	6334282	587847	6335200	1539200	8	H	0.4
Indalsälven Bergeforsen	6934501	623040	6935870	1582050	22	Y	0.3
Delångersån Iggesund	6835609	610559	6836610	1567930	21	X	0.5
Gothemsån Hörsne	6385253	715277	6384910	1667210	9	I	0.01
Ljungbyån Ljungbyholm	6277028	571895	6278310	1522550	8	H	0.5