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Occurrence of organic micropollutants and hormones in Swedish surface water

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ABSTRACT

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The occurrence and source distribution of organic micropollutants (OMPs) have been investigated in Swedish surface waters, in 23 rivers connected to the lakes Vänern, Vättern and Mälaren, 3 Wastewater treatment plants (WWTPs) and 3 Drinking water plants (DWTPs) located in the middle of Sweden was sampled. Compounds such as pharmaceuticals, industrial chemicals, pesticides, personal care products, hormones, Per- and polyflouroalkyl substances (PFASs), isoflavones, stimulants and parabens were selected. The analysis was done by using solid phase extraction (SPE) and Ultra-performance liquid chromatography tandem mass spectrometry (UPLC-MS/MS).

Of the 121 studied compounds 91 was detected in concentration levels varying between a few ng/L up to 160 µg/L in wastewater effluent. The detected concentrations of 80 compounds in surface water from rivers varied from low ng L^{-1} up to 3.3 µg/L, 43 OMPs within the range from low ng/L up to 370 ng/ L could be detected in the lakes and 35 OMPs could be found in levels from low ng/L up to 2.9 µg/L in the drinking water. The number of detected compounds and concentration levels clearly decreases from wastewater influent to effluent, rivers, lakes and lastly to drinking water.

The concentration levels of OMPs in the surface water samples varied between sampling sites and the three lakes making it clear that Lake Mälaren is the most contaminated one out of these three. OMPs such as antibiotics, antidepressants and personal care products were most frequently detected in all samples. The highest total OMP concentration levels were found in Enköping river (79 µg/L), Lövsta river (33 µg/L), Ösan (16 µg/L) and Lillån (13 µg/L).

A risk assessment for drinking water with regard to human health was conducted for two compounds by calculating the Benchmark Quotient (BQ) using drinking water equivalent levels (DWELs). Two compounds, carbamazepine and bezafibrate, was selected based on detection frequency and available toxicity data. While bezafibrate didn't show any indications of risk to human health, carbamazepine had a BQ of 1.47 which indicates a risk to human health when humans are exposed to these concentration levels over a period of a lifetime.

Keywords: surface water, wastewater, SPE, pharmaceuticals, target analysis

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REFEREAT

Förekomst av organiska mikroföroreningar och hormoner i svenska ytvatten
Malin Forsberg

Genom att använda en målanalys har förekomsten och fördelningen av organiska mikroföroreningar i svenska ytvatten studerats. Vattenprover från 23 vattendrag som antingen mynnar ut i eller börjar i någon av sjöarna Vänern, Vättern eller Mälaren, tre avloppsreningsverk och tre dricksvattenverk i mellersta Sverige har samlats in. Ämnen så som läkemedel, industriella kemikalier, pesticider, hudvårdsprodukter, hormoner, högflorerade ämnen (PFAS), isoflavoner, stimulanter och parabener valdes ut och analyserades med hjälp av fastfasextraktion och vätskekromatografi kopplad till masspektrometer (UPLC-MS/MS).

Av de 121 utvalda ämnena kunde 91 av dessa detekteras i koncentrationer som varierade mellan några få ng L^{-1}upp till 160 µg/L i utgående avloppsvatten. I vattendragen kunde 80 av de organiska mikroföroreningarna detekteras i koncentrationer mellan låga ng/L upp till 3.3 µg/L medan endast 43 kunde detekteras i sjöarna inom koncentrationsintervallet låga ng/L till 370 ng/L. Slutligen detekterades 29 mikroföroreningar i dricksvattnet där koncentrationerna varierade mellan några få ng/L upp till 2.9 µg/L. Resultatet visar att antalet detekterade organiska mikroföroreningar och deras respektive koncentrationer tydligt minskar vid jämförelse av de olika matriserna från ingående avloppsvatten till utgående, vattendrag, sjöar och slutligen i dricksvattnet.

I ytvattenproverna varierade koncentrationsnivåerna av organiska mikroföroreningar mellan de olika vattendragen och det var tydligt att Mälaren är mer kontaminerad än Vänern och Vättern. Det gick också att se tydliga trender i vilka ämnen som vanligen detekterades i de olika proverna, särskilt bland läkemedlen då ämnen som är antibiotika-klassade eller hör till gruppen antidepressiva var vanligast förekommande. De högsta totala koncentrationerna av organiska mikroföroreningar kunde hittas i Enköpingsån (79 µg/L), Lövstaån (33 µg/L), Ösan (16 µg/L) samt Lillån (13 µg/L). Dessa fyra vattendrag är därmed de mest förorenade i denna studie och kan därför ses som särskilt förorenade.

En riskanalys med hänsyn till människors hälsa gjordes på dricksvattnet genom att beräkna en referenskvot (BQ) med hjälp av ekvivalenta dricksvatten-nivåer (DWELs). De två ämnena karbamazepin och bezafibrat valdes på grund av deras detektionsfrekvens (FD) och tillgänglighet av toxicitetsdata. Bezafibrat visade ingen potentiell risk medan karbamazepin hade ett BQ-värde på 1,47 vilket indikerar en potentiell risk till människors hälsa om man utsätts för de funna koncentrationerna under hela sin livstid.

Nyckelord: ytvatten, avloppsvatten, SPE, läkemedel, målanalys

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PREFACE

This thesis was written as the conclusive part of the Master's Programme in Environmental and Water Engineering at Uppsala University (UU) and the Swedish University of Agricultural Sciences (SLU), holding 30 credits. Supervisor was Oksana Golovko and subject reader was Lutz Ahrens from the Department of Aquatic Sciences and Assessment.

First I would like to thank my supervisor Oksana and subject reader Lutz for this opportunity, for your valuable feedback and guidance throughout my thesis. Their patience and goodwill to answer my questions and willingness to always lend a hand when needed has been invaluable throughout this entire process. Thank you.

I would also like to thank my friends and family for their constant support and encouragement throughout my entire education, I could not have done this without you. During my time at UU and SLU I've had the pleasure of getting to know people who've inspired me, both personally and professionally. You have given me the energy to keep on going and have helped me finding my own motivation during late nights studying for exams and over endless cups of coffee. Thank you for always believing in me.

Lastly, I would like to thank my own stubbornness for always making me want to try just one more time.

Malin Forsberg
Uppsala, January 2022

POPULAR SCIENCE SUMMARY

Water is one of our most valuable resources, and is vital for all living things. Water is also an important part of many human activities such as showering, flushing toilets, etc. In order to have clean water in the environment and in our taps, all wastewater has to be treated in wastewater treatment plants (WWTPs) before released into the environment as wastewater effluent. Other sources for the occurrence of OMPs in surface water is agricultural run-offs, effluents from hospitals or industries. When released into the receiving surface waters such as rivers and lakes, the effluent still contains compounds which are toxic to the aquatic environment. The same surface waters are used for producing drinking water in drinking water treatment plants (DWTPs) before getting to our taps.

Organic micropollutants (OMPs) is a group of compounds which includes pharmaceuticals, hormones, PFASs, pesticides, industrial chemicals, etc. They are used in everyday life for human and/or veterinary purposes and they are often persistent to degradation. These properties make the removal process in the WWTPs difficult which leads to a leakage of OMPs into the environment. Microorganisms can to some extent degrade OMPs in both WWTPs and in the environment, or the OMPs can be degraded as a result of sunlight, by sorption onto biomass in the WWTP or sorption into sediments when present in the environment. With microorganisms present, different bi- or transformation products can be formed and might cause negative effects on the aquatic environment. When present in the environment these OMP compounds and their biproducts can cause negative effects on aquatic organisms such as fish, mussels, algae, etc. As an example, painkillers and beta blockers have been shown to have negative physiological effects on mussels in the Baltic Sea.

OMPs and hormones do not occur individually in the environment, but as a mixture of numerous other compounds at varying concentration levels. Individually, these compounds may occur at harmless concentrations whereas the complicated combinations in the mixtures may be harmful. Therefore, it is important to study the occurrence and source distribution of these compounds in surface waters.

The main aim of this project was to study the occurrence and source distribution of OMPs and hormones in Swedish surface waters. Water samples were collected from three lakes, 23 rivers, three WWTPs and three DWTPs. The study was executed in order to assess the current state of the contamination caused by OMPs and hormones in rivers connected to either lake Vänern, Vättern or Mälaren.

The results showed a clear decrease in the concentrations and amount of detected OMPs and hormones from wastewater influent to drinking water.

Results from the river samples showed that various OMPs and hormones of different concentrations could be found in all samples proving that more advanced treatment techniques are needed in order to reduce the occurrence and concentrations of these compounds in surface water.

ABBREVIATIONS

ARF	Average response factor
BAM	Dichlorobenzamide
BQ	Benchmark Quotient
DEET	Dietyltoluamide
DWEL	Drinking water equivalent level
DWTP	Drinking water treatment plant
EQS	Environmental quality standards
FD	Frequency of detection
HPLC	High performance liquid chromatography
IC	Industrial chemical
IS	Internal standard
LC	Liquid chromatography
LOQ	Limit of quantification
ME	Matrix effect
MQ	Milli-Q water
MS	Mass spectrometry
MST	Matrix matching standard
NS	Native standard
NSAID	Non-Steroidal Anti-Inflammatory Drug
OMP	Organic micropollutant
PE	Population equivalent
PFASs	Per- and polyflouroalkyl Substances
PP	Polypropylene
SPE	Solid phase extraction
UPLC-MS/MS	Ultra-high-Pressure Liquid Chromatography tandem Mass Spectrometry
WFD	Water Frame Directive
WWTP	Wastewater treatment plant

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1 Introduction

In the modern society, organic micropollutants (OMPs) are used in large quantities all over the world. However, the impact of OMPs on the aquatic environment has not yet gotten the attention it needs. The Water Framework Directive (WFD) came into force in December 2000 and establishes a framework in order to protect inland surface waters, coastal waters, transitional waters and groundwater. Improving the aquatic environment through measures against priority substances, substances with a significant risk to or transported via the aquatic environment, is one of the objectives of the WFD (Whalley et al., 2018).

Pharmaceuticals (antidepressants, painkillers, antibiotics, etc.) and hormonal drugs (contraceptive pills, thyroid drugs, etc.) are used on a daily basis for treatment of different diseases or symptoms for human or veterinary purposes. Many of these compounds are designed to be more or less persistent to degradation. The substances reach the wastewater treatment plants and are thereafter spread into the environment. Take antibiotic substances, they are widely used and when secreted they entail release of substances which increases the risk for development of antibiotic resistant bacteria (Helmfrid et al., 2006).

1.1 Aim of the study

The main aim of this master project is to study the occurrence and source distribution of OMPs in Swedish surface waters by answering the following questions

I. Is there a clear decrease in the concentrations of OMPs and hormones from wastewater to drinking water?
II. Is there a clear difference in occurrence and concentrations of OMPs and hormones in rivers connected to the lakes Vänern, Vättern and Mälaren and which is the most polluted lake?
III. Are there any risks to human health related to OMPs and hormones in drinking water from drinking water plants (DWTPs) connected to lake Vänern, Vättern or Mälaren?

1.2 Limitations

Limitations for this project is a target analysis. In this study, a total amount of 121 compounds were analysed and the selection of compounds was done based on the previous study by Rehrl et al. (2020). This limitation was set since the true number of occurring compounds in the water bodies are impossible to know and therefore a non target analysis should be performed.

2 Background and Theory

2.1 OMPs in the environment

Water is a very important resource for all living organisms and human activities like industry, agriculture and domestic use. However, people often take this resource for granted and several organic micropollutants (OMPs) end up in environmental compartments due to reasons like human ignorance and lack of legislation (Barbosa et al., 2016; Whalley et al., 2018). Several studies have shown the occurrence of OMPs in the aquatic environment such as surface water, groundwater and even drinking water at concentrations varying between ng/L up to µg/L (Barbosa et al., 2016; Ericson et al., 2010; Fick et al., 2010; Petrie et al., 2015; Ternes et al., 2015).

It is well known that OMPs have a negative impact on the aquatic environment including aquatic organisms such as fish, mussels, algae, etc. (Ericson et al., 2010; Helmfrid et al., 2006). The known effects are almost exclusively negative for the aquatic environment. It was shown that well known non-steroidal anti-inflammatory drugs (NSAIDs) such as ibuprofen and diclofenac and beta blocker propranolol have negative physiological effects on Baltic Sea blue mussels (Ericson et al., 2010). The same study showed that mussels exposed to concentrations of these compounds both individually (diclofenac 100 µg/L, ibuprofen 1000 and propranolol 5000 µg/L) and as a mixture (25/75 combination of propranolol and diclofenac in the concentrations 1000 µg/L) for two weeks, had a lower scope of growth due to less available energy for metabolism. Additionally, the mussels had a lower byssus strength and a lower abundancy of byssus threads, which reduces the mussel' ability to attach to the underlying surface. Psychiatric pharmaceuticals such as anxiolytics and antidepressants have been shown to bioconcentrate in fish tissue such as the brain and liver (McCallum et al., 2017). McCallum et al., (2017) showed that oxazepam increased boldness in European perch while fluoxetine made guppies slower in their response to threats by reducing the predator response behaviours. However, in the environment, the compounds occur as a complex mixture of different OMPs such as pharmaceuticals, residues, transformation products, pesticides, industrial chemicals, hormones, PFASs, etc. and all in varying concentrations of individual compounds which makes it almost impossible to predict the actual effects on the aquatic environment (Barbosa et al., 2016; Wallberg et al., 2016; Whalley et al., 2018). This phenomenon is usually referred to as the cocktail effect, whereby mixtures of compounds that may individually occur at harmless concentrations may affect health and other due to formed complicated combinations (Whalley et al., 2018).

2.2 Wastewater treatment plants

Municipal wastewater treatment plants are designed to treat wastewater derived from households, which basically means they are supposed to treat water with oxygen-consuming substances, easily degraded organic matter (DOM), nitrogen and phosphorus (Helmfrid et al., 2010, 2006). The majority of the WWTPs in Sweden are so called conventional WWTPs and include a combination of mechanical, chemical and biological treatment steps. The first step is the mechanical which separates solid particles like toilet paper, cotton swabs, etc. In the second step, the chemical cleaning, a chemical coagulant is added in order to remove the phosphorus by precipitation. The precipitate forms a sludge which is removed and treated separately while the water continues to the third step which is the biological. Microorganisms remove nitrogen, organic material and remaining phosphorus, often in an so-called activated sludge process (Naturvårdsverket, 2017). Pharmaceutical residues and other organic micropollutants will therefore partially pass the WWTPs and reach the recipient water unchanged and undegraded.

Many OMPs are persistent and most of the pharmaceuticals are designed to endure transport and storing in order to reach its organ of target in the human body without degrading (Wallberg et al., 2016). In order to be secreted most of the pharmaceuticals have a high water solubility, described as log K_{ow} (or sometimes log P_{ow} or log P) which also affects their ability to bioaccumulate (Wallberg et al., 2016).

The concentrations of different OMPs in the environment depends not only on usage and the WWTPs ability to remove them, but also on the physical-chemical properties of the compounds. Several studies show higher concentrations and amount of detected compounds in the influent wastewater as compared with the effluent, but the effluent water still contains a large number of both parent compounds and their metabolites (Helmfrid et al., 2010, 2006; Petrie et al., 2015). Humans often consume the parent compound which then gets excreted from the human body as a number of correlated metabolites but some compounds will pass the body completely intact (Helmfrid et al., 2006; Petrie et al., 2015). Ibuprofen is one example, it gets excreted as a mixture of only 1 % unchanged drug (parent compound) and different metabolites after ingestion (Petrie et al., 2015).

Like the parent compounds, the corresponding metabolites can be very persistent, and, in some cases, they can be transformed back to the active substances (parent compounds). This makes them especially hard to remove during the secondary wastewater treatment which results in their release into the environment (Helmfrid et al., 2006; Petrie et al., 2015; Wallberg et al., 2016).

The removal in the WWTPs can vary between different OMPs from a physically driven process (adsorption) to biologically mediated enzymatic reactions (biodegradation) (Petrie et al., 2015). The physical-chemical properties such as hydrophobicity and water solubility, plays a crucial role in the fate of the compound and determines how and if it will degrade. Sorption onto biomass during the treatment in WWTP or onto the sediments when present in the environment is one option for some compounds (Wallberg et al., 2016). This will however only result in a decrease of the compound in one phase (liquid) and an increase in another (solid). Some antibiotics have a high affinity to solid organic matter which results in their sorption in the WWTP.

Biodegradation is another common possibility for removing OMPs from the aqueous phase of both wastewater and surface waters. However, this process causes the formation of a number of different degradation or transformation products (Petrie et al., 2015; Wallberg et al., 2016). Degradation due to photolysis is also a possibility and this has been proven to be successful for several compounds (Petrie et al., 2015). Nonetheless, as with biological degradation, the removal is not an indication of complete mineralisation and the occurrence of transformation products may be observed. Studies show that even if the parent compound is removed, the result may not be equal to a reduction in toxicity (Petrie et al., 2015; Wallberg et al., 2016)

Fick et al. (2011) performed a national screening in Sweden during 2010 where they included a total of 101 pharmaceuticals and the results showed 92 detected pharmaceuticals in WWTP influent. The found levels ranged from low ng/L up to 540 µg/L. However, the removal efficiencies in this study could not be calculated for all compounds since some were only detected in influent and not effluent wastewater. They also showed negative removal rates which indicates an increase in concentrations due to deconjugation of metabolites.

2.3 Surface water

Surface waters include all waters found on the Earth's surface such as rivers and lakes. These water bodies are of outmost importance for all living organisms on Earth and human activities

such as agriculture, industrial use and drinking water. OMPs in surface waters originate from sources such as industrial wastewater, agricultural runoff, livestock and agriculture, landfill leakage, domestic and hospital effluents (Barbosa et al., 2016). The concentrations of many OMPs decreases in the WWTPs, as described above, brownification is however a growing problem for the photodegradation in northern Europe and North America. The presence of dissolved organic matter and other particles may negatively affect the degradation kinetics of some compounds in surface waters by clouding the sunlight intensity (Petrie et al., 2015; Vinterstare, 2016).

Implemented regulations on management of industrial effluents has improved the surface water quality in several European countries but an improvement and stricter regulations in other regions of the world are still needed (Barbosa et al., 2016). Although the monitoring of discharges is improving there's still a lack of proper European Union legislation that obligate surface water quality monitoring of OMPs (Lindim et al., 2016). Screening surveys have however been conducted and Petrie et al. (2015) reported that approx. 70 different pharmaceuticals of variable therapeutic classes have been detected in UK surface waters. According to another screening programme, Fick et al. (2011) found 66 pharmaceuticals in the range from low ng/L up to 1.8 µg/L in surface water samples. The detected concentrations were in a comparable range with lower ranges found in a European-wide study (Fick et al., 2011).

A lack in knowledge of disposed wastewater effluent volume and discharge of the river at the sampling point makes the comparison of detected OMP concentrations in wastewater effluent and the recipient surface water difficult. Assumptions can still be made based on the fact that higher effluent concentrations means higher emissions resulting in higher concentration levels in rivers (Lindim et al., 2016). Concentration levels found in the rivers are however much lower than in the effluent due to a higher flow rate which leads to dilution (Barbosa et al., 2016; Sörengård et al., 2019).

2.4 Drinking water treatment plants

Modern treatment processes exist in order to provide lines of defence (or so-called barriers) between waterborne diseases and the consumer. The treatment process train of the Drinking water treatment plant (DWTP) depend on the raw water source (type and contamination levels) (Gerba, 2009; Svenskt Vatten, n.d.). The raw water sources used for drinking water in Sweden are almost equally divided between surface water and groundwater where approximately 50 % of the groundwater fraction comes from artificial groundwater (Tröger et al., 2018). Artificial groundwater is another expression for infiltrated surface water. An increasing number of OMPs in the water sources obstructs production of drinking water and calls for more advanced treatment. Sand filtration and flocculation are two examples of conventional treatment processes primarily developed and used in order to remove pathogens and nutrients. However, their ability to remove OMPs have been proven insufficient. Nanofiltration and reverse osmosis membranes are two examples of modern treatment techniques that have been proven to be effective in removal of OMPs while other techniques such as granulated active carbon (GAC) filtration only decrease the levels. The effectiveness of GAC generally decreases with time of use and complete removal of OMPs cannot be achieved. The effective treatment techniques can

be efficient in small-scale but are impractical in full-scale DWTPs due to a high concentration of OMPs in the retentate (Tröger et al., 2018).

When DWTPs are insufficient in their removal of OMPs human exposure and bioaccumulation of hazardous compounds may increase. Furthermore, new transformation products can be formed during the treatment processes, especially during the disinfection when the disinfectants (such as chlorine, chloramines, ozone, etc.) reacts with natural organic matter (NOM) and bromide or iodide (Richardson and Ternes, 2014). These biproducts may also form as a result of a reaction between other organic contaminants and disinfectants (Richardson and Ternes, 2014). In addition to insufficient removal, Swedish DWTPs are required to monitor only a limited number of organic compounds (20 OMPs, besides pesticides) due to Swedish regulations (Tröger et al., 2018).

As previously stated, OMPs can be found in surface waters and since many DWTPs use surface water as raw water source, low levels of OMPs can still be detected in some drinking waters. However, the levels are in the low ng/L range and the amount of detected compounds are low. According to the screening programme conducted by Fick et al. (2011) low ng/L levels of 26 pharmaceuticals could be detected in the drinking water in Stockholm. They also found a significant difference when comparing samples from Umeå to samples from Stockholm. The samples from Umeå contained low ng/L levels of only 2 pharmaceuticals and one explanation could be differences in raw water source.since DWTPs in Stockholm is using surface water from lake Mälaren while Umeå uses artificial bank filtrated groundwater (Fick et al., 2011). The detected amount of compounds and their levels were, as with surface waters, in a comparable range with lower ranges found in a European-wide study (Fick et al., 2011).

3 Materials and Method

3.1 Chemicals and reagents

Ultrapure water was used for the chemical analysis and generated by a Milli-Q (MQ) Advantage Ultrapure Water purification system and then filtered through a 0.22 µm Millipak Express membrane and an LC-Pak polishing unit (Merk Millipore, Billerica, MA). Methanol, acetonitrile, ammonium acetate and ethyl acetate of high analytical grade were obtained from Sigma-Aldrich (Sweden).

All analytical standards that were used for analysis were of high purity grade (>95 %). The native standards (NSs) (n=121) originated from Sigma-Aldrich (Sweden) and the isotopically labelled standards (ISs) (n=26) for the target compounds were acquired from Wellington Laboratories (Canada), Teknolab AB (Kungsbacka, Sweden), Sigma-Aldrich (Sweden) and Toronto Research Chemicals (Toronto, Canada). Additional and detailed information about the native and internal standards can be found elsewhere (Rostvall et al., 2018).

All samples were filtered through a glass microfibre filter (grade GF/F, Whatman, thickness 0.42 mm, pore size 0.7 µm) purchased from Millipore (Cork, Ireland). Oasis HLB SPE cartridges (200 mg, 6 mL) were used for the solid phase extraction (SPE) and purchased from Waters Oasis, MA, USA.

3.2 Selected compounds

A total amount of 121 compounds were selected for evaluation in this project, including 75 pharmaceuticals, 13 hormones, 13 PFASs, 8 industrial chemicals, 4 personal care products, 3 parabens, 2 stimulants, 2 pesticides and 1 isoflavone. The pharmaceuticals cover a number of therapeutic groups like antibiotics, anticancer, antidepressants, antidiabetics, antidiarrheal, antifungals, antihistamines, antihypertensives, antilipemic agents, antipsychotics, antisecretory agents, beta blockers, diuretics, non-steroidal anti-inflammatory drugs (NSAID) and sedatives. Target compounds were selected based on information in the literature, on their occurrence and ubiquity in aquatic environments and on their usage and consumption. A list of selected compounds can be found in Table A1 in Appendix.

3.3 Study sites description

Vänern is the largest lake in Sweden with its area of 5 450 km^2 and the third largest in Europe (SMHI, n.d.). The lake reaches from Karlstad in the north to Trollhättan in the south and surrounded by Gullspång and Götene among others in the east and Säffle and Vänersborg among others in the west. Vänern provides around 800 000 pe with drinking water, has a maximum depth of 106 m, water residence time is 8—9 years and the drainage basin covers 10 % of Sweden's land area (Christensen et al., 2007; SMHI, n.d.). The drainage basin is dominated by forest area with just over 60 % and mostly agricultural area in the south. Five rivers connected to Lake Vänern were selected and sampled: Göta river, Tidan, and three different sites in Klar river.

Lake Vättern has an area of ca 1 900 km^2 which makes it the second largest lake in Sweden and reaches from Askersund in the north to Jönköping in the south. Maximum depth is 128 m, the water residence time is 58—60 years and it provides around 250 000 pe with drinking water (Christensen et al., 2007). It has a small drainage basin for its size and that's mainly due to its topographic location in comparison with the enclosing land area. The drainage basin covers almost 1 % of Sweden's land area and consists mainly of forest and agricultural areas (Christensen et al., 2007). There are 148 incoming rivers where the biggest one in Huskvarna river and the outlet of the lake is mainly Motala stream (SMHI, n.d.). Four rivers connected to Lake Vättern were selected and sampled: Lillån, Munksjön, Huskvarna river and Motala stream.

Lake Mälaren is the third largest in Sweden with its surface area of 1 140 km^2 maximum depth of 64 m. Water residence time is 2.2 years and the drainage basin covers ca 5 % of Sweden’s land area and is characterized by 57 % forest area, 20 % agricultural area and 11 % water bodies (Sonesten et al., 2013). Surrounded by cities such as Västerås in the west, Uppsala in the north, Stockholm in the east and Eskilstuna and Södertälje in the south, this area is considered to be one of the fastest economically expanding regions in Sweden. The population increase in Stockholm is also considered to be one of the greatest increases during the next five years in Europe (“Stockholms Handelskammare - Stockholm is fastest growing city in Europe,” n.d.). Since the lake is surrounded by a large number of cities it is affected by a number of wastewater discharges and is the main source for drinking water in the Stockholm area (Naturvårdsverket, 2017). The thirteen sampled rivers connected to Mälaren were: Fyrisån, Örsundaån,

Enköpingsån, Arbogaån, Oxundnaån, Kolbäcksån, Sagaån, Lövstaån, Märstaån, Norrström, Svartån, Hedströmmen and Eskilstunaån.

All sampling points around the three lakes can be seen in Figure 1 (A, B, C) and a complete list of all surface water samples can be found in table B1 in Appendix B.

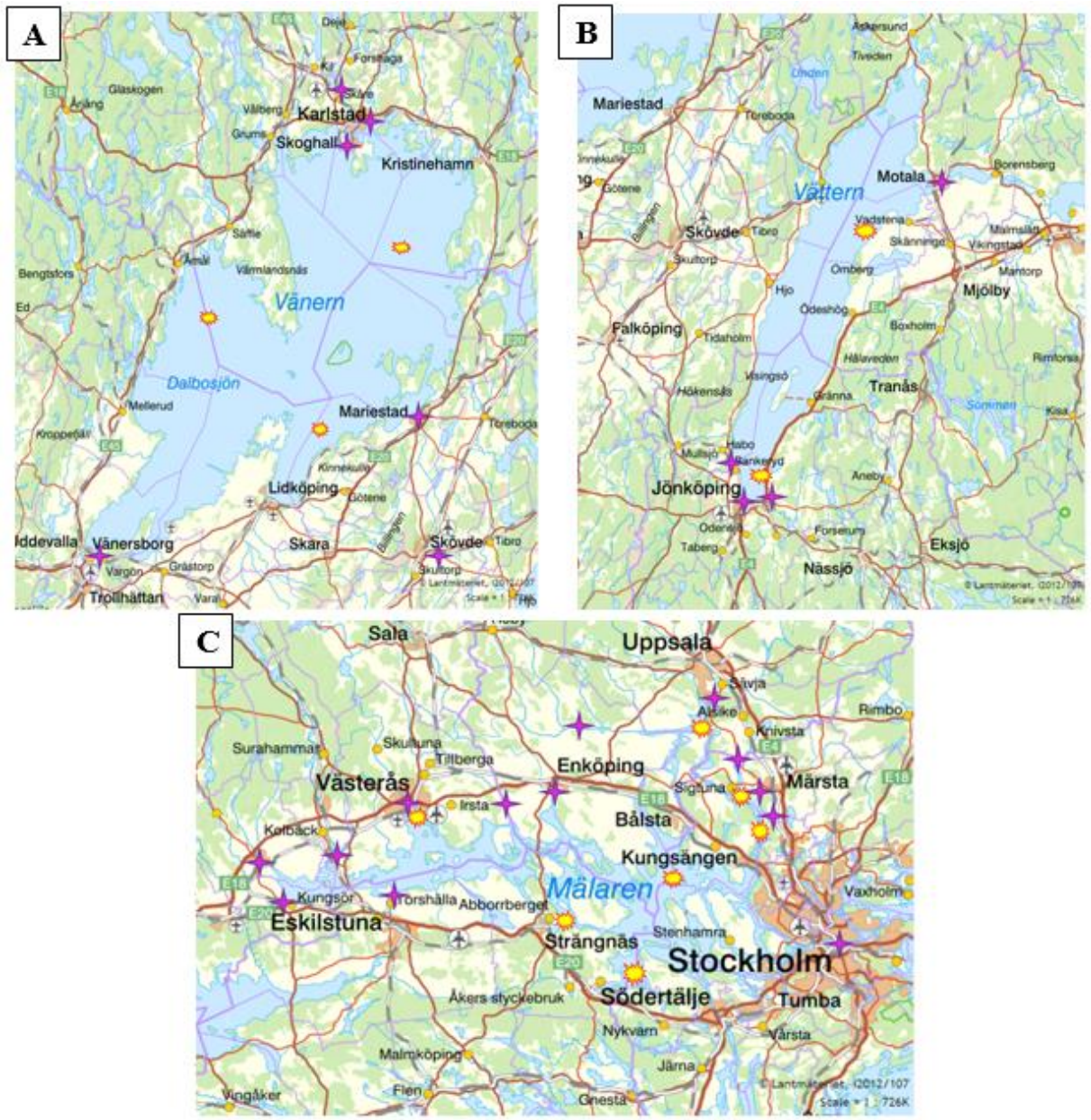

Figure 1: All sampling sites around the three lakes Vänern (A), Vättern (B) and Mälaren (C) where the surface water samples were collected. Sampling sites for river samples are marked with a pink star and the lake samples are marked with a yellow explosion. Miljödata MVM [2020]. Swedish University of Agricultultural Sciences (SLU). National data host lakes and watercourses, and national data host agricultural land. http://miljodata.slu.se/mvm/[2020-01-07]

3.4 Sample collection

Within this project we have decided only to provide a list of DWTP- and WWTP-codes and not a map and full information about the facilities since we would like to keep information about their locations confidential.

The wastewater samples were collected from 3 WWTPs as grab samples in September 2019 and the surface water samples during one week in October 2019. The sampling bottles were rinsed three times with water from the sampling location before being filled with the samples. All samples were then stored at -20 °C at the Department for Aquatic Sciences and Assessment at SLU.

Wastewater influent and effluent were collected from 3 WWTPs individually connected to one of the three lakes.

Surface water was collected in 1 L PP bottles as grab samples from 23 rivers connected to either Vänern (n=6), Vättern (n=4) or Mälaren (n=13). In addition to the surface water samples, lake samples from Vänern (n=3), Vänern (n=2) and Mälaren (n=7) were also collected as grab samples. The lakes are the three biggest lakes in Sweden and are major suppliers for drinking water production in the area.

Drinking water samples were collected as grab samples from three DWTPs individually connected to one of the three lakes.

3.5 Sample preparation

The sample preparation and analysis was performed on the dissolved aqueous phase with solid phase extraction (SPE) using a validated method described by Rehrl et al. (2020). All water samples (approximately 500 mL aliquot) including blanks (n=3) were extracted by SPE.

In short, all water samples were filtered with pre-baked (550 ˚C for 24 h) glass fibre filters (GFF, 0.45 µm, What-man, GE Healthcare, IL, USA). Aliquots of 500 mL for each sample were transferred to pre-rinsed (methanol) 1 L PP bottles. Every sample was spiked with 20 ng of the ISs mixtures per aliquot of the samples (Sörengård et al., 2019).

For the SPE, 200 mg HLB cartridges (Waters Oasis, MA, USA) were used for all samples. The cartridges were all pre-conditioned with 6 mL methanol followed by 6 mL Milli-Q water by gravity. The samples were then loaded onto the SPE reservoirs and was loaded on the SPE cartridges at a rate of approx. one drop per second. The SPE cartridges were dried and thereafter eluted two times with 4 mL methanol into 15 mL PP-tubes (Corning™). A gentle stream of nitrogen gas was then used to evaporate all eluted samples until reaching a volume of 0.5 mL. The extracts were then transferred to 1.5 mL auto-injector glass vials (Eppendorf, Germany) and the walls of the PP-tubes were rinsed thrice with 200 µL methanol before being transferred to the same vials. The extracts was evaporated until a volume of 0.5 mL and a volume of 0.5 mL Milli-Q was added to the extracts before being vortexed for 30 s before analysis (Sörengård et al., 2019).

3.6 Instrumental analysis

The different water samples were analysed by a DIONEX UltiMate 3000 ultra-performance liquid chromatography (UPLC) system (Thermo Scientific, Waltham, MA, USA) coupled to a triple quadrupole mass spectrometer (MS/MS) (TSQ QUANTIVA, Thermo Fisher Scientific, Waltham, MA, USA). As analytical column an Acquity UPLC BEH-C18 column (50 mm × 2.1 i.d., 1.7 µm, Waters Corporation, Manchester, UK) was used for chromatographic separation of target OMPs. The mobile phase consisted of Milli-Q with 5 mM ammonium acetate and acetonitrile. The flow rate was 0.5 mL/min and run time was 15 min using switching positive and negative electrospray ionization modes. A 11-point calibration curve from 0.01 to 500

ng/mL were prepared for the data evaluation. Using TraceFinder™ software (Thermo Fisher Scientific, MA, USA) the instrumental data was evaluated using.

3.7 Quality assurance

In order to test the performance of the method linearity, limit of quantification (LOQs), relative recovery, precision, blanks and matrix effect (ME) were assessed. An eleven-point calibration curve in the concentration range from 0.01 ng/L to 500 ng/L was prepared in order to test the linearity. The linearity of the calibration curve was assessed by calculating the coefficient of determination (R^2). The linearity parameters of each compound can be found in in Table D1 in Appendix D.

LOQ values was calculated as half of the lowest calibration point in the calibration curve where the standard deviation of the average response factor (ARF) was < 30 %. The corresponding peak area to this concentration was then used for calculating LOQ for each individual compound in each sample, see Table D1 in Appendix D.

The absolute recovery describes the efficiency of the sample preparation step by showing the proportion of obtained analyte from the sample during the sample preparation (Kruve et al., 2015). The performance of the extraction method (SPE and UPLC-MS/MS) was done by calculating the absolute recovery by creating so-called fortified samples. Fortified samples were prepared by spiking a known concentration of NS to the samples before SPE extraction, and then correlating it with the detected concentration after extraction and analysis. The fortified samples were spiked with 100 ng of NS and 20 ng of ISs per aliquots of the sample. The average absolute recovery for each analyte can be found in Table D1 in Appendix D.

The repeatability of the study is a way of evaluating the precision of the method and was done by preparing duplicates for every tenth sample. The resulting values enables a comparison of the analysis within a batch of samples and between different batches.

Both the mass and the retention time of a compound is relevant for the detection by the instrument (UPLC-MS/MS). Therefore, using isotopically labelled standards is the optimal approach (European Commission, 2002). That is the ideal case but due to inaccessibility some target compounds in this study could not be matched with the perfectly designed IS, therefore a replacement IS had to be selected. The replacement IS has to have as similar physical-chemical properties, retention time and categorial grouping of the compound as possible in order to achieve acceptable recovery rates for the compounds (European Commission, 2002)

Environmental water samples are not pure water but a mixture of wanted or expected target compounds, the samples also contain unknown compounds which must be taken into consideration. The exact content of the water is impossible to predict since it's a mixture of various endogenous substances like lipids, proteins, salts, minerals etc. that together or individually can greatly affect both the extraction and analysis. This is generally referred to as matrix effect and can result in a suppressive or enhancing ion effect. In order to address the matrix effect matrix matching standards (MSTs) were prepared and used. Since the matrix effect is different for every type of sample five different matrices (wastewater influent, wastewater effluent, rivers, lakes, drinking water) were used when comparing all types of

samples, and three different matrices (Vänern, Vättern, Mälaren) were used when comparing the surface waters.

MSTs were prepared for each matrix by spiking 20 ng of the ISs and 100 ng of NS per aliquot of sample before analysis.

The ME was calculated by subtracting the peak area/IS ratio determined in non-spiked samples from the peak area/IS ratio in MST samples. Matrix effects were calculated in order to see if there was an ion enhancement or suppression, Table D1 in Appendix D. Negative values indicates an ion suppression while positive values indicates an ion enhancement.

Each batch of analysis included two blanks containing MQ water and MeOH. This was done in order to eliminate any concerns of contamination and to facilitate memory effects during analysis in the instrument. During the extraction all PP-bottles and SPE reservoirs were rinsed three times with methanol to avoid any contamination. Adapters and stop-cocks from the SPE and needles from the evaporation step were ultrasonicated for 20 mins, twice with methanol or three times with ethanol. Additionally, all analytical work was operated whilst wearing gloves.

3.8 Risk assessment

OMPs doesn't only have negative effects on the aquatic environment, when present in drinking water they can impose a risk on human health (Couto et al., 2019a). Many of them have guidelines which describes the highest concentration of which the compound can appear in drinking water, without any negative effects on human health. In order to get a risk assessment of the OMPs, the drinking water equivalent levels (DWELs) were calculated with Eq. (1)

$$DWEL = \frac{TDI * M * f}{V} \qquad (1)$$

Where *TDI* represents the Tolerable Daily Intake (µg/kg bw/day), *M* is the body weight (60 kg), *f* represents the drinking water allocation (adopted value 0.2) and *V* represents the personal drinking water consumption (2 L/day) (Couto et al., 2019a). The risk was then assessed by calculating the Benchmark Quotient (BQ) as a ratio between the maximum or mean drinking water concentration and the DWEL value. BQ values of 1 represents a perfect match with the DWEL which makes the water potable. If the BQ ≥ 1 in the drinking water, a potential risk to human health can be observed if exposed to this concentrations over a period of life (Couto et al., 2019a).

4 Results

A total number of 121 OMPs have been analysed in five different matrices (wastewater influent, wastewater effluent, rivers, lakes and drinking water).

4.1 Differences between matrices

The occurrence of OMPs in the studied water samples is shown in Figure 2. The concentrations in each sample has been summarised into a cumulative concentration and before plotted in a boxplot the log10 was used. Negative values represent concentrations in the range between 0—1 ng/L and the logarithmic values were set to 1 for the cumulative concentrations equal to zero. It is clear that all three groups (OMPs, hormones and PFASs) of compounds are present in wastewater influent, effluent, rivers and lakes. It can be argued that PFASs are stable in the

same matrices since the boxplots are similar for these cases (Mazzoni et al., 2019). OMPs and hormones on the other hand, decrease in concentrations in the wastewater and rivers, whereas the majority of the compounds were absent in both lakes and drinking water. This may be explained by the dilution effect since the water volume in the river is big, moving and due to larger distance from the effluent discharges.

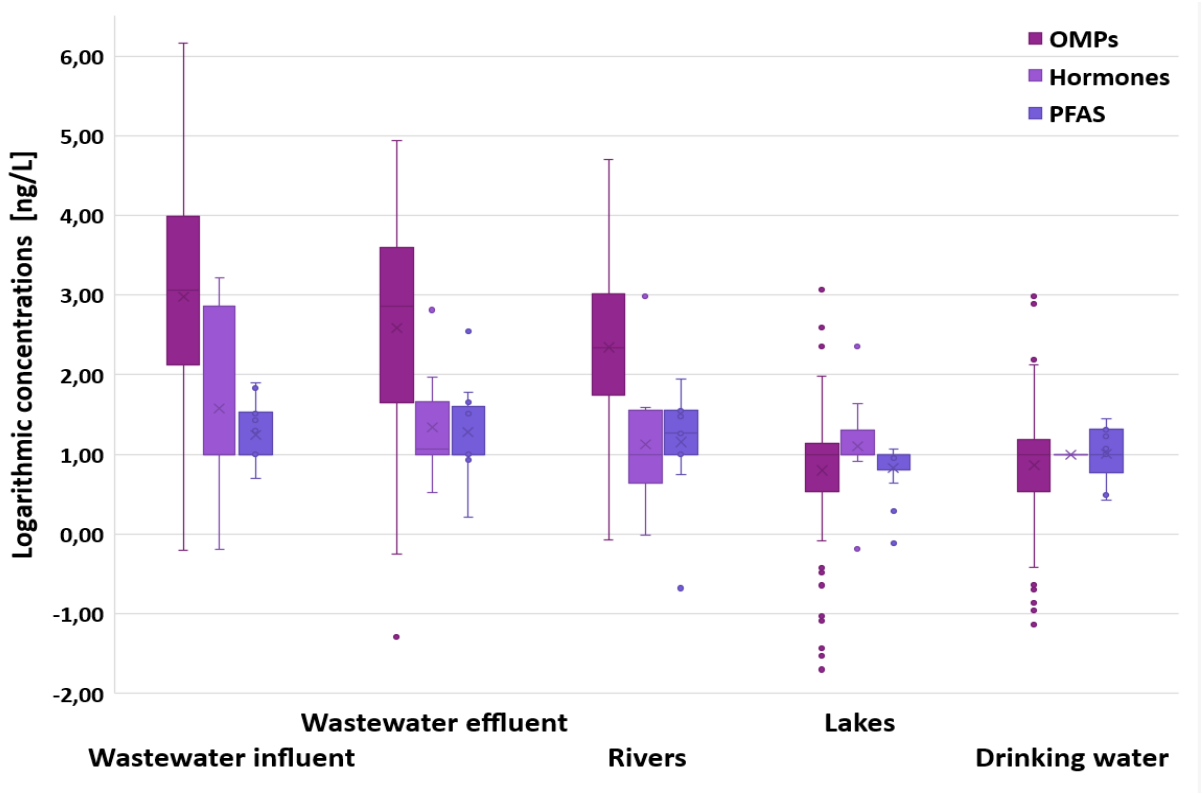

Figure 2: Boxplot showing logarithmic cumulative concentrations of OMPs (n=95), Hormones (n=13) and PFASs (n=13) in different matrices (n=5). It clearly shows a decrease in the concentrations from wastewater to drinking water.

4.2 Frequency of detection

Frequency of detection (FD) was calculated for every compound in all five matrices in order to see how often they were detected in the samples. This was done by dividing the number of positive samples for each compound by the total number of samples.

In general the FDs were higher in the wastewater influent than the other matrices, 92 of the 121 compounds could be detected with an FD > 50 %. The effluent wastewater is a close second with 91 detected compounds, 80 compounds were detected in the river matrix, 43 in the lake and 29 in the drinking water. Comparing the five matrices only 26 compounds could be found with an FD > 50 % in all matrices and can be seen in Table 1. A complete list of the FDs can be found in Table C1 in Appendix C.

4-Chloro-3-methylphenol and ethylparaben were only detected in the influent wastewater which could suggest a successful removal in the WWTPs. Looking at Valproic acid and Propylparaben the results indicate a lower detection in the effluent which also could be a result of removal but it could also be a coincidence since only three WWTPs were sampled.

Table 1: Calculated FDs for the 26 compounds that had an FD > 50% in all five matrices.

Compound	WW IN	WW OUT	Rivers	Lakes	DW
BAM (Dichlorobenzamide)	100%	100%	100%	95%	97%
Bicalutamide	100%	100%	100%	100%	79%
Caffeine	100%	100%	100%	100%	88%
Carbamazepine	100%	100%	100%	100%	94%
Cetirizine	100%	100%	96%	100%	74%
DEET	100%	100%	100%	100%	97%
Desvenlafaxine	100%	100%	100%	100%	97%
Fexofenadine	100%	100%	100%	95%	53%
Fluconazole	100%	100%	96%	95%	97%
Lamotrigine	100%	100%	91%	100%	91%
Laurilsulfate	95%	100%	87%	100%	97%
Lidocaine	100%	100%	91%	100%	68%
Mefenamic acid	100%	100%	100%	100%	97%
Metformin	100%	100%	91%	90%	82%
Nicotine	100%	100%	100%	95%	62%
Norsertraline	100%	100%	96%	100%	76%
Oxybenzone (Benzophenone-3)	100%	95%	78%	81%	85%
PFHpA	67%	100%	83%	62%	83%
PFHxS	67%	100%	87%	95%	83%
PFOA	100%	100%	96%	100%	100%
Propylparaben	95%	81%	70%	57%	50%
Sucralose	100%	100%	100%	57%	62%
Tolytriazole	100%	100%	83%	90%	74%
Tributyl citrate acetate	100%	100%	100%	100%	97%
Triisopropanolamine	100%	100%	96%	100%	97%
Valproic acid	100%	71%	65%	100%	71%

The FDs are generally lower in the river samples and the number of compounds with a frequency of detection greater than 50 % in the rivers was, as previously stated, 80, see Table C1 in Appendix C. The lower FDs agrees with previous studies suggesting a lower amount of detected OMPs and concentrations in surface waters. Methylparaben and Ifosfamide showed higher FDs in the river samples than wastewater samples (Methylparaben: 87 % in surface water, 67 % in wastewater effluent and Ifosfamide: 74 % in surface water, 29 % in wastewater effluent).

In figure 3 only the hormones with a frequency of detection >50 % is shown. When studying the figure, 11 out of 13 compounds could be detected in the samples. It is clear that 17α-ethynylestradiol has the highest frequency of detection while estriol and norethindrone has the lowest.

17α-ethynylestradiol is an estrogenic compound with low water solubility often used in contraceptive pills which might explain the high FD (Lindim et al., 2016), but other factors may also affect these findings. Estriol on the other hand is a weak oestrogen and a minor female sex hormone almost only detectable in pregnant women, which might explain why this compound wasn't found in the samples (Velicu and Suri, 2009).

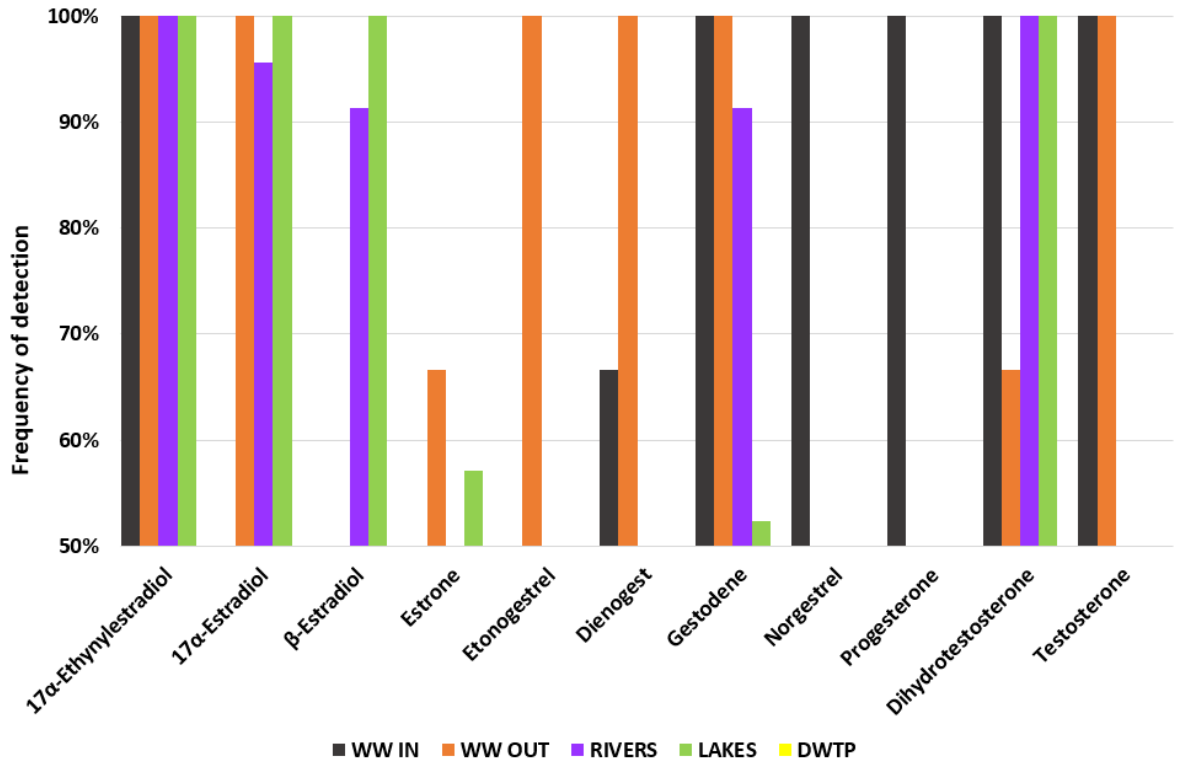

Figure 3: Column chart showing the frequency of detection (>50 %) of hormones (n=13) in different matrices (n=5). 17α-Ethynylestradiol, Gestodene, Dihydrotestosterone and 17α-Estradiol has the highest FDs.

4.3 Distribution of OMPs, PFASs and hormones in Wastewater

The detected compounds have been divided into 18 categories according to their therapeutic groups and shown as total (cumulative) amount per sample. These 18 categories consist of analgesics (n=3), antibiotics (n=11), anticonvulsants (n=4), antidepressants (n=9), antifungal (n=5), antihypertensive (n=5), antilipidemic (n=3), antineoplastic agents (n=3), beta blockers (n=7), hormones (n=13), industrial chemicals (n=8), NSAID (n=6), opiates (n=3), other (n=18), personal care products (n=5), pesticides (n=2), PFASs (n=13) and stimulants (n=2).

Results from the wastewater samples are shown in figure 4. The bars clearly shows a high occurrence of analgesics, industrial chemicals, personal care products and stimulants, in both influent and effluent wastewater. The concentrations however, seem to be lower in the effluent, which is expected due to treatment. One can clearly see the difference between influent and effluent when comparing the analgesics and stimulants while the difference for industrial chemicals is not as clear. When comparing the different lakes the higher concentrations connected to lake Mälaren is easy to recognize, in both influent and effluent WW.

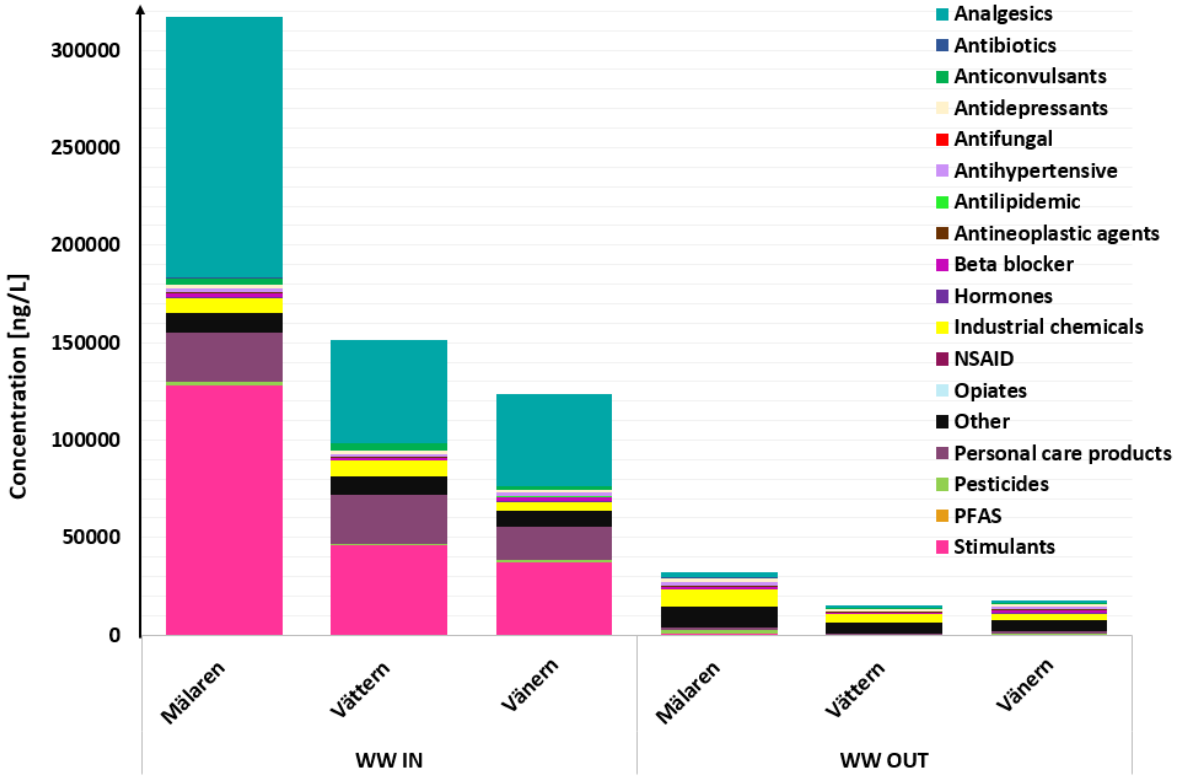

Figure 4: Bar chart with cumulative concentrations of OMPs, PFASs and hormones in the three different WWTPs connected to lakes Mälaren, Vänern and Vättern. The total concentrations are much higher in WW IN than WW OUT and samples connected to Mälaren are the highest.

4.4 Distribution of OMPs, PFASs and hormones in surface water

4.4.1 Rivers

The distribution of all detected target compounds in all 23 rivers can be seen in figure 5. The target compounds are divided into 18 groups depending on their physical-chemical properties and usage, in the same way as for the wastewater samples. The river samples are sorted by corresponding lake (Vänern, Vättern, Mälaren) in order to compare the three different lakes to each other. Since both LIII_R3 and LIII_R13 have higher cumulative concentrations of OMPs they were placed to the right with a different y-axis.

The majority (14) of the river samples in figure 5 has a cumulative OMP concentration ≤ 2 mg/L per sample, while the other seven rivers (excluding LIII_R3 and LIII_R13) vary in the concentration range of 2 mg/L up to just below 16 mg/L, see table 2. River LII_R4 connected to Vättern has the lowest cumulative concentration with a value of 0.45 mg/L and LIII_R8 connected to Mälaren is a close second with a cumulative concentration of 0.49 mg/L

The rivers connected to lake Mälaren has relatively low cumulative OMP concentrations, but also the two samples with the highest concentrations, as compared to the other two lakes. In sample LIII_R3 the cumulative OMP concentration reaches a value just below 78.8 mg/L which is really high for a surface water sample. LIII_R13 is with its 33.2 mg/L the second most contaminated river according to these findings.

Samples connected to Vänern and Vättern are seemingly similar in comparison however, when excluding sample LI_R5 and LII_R1 lake Vättern actually has higher average cumulative

concentrations. Therefore, it can be argued that the area surrounding the sampling sites have a big impact on the concentrations found in the samples.

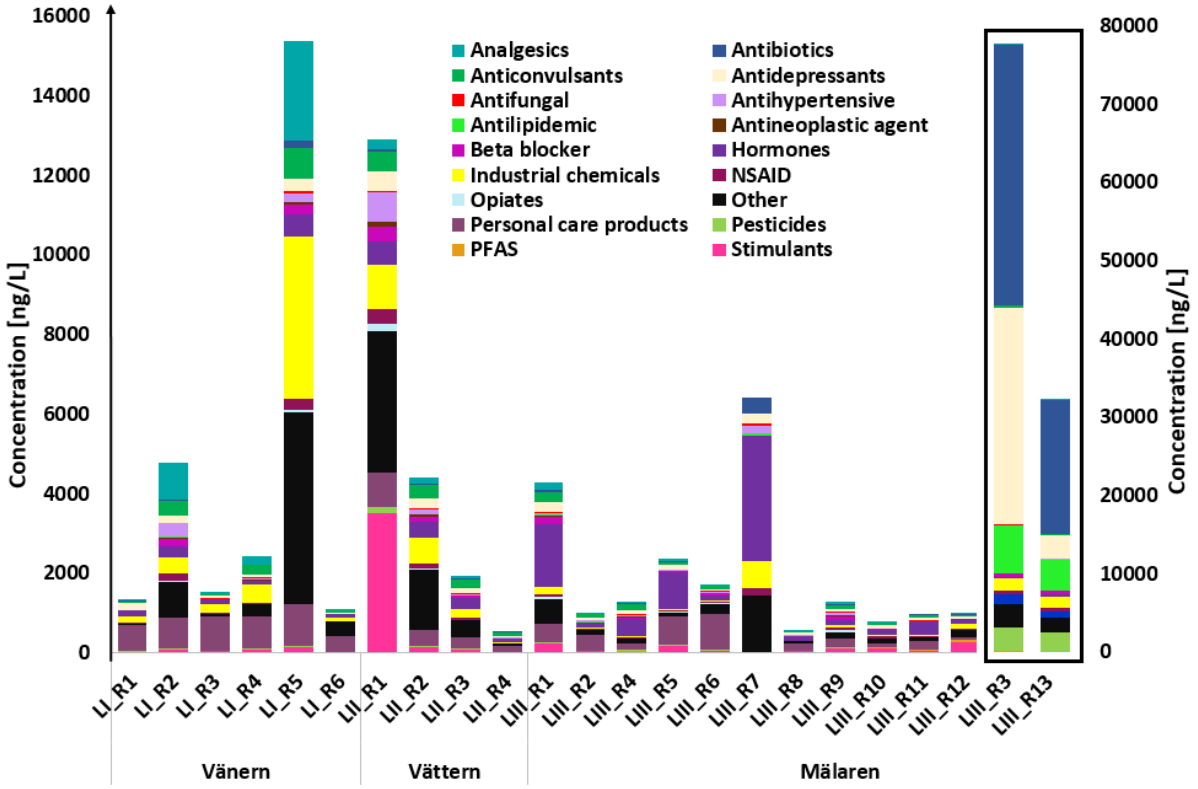

Figure 5: Bar chart showing the cumulative OMP concentrations in surface water samples from all sampled rivers connected to lake Vänern. Vättern and Mälaren. River LIII_R3 and LIII_R13 had considerably higher cumulative concentrations and were therefore moved to the right and put inside the black rectangle with a different y-axis.

The total OMP concentration is, as can be seen in Table 2 and figure 5, highest in the sample LIII_R3 from (79 µg/L) and lowest in sample LIII_R8 (0.45 µg/L).

Table 2: Detected concentrations of pharmaceuticals, PFAS, hormones, industrial chemicals, pesticides and stimulants in the 23 different river samples. The total concentrations are in mg/L whereas the other concentrations are in ng/l.

Sample	Total OMP [µg/L]	Pharmaceuticals [ng/L]	PFAS [µg/L]	Hormones [µg/L]	Industrial chemicals [µg/L]	PCPs [µg/L]	Pesticides [µg/L]	Stimulants [µg/L]
LI_R1	1.2	310	8.1	13	140	670	8.5	28
LI_R2	4.7	3400	4.6	26	420	760	37	77
LI_R3	1.4	310	4.1	14	210	850	9.9	50
LI_R4	2.5	1100	4.3	27	450	820	11	87
LI_R5	16.0	10 000	6	95	4100	1100	45	130
LI_R6	1.0	510	5.7	13	91	380	9.3	18
LII_R1	13.0	6800	5.8	48	1100	860	140	3500
LII_R2	4.4	3000	7.2	97	660	400	40	140
LII_R3	1.9	1200	13	45	240	280	19	75
LII_R4	0.45	220	3.7	25	27	160	10	9.4
LIII_R1	3.0	2000	8.3	130	190	480	20	230
LIII_R2	0.94	450	5	20	28	390	17	38
LIII_R3	79.0	74 000	38	95	1500	75	3000	7.9
LIII_R4	1.0	690	36	44	46	170	15	27
LIII_R5	1.5	560	11	13	46	710	16	170
LIII_R6	1.6	590	9.7	20	37	900	20	50

LIII_R7	3.3	2600	3	11	690	0.95	9.6	15
LIII_R8	0.49	200	6.2	36	16	180	9.7	44
LIII_R9	1.2	760	12	56	59	230	24	100
LIII_R10	0.74	430	13	34	36	86	13	130
LIII_R11	0.68	340	11	23	25	210	11	62
LIII_R12	0.92	380	58	25	120	68	13	270
LIII_R13	33.0	29 000	24	140	1500	32	2400	9.6

4.4.1.1 Rivers connected to Lake Vänern

Looking at the bar chart including samples from rivers connected to lake Vänern, figure 6, a pattern with high occurrence of analgesics, industrial chemicals, personal care products and the group other can be seen. However, the cumulative concentrations of OMPs and hormones are generally low with the exception of sample LI_R5 which entails a large amount of industrial chemicals and the group other. The results could indicate a number of industries in the area close to the sampling point, or inside the catchment area. As it happens the sampling point LI_R5 is located downstream the WWTP effluent discharge and the WWTP is the recipient of hospital waste, which might explain the high occurrence and concentrations of different pharmaceuticals and hormones.

Sample LI_R6 has the lowest cumulative concentration which might be explained by the size

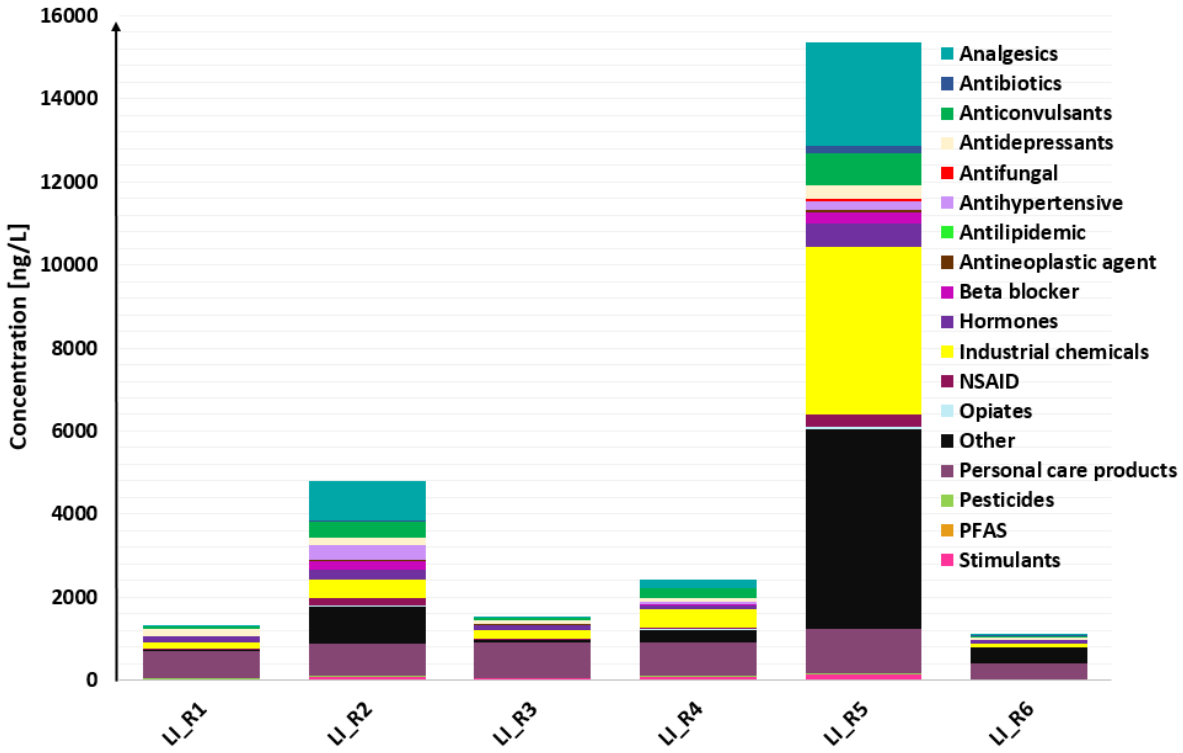

Figure 6: Bar chart of cumulative concentrations of target compounds in surface water samples from rivers connected to lake Vänern. The sample with the highest concentrations belong to LI_R5 and the lowest concentrations belong to LI_R6. Personal care products, industrial chemicals, other and analgesics are the most common groups of detected compounds.

of this river, it is very broad which causes dilution due to the amount of water.

4.4.1.2 *Rivers connected to lake Vättern*

It is harder to see a similar pattern in the rivers connected to Vättern, see figure 7. Stimulants, other, industrial chemicals and personal care products can however be pinpointed as the most frequently detected groups in these four rivers. Sample LII_R1 is the most polluted one and LII_R4 has the lowest cumulative concentrations. The LII_R1 river is the recipient of WWTP and the sampling point was downstream the effluent discharge. In combination with a lower water flow than LII_R4 it might be one explanation for the difference. Another reason could be that the sampling point LII_R1 is close to the inlet to Vättern while the sampling point for LII_R4 was close to the outlet.

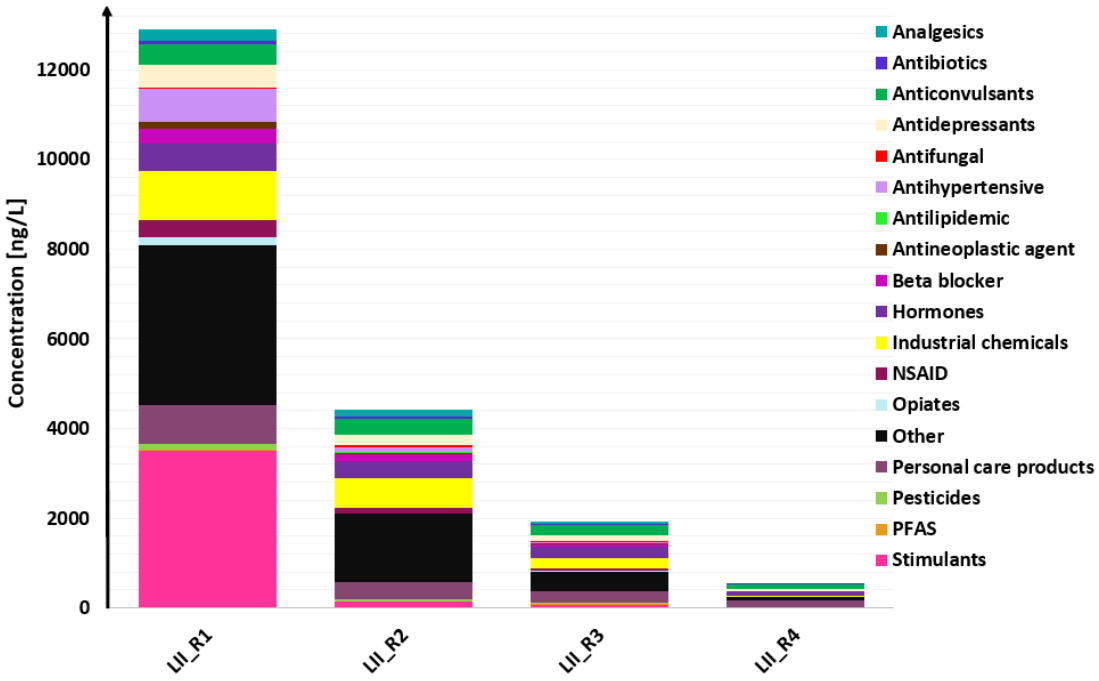

Figure 7: The barchart shows cumulative concentrations of OMPs found in the samples from rivers connected to the lake Vättern. LII_R1 has much higher concentrations than the other rivers and LII_R4 has the lowest. Stimulants, other, industrial chemicals and personal care products are the most common groups.

4.4.1.3 *Rivers connected to lake Mälaren*

In the 11 rivers to the left in figure 8, the categories other, industrial chemicals and personal care products are the ones that stand out, while the antibiotics, antidepressants and antilipidemic compounds stand out in the two rivers to the left. LIII_R8 has the lowest cumulative concentration of all samples which might be an effect of no bigger cities in the catchment area, the river is the recipient of WWTP effluent but the WWTP is small with 10 500 PE. Differences could be seen when comparing this river sample with LIII_R1 which has higher concentrations and is also a recipient of WWTP effluent for 180 000 PE. However, the amount of PE is not the only reason for differences since sample LIII_R3 was found to be the most polluted river in this study, but this river is the recipient of WWTP effluent with 105 000 PE. This sampling point is however, downstream both industrial area and a WWTP which is the recipient of hospital wastewater. That might explain the high concentrations of both antibiotics and antidepressants in the sampled water. LIII_R13 also contain high concentrations of antibiotics but this river is

not the recipient of hospital waste and therefore these compounds most likely comes from households or something else.

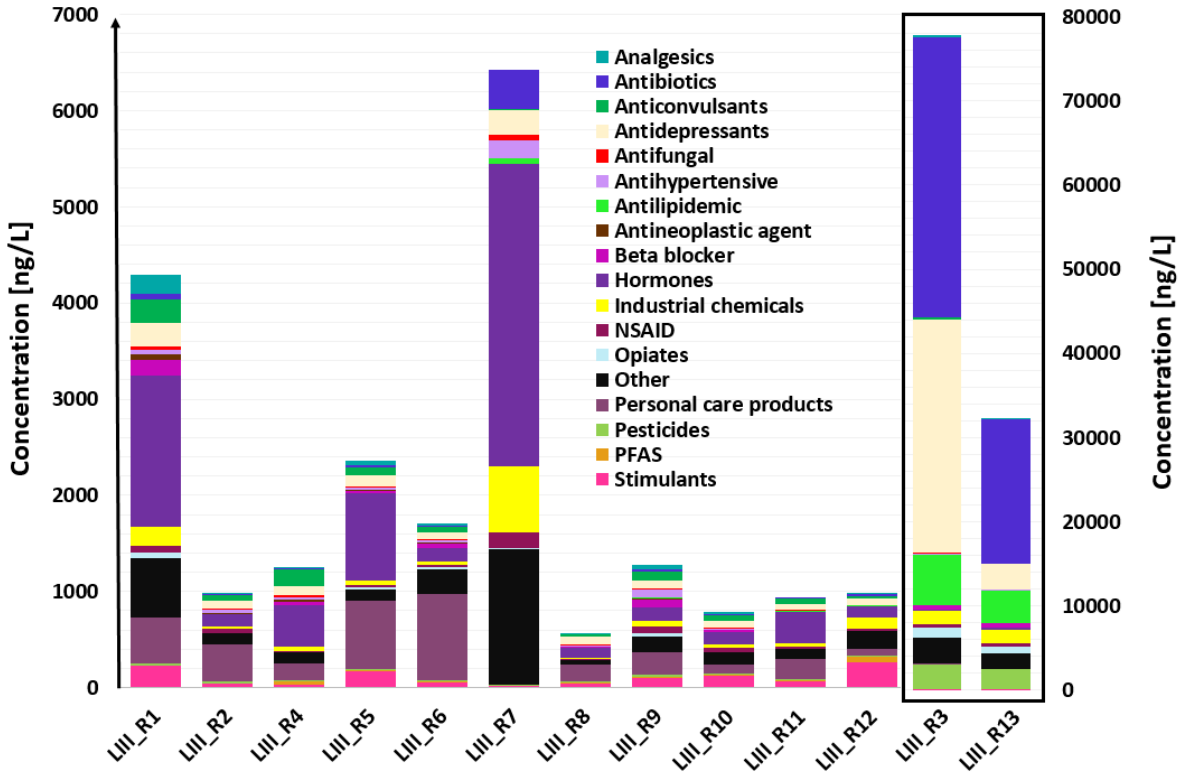

Figure 8: Bar chart showing results from the sampled rivers connected to lake Mälaren. Since the samples LIII_R3 and LIII_R13 has considerably higher cumulative concentrations than the other 11 samples, these two can be found inside the black rectangle to the right. These two samples also have their own y-axis. Lowest concentrations could be found in sample LIII_R8. The most common groups in the 11 samples to the left seem to be stimulants, personal care products, hormones, other and industrial chemicals. In the two samples to the right however, antibiotics, antidepressants, antilipidemic and pesticides seem to be the most common ones.

4.4.2 Lakes

The results from the lake samples can be seen in figure 5 and looking at the bars one can easily see the difference between the three lakes. It can be seen that lake Mälaren contains higher concentrations of all OMPs. One can also see a higher concentration of industrial chemicals in all samples from Mälaren, samples from lake Vättern contains higher concentrations than lake Vänern. Anticonvulsants, antidepressants, hormones, industrial chemicals, pesticides and stimulants are categories that are easily spotted in all sites. One difference between the three lakes can be seen when comparing the amount of industrial chemicals found in the samples from the different sites. It is clear that the highest amount of industrial chemicals can be found in lake Mälaren. This could very well be a result of the differences in size between the lakes and the surrounding areas where lake Mälaren has a higher urban area density than both Vänern and Vättern. The higher concentrations in Mälaren could also be connected to dilution effect since lake Mälaren is smaller than the other two lakes, which means the concentrations in the bigger lakes are more diluted (Tröger et al., 2018). This might explain the differences between the three lakes when comparing the hormones or the industrial chemicals, which are higher in lake Mälaren than lake Vättern and lake Vänern.

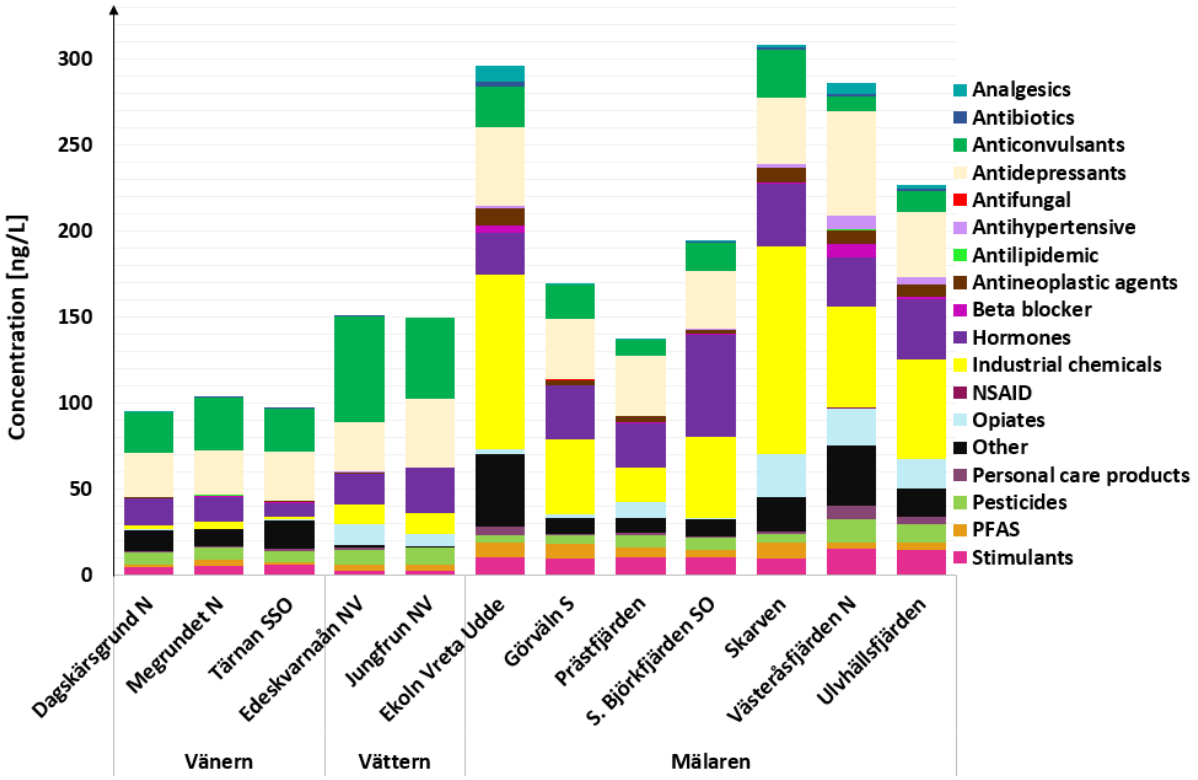

Figure 9: Bar chart with results from the lake samples indicate higher cumulative concentrations in the samples from lake Mälaren. The samples from Ekoln Vreta udde, Skarven, Västeråsfjärden N and Ulvhällsfjärden has the highest concentrations while the lowest can be found in samples from Dagskärsgrund N, Tärnan SSO and Megrundet N. Anticonvulsants, antidepressants, hormones, industrial chemicals, other and pesticides can easily be spotted in all samples.

4.5 DWEL

DWEL was calculated using eq. (1) for two compounds which were detected in the samples from DWTPs. BQs was calculated as a ratio between the maximum or mean concentration of detected compound and the calculated DWEL, resulting in BQ_max where maximum values were used and BQ_mean where mean values were used. Carbamazepine had an FD of 100 % and Erythromycin an FD of 17 % in the three analysed DWTPs. The results can be seen in Table 3. Only Carbamazepine had a BQ ≥ 1 with its BQ_max =1.47 which indicates a potential risk to human health when exposed to these levels for a period of life (Couto et al., 2019a).

Table 3: Calculated DWEL-values for five detected compounds. TDI values from Couto et al. (2019).

Compound	TDI	DWEL	BQ_max	BQ_mean
Carbamazepine	0.34	2.04	1.47	0.50
Erythromycin	4.3	25.8	0.54	0.54

5 Discussion

A total of 91 out of the 121 analysed compounds were detected with a FD ≥ 50 % in the wastewater effluent in concentration levels from low ng/L up to 160 µg/L. In the surface water samples 80 of the 121 target compounds were found at concentrations from low µg/L up to 3.3 µg/L. 35 OMPs were detected at levels between low µg/L up to 2.9 µg/L. These findings are similar to ones in previous studies, see table E1 in Appenfdix E. (Ahrens et al., n.d.; Couto et al., 2019b; Fick et al., 2011; Helmfrid et al., 2010, 2006; Loos et al., 2009; Malnes et al., 2021;

Petrie et al., 2015). The concentration levels are however slightly lower than concentrations found in surface waters outside of Sweden (Petrie et al., 2015). This could be a result of differences in consumption rate and differences in legislations or restrictions regarding the handling and discharge of OMPs (Naturvårdsverket, 2017). The Swedish Environmental Code for example, states that all activities that may inflict harm or inconvenience to the environment, humans or health should be regulated and carried out in best way possible (Naturvårdsverket, 2003). Differences in climate conditions negatively effects the biological activity and/or the biodegradation in WWTPs resulting in a lower removal of OMPs (Hey et al., 2012). Thus, the lower concentrations detected in Swedish wastewater effluent may be explained by a colder climate as compared to some of the other countries included in the European wide surveys performed and described by Loos et al. (2009) and Petrie et al. (2015).

The results have shown decreasing of OMP and hormone concentrations from wastewater to drinking water, where the highest concentrations could be found in wastewater and the lowest in drinking water. Even the number of detected compounds in the different matrices decreased when following the water from wastewater to drinking water. It could be explained by the fact that wastewater influent is a complex matrix with loads of different compounds which reduces in both concentrations and amount during the treatment steps. Once the effluent wastewater is discharged into recipient surface water systems the concentrations will decrease even more due to different degradation pathways and dilution effect (Petrie et al., 2015; Wallberg et al., 2016).

It is difficult to explain the occurrence of some studied compounds at different concentration levels in a particular river compared to another. Low concentrations in the surface waters can also depend on the catchment area, amount of WWTP discharges, the treatment steps at the WWTPs, temperature and pH of the sampled water, water flow rate in the different rivers, etc. (Petrie et al., 2015). This can especially be seen in sample LIII_R3 which is the recipient of WWTP of 105 000 PE, hospital waste and a catchment area which included industries and agricultural land. Higher concentrations of pharmaceuticals such as antibiotics are expected due to the hospital waste, industrial chemicals due to the industries and pesticides such as BAM (2,6-dichlorobenzamide) due to the agricultural run-offs. BAM is a metabolite of the substance Dichlobenil, which usage is banned in the European Union countries but due to the compound's persistency, is still frequently found in countries like Sweden, Finland and Denmark (Barbosa et al., 2016; Pukkila and Kontro, 2014; Whalley et al., 2018). Nevertheless, some cases are harder to trace back to the sources, as in the case with sample LI_R5, sampled from river Ösan, where the concentrations of OMPs where much higher as compared to the other rivers connected to Vänern. This river is the recipient of WWTP containing hospital waste which would explain the higher concentrations of both pharmaceuticals and personal care products such as Sulisobenzone and Oxybenzone but not the relatively high concentrations of industrial chemicals such as Tris(2-butoxylethyl) phosphate and Sucralose. Tris(2-butoxylethyl) phosphate is commonly used in plastics, floor finishes, waxes etc. and highly soluble in water (PubChem, n.d.) and the high concentrations may indicate discharges directly into the river.

The sample from river LIII_R3 is by far the most contaminated sample in this study. This sampling site locates in Enköping river and it is close to the WWTP discharge which possibly affects the found concentration levels. High concentrations of antidepressants such as Amitriptyline and Norsertaline and antibiotics such as Chlorampenicol (commonly used for treatment of numerous bacterial infections) were found in this sample. This indicates a higher consumption of these substances and the possible presence of hospital waste in the WWTP

effluent or the occurrence of a hospital discharge in the nearby area. A hospital is in fact located in the nearby area of this sampling point and therefore it's reasonable to assume that hospital waste also reaches the WWTP. The sample site is also close to the wastewater discharge, a small marina, a city with industries, roads and agricultural land area which could affect the mixture of compounds. Thus, higher concentration levels in this sample is reasonable. Industrial chemicals in this study also includes compounds such as Di-(2-ethylhexyl) phosphoric acid which is commonly used in corrosion inhibitors. This could explain why industrial chemicals like this one is found in samples from sites close to marinas.

This study shows a clear difference in concentrations between the three lakes. A previous study have shown Mälaren lake to be the most polluted (Rehrl et al., 2020) and based on the results of this study, this can be confirmed. The results suggest that Enköping river has the highest total OMP concentration with 79 µg/L and Lövsta river are the second most polluted one with 33 µg/L. These two are connected to lake Mälaren and are more polluted than any of the other Mälaren rivers which has relatively low total OMP concentrations. Ösan (16 µg/L) and Lillån (13 µg/L) are the most polluted rivers connected to lake Vänern and Vättern. These results make Enköping river, Lövsta river, Ösan and Lillån hot spots for OMPs in this study. Lillån and Lövsta river were relatively small as compared to Ösan and Enköping rivers suggesting that water flow rate has an impact on the concentration levels. The four rivers are all recipients of WWTP effluents which could be seen as a confirmation of the impact wastewater discharges has on the concentration levels.

Since OMPs and some hormones could be detected in the surface water it is clear that some compounds are more persistent to the wastewater treatment than others. It is also obvious that the OMPs and hormones does not occur separately in the samples, but in a complex mixture of at least 121 different compounds. Since modern technology are not yet able to detect and identify all compounds that occur in environmental waters, it is not possible to know for certain, which effects these compounds pose to humans, aquatic organisms or others. Resulting effects and risks on the aquatic environment may be known when compounds are found individually but, as previously told, when found in various mixtures the risks and effects are very complex.

The resulting effects and risks on the aquatic environment may be known for individually occurring compounds (Barbosa et al., 2016; Wallberg et al., 2016; Whalley et al., 2018). In reality the compounds occur in various mixtures which makes the risks and effects very complex to foresee and calculate. Extended research on relevant compounds and their toxicity has to be made in order to assess the actual and true effects. In fact 95-99 % of all occurring effects comes from these unknown substances (Lundqvist and Oskarsson, 2020) indicating more advanced treatment processes and methods for detection is needed (Wallberg et al., 2016).

The risk assessment for drinking water samples were calculated for only two compounds, Carbamazepine and Bezafibrate. These two compounds were selected based on available toxicity data and their detected concentrations in the analysed drinking water. Only Carbamazepine showed a BQ (1.47) that implies a potential risk to human health when exposed to the compound in this concentration during a lifetime. Sources of error exists since not every human weigh 60 kg and drinks 2 L of drinking water every day, but those assumptions were made in order to calculate the BQ value. In this study, only one compound implied a risk to human health, therefore it can only be seen as an potential indicator of the problems that OMPs and hormones causes when present in the environmental waters. Couto et al. (2019) came to

similar conclusions regarding Carbamazepine in drinking water. Carbamazepine is listed as a high priority compound in the Global Water Research Coalition (GWRC) due to its physical-chemical properties that makes it very persistent to treatment among others (KIWA Water Research et al., 2008).

6 Conclusions

This study shows a clear decrease in concentration levels of OMPs and hormones in samples from the five different matrices. Highest concentrations could be found in wastewater influent and the lowest could be found in the drinking water.

A risk assessment regarding human health issues derived from drinking tap water showed that only carbamazepine poses a threat to human health. Carbamazepine had a BQ of 1.47 indicating that when exposed to these levels for a period of a lifetime, human health may be negatively affected.

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Appendix A – List of compounds

Compounds selected for analysis, their respective category and type are listed in Table A1.

Table A1: List of compounds selected for analysis.

Compound	Category	Type
2,2'-Dimorpholinyldiethyl-ether	Industrial chemical	
3-(4-Methylbenzylidene)camphor	Personal care product	
4-Chloro-2-isopropyl-5-methylphenol	Industrial chemical	
4-Chloro-3-methylphenol	Industrial chemical	
Aceclofenac	Pharmaceutical	NSAID (nonsteroidal anti-inflammatory drug)
Acetaminophen (Paracetamol)	Pharmaceutical	Analgesics (painkiller)
Albuterol (Salbutamol)	Pharmaceutical	Beta blocker
Amitriptyline	Pharmaceutical	Antidepressant
Amoxicillin *	Pharmaceutical	Antibiotic
Atenolol	Pharmaceutical	Beta blocker
Atorvastatin	Pharmaceutical	Antilipidemic Agents
Azithromycin *	Pharmaceutical	Antibiotic
BAM (Dichlorobenzamide)	Pesticide	Metabolite of dichlobenil
Bezafibrate	Pharmaceutical	Antilipemic drug
Bicalutamide	Pharmaceutical	
Bisoprolol	Pharmaceutical	Beta blocker
Caffeine	Stimulant	
Carazolol	Pharmaceutical	
Carbamazepine	Pharmaceutical	Antiepileptic
Cetirizine	Pharmaceutical	Antihistamine
Chloramphenicol	Pharmaceutical	Antibiotic
Chlorzoxazone	Pharmaceutical	
Ciprofloxacin *,**	Pharmaceutical	Antibiotic
Citalopram	Pharmaceutical	Antidepressant
Clarithromycin *	Pharmaceutical	Antibiotic
Climbazole	Pharmaceutical	Antifungal
Clindamycin	Pharmaceutical	Antibiotic
Clozapine	Pharmaceutical	Antipsychotic
Codeine	Pharmaceutical	Opiates, opioids and metabolites
Daidzein	Isoflavone	
DEET (diethyltoluamide)	Pesticide	Insect repellent

Compound	Category	Type
Desvenlafaxine	Pharmaceutical	Antidepressant
Di-(2-ethylhexyl)phosphoric acid	Industrial chemical	
Diazepam	Pharmaceutical	Sedative
Diclofenac *,**	Pharmaceutical	NSAID (nonsteroidal anti-inflammatory drug)
Diltiazem	Pharmaceutical	Antihypertensive
Erytromycin *	Pharmaceutical	Antibiotic
Ethylparaben	Paraben	Antifungal preservative
Fexofenadine	Pharmaceutical	Antihistamine
Fluconazole	Pharmaceutical	Antifungal
Fluoxetine	Pharmaceutical	Antidepressant
FOSA (perfluorooctane sulfonamide)	PFAS	
Furosemide	Pharmaceutical	Diuretics
Gemfibrozil	Pharmaceutical	Antilipidemic Agents
Hydrochlorothiazide	Pharmaceutical	Diuretics
Ibuprofen	Pharmaceutical	NSAID (nonsteroidal anti-inflammatory drug)
Ifosfamide	Pharmaceutical	Anticancer
Irbesartan	Pharmaceutical	Antihypertensive
Lamotrigine	Pharmaceutical	Antiepileptic
Laurilsulfate	Personal care product	
Lidocaine	Pharmaceutical	Anesthetic
Loperamide	Pharmaceutical	
Losartan	Pharmaceutical	Antihypertensive
Meclofenamic acid	Pharmaceutical	NSAID (nonsteroidal anti-inflammatory drug)
Mefenamic Acid	Pharmaceutical	NSAID (nonsteroidal anti-inflammatory drug)
Memantine	Pharmaceutical	
Metformin	Pharmaceutical	Antidiabetic
Methylparaben	Paraben	Antifungal preservative
Metoprolol	Pharmaceutical	Beta blocker
Metronidazole	Pharmaceutical	Antibiotic
Mirtazapine	Pharmaceutical	Antidepressant
Nicotine	Stimulant	
Norsertraline	Pharmaceutical	Antidepressant
Omeprazole	Pharmaceutical	Antisecretory Agent

Compound	Category	Type
Oxazepam	Pharmaceutical	Sedative
Oxybenzone (Benzophenone-3)	Personal care product	UV filter
Oxycodone	Pharmaceutical	Opiates, opioids and metabolites
Panthenol	Pharmaceutical	
Paroxetine	Pharmaceutical	Antidepressant
PFBA (perfluorobutanoic acid)	PFAS	
PFBS (perfluorobutanesulfonic acid)	PFAS	
PFDA (perfluorodecanoic acid)	PFAS	
PFDoDA (perfluorododecanoic acid)	PFAS	
PFHpA (perfluoroheptanoic acid)	PFAS	
PFHxA (perfluorohexanoic acid)	PFAS	
PFHxS (perfluorohexanesulfonic acid)	PFAS	
PFNA (perfluorononanoic acid)	PFAS	
PFOA (perfluorooctanoic acid)	PFAS	
PFOS (perfluorooctanesulfonic acid)	PFAS	
PFPeA (perfluoropentanoic acid)	PFAS	
PFTeDA (perfluorotetradecanoic acid)	PFAS	
PFUnDA (perfluoroundecanoic acid)	PFAS	
Primidone	Pharmaceutical	Antiepileptic
Propranolol	Pharmaceutical	Beta blocker
Propylparaben	Paraben	Antifungal preservative
Pyrimethamine	Pharmaceutical	
Ramipril	Pharmaceutical	
Ranitidine	Pharmaceutical	Antisecretory Agent
Ricinoleic acid	Pharmaceutical	
Roxithromycin	Pharmaceutical	Antibiotic
Salicylic acid	Pharmaceutical	NSAID (nonsteroidal anti-inflammatory drug)
Sertraline	Pharmaceutical	Antidepressant
Simvastatin	Pharmaceutical	Antilipidemic Agents
Sotalol	Pharmaceutical	Beta blocker
Sucralose	Artificial sweetener	
Sulfamethoxazole	Pharmaceutical	Antibiotic
Sulisobenzone	Personal care product	
Tamoxifen	Pharmaceutical	

Compound	Category	Type
Terbutaline	Pharmaceutical	
Thiabendazole	Pharmaceutical	
Tolytriazole	Pharmaceutical	
Tramadol	Pharmaceutical	Analgesics (painkiller)
Tributyl citrate acetate	Industrial chemical	
Triisopropanolamine	Industrial chemical	
Trimethoprim	Pharmaceutical	Antibiotic
Tris(2-butoxylethyl) phosphate	Industrial chemical	
Valproic acid	Pharmaceutical	Antiepileptic
Valsartan	Pharmaceutical	Antihypertensive
Venlafaxine	Pharmaceutical	Antidepressant
17-Alpha-ethinylestradiol (EE2) *, **	Hormone	
17-Beta-estradiol (E2) *, **	Hormone	
Estrone (E1)	Hormone	
Estradiol *	Hormone	
Etinylestradiol *	Hormone	
Dienogest	Hormone	
Dihydrotestosterone	Hormone	
Gestodene	Hormone	
Norethindrone	Hormone	
Norgestrel	Hormone	
Progesterone	Hormone	
Testosterone	Hormone	

***Watch list EU (WFD)**

**** CEC – Contaminants of emerging concern (from WFD)**

Appendix B – Surface water samples

All surface water samples are listed with extraction code, sampling site and extraction code in Table B1.

Table B1: List of all sampled surface water in rivers and their extraction codes.

Lake	Extraction code	Sampling site
Vänern	LI_R1	Klarälven Almar
	LI_R2	Klarälven Skoghall, bron vid kemiska fabriken
	LI_R3	Klarälven Karlstad
	LI_R4	Tidan, Stadkvarnen i Mariestad
	LI_R5	Ösan, bron vid Asketorp
	LI_R6	Göta älv Vargön
Vättern	LII_R1	Lillån Bankeryd, outlet Vättern
	LII_R2	Munksjöns outlet
	LII_R3	Huskvarnaån
	LII_R4	Motala ström
Mälaren	LIII_R1	Fyrisån Flottsund
	LIII_R2	Örsundaån
	LIII_R3	Enköpingsån
	LIII_R4	Sagån
	LIII_R5	Svartån Västerås, Turbinbron
	LIII_R6	Kolbäcksån, Strömsholm
	LIII_R7	Hedströmmen
	LIII_R8	Arbogaån Kungsör
	LIII_R9	Eskilstunsån
	LIII_R10	Norrström (outlet)
	LIII_R11	Oxundnaån
	LIII_R12	Märstaån outlet
	LIII_R13	Lövstaån

Appendix C – Frequency of detection

The frequencies of detection (FDs) were calculated for all compounds in every matrix and are listed in Table C1.

Table C1: Calculated frequencies of detection for all analysed compounds in the five different matrices. No percentage indicates that the compound was not detected,

Compound	WW IN	WW OUT	Rivers	Lakes	DW
17α-Estradiol		100%	96%	100%	33%
17α-Ethynylestradiol	100%	100%	100%	100%	17%
2,2'-Dimorpholinyldiethyl-ether	90%	95%			
3-(4-Methylbenzylidene)camphor					
4-Chloro-2-isopropyl-5-methylphenol			13%		
4-Chloro-3-methylphenol	57%		9%		
Aceclofenac					
Acetaminophen	100%	95%			
Albuterol (Salbutamol)	100%	100%			
Amitriptyline	100%	100%			
Amoxicillin					
Atenolol	100%	100%	87%		
Atorvastatin (Lipitor)	100%	95%	61%		
Azithromycin	100%	100%	61%		
BAM (Dichlorobenzamide)	100%	100%	100%	95%	97%
Bezafibrate	95%	100%	78%		
Bicalutamide	100%	100%	100%	100%	79%
Bisoprolol	100%	100%	83%		
Caffeine	100%	100%	100%	100%	88%
Carazolol	76%	24%	26%	19%	9%
Carbamazepine	100%	100%	100%	100%	94%
Cetirizine	100%	100%	96%	100%	74%
Chloramphenicol	10%	19%	61%		3%
Chlorzoxazone	100%	100%	52%		
Ciprofloxacin					
Citalopram	100%	100%	91%		
Clarithromycin	95%	100%	70%		
Climbazole	100%	100%	74%		
Clindamycin	100%	100%	87%	62%	
Clozapine	95%	100%	65%		
Codeine	100%	100%	91%		
Daidzein	100%	81%			
DEET	100%	100%	100%	100%	97%
Desvenlafaxine	100%	100%	100%	100%	97%
Di-(2-ethylhexyl)phosphoric acid	100%	90%	57%		
Diazepam	86%	95%	52%		
Diclofenac	100%	100%	96%		
Dienogest	67%	100%	4%		
Dihydrotestosterone	100%	67%	100%	100%	

Compound	WW IN	WW OUT	Rivers	Lakes	DW
Diltiazem	100%	100%	61%		
Erythromycin	100%	100%	83%		
Estriol			4%		
Estrone		67%	43%	57%	
Ethylparaben	57%		13%		
Etonogestrel	33%	100%	30%		
Fexofenadine	100%	100%	100%	95%	53%
Fluconazole	100%	100%	96%	95%	97%
Fluoxetine	24%	29%	9%		
FOSA			4%	14%	
Furosemide	100%	100%	83%		
Gemfibrozil	76%	52%			
Gestodene	100%	100%	91%	52%	
Hydrochlorothiazide (HCTZ)	100%	100%	96%		
Ibuprofen	100%	81%	61%		
Ifosfamide	14%	29%	74%	38%	18%
Irbesartan	100%	100%	70%		
Lamotrigine	100%	100%	91%	100%	91%
Laurilsulfate	95%	100%	87%	100%	97%
Lidocaine	100%	100%	91%	100%	68%
Loperamide	95%	100%			
Losartan	100%	100%	87%		
Meclofenamic acid	14%	10%	22%		9%
Mefenamic acid	100%	100%	100%	100%	97%
Memantine	100%	100%	78%		
Metformin	100%	100%	91%	90%	82%
Methylparaben	67%		87%		
Metoprolol	100%	100%	91%	100%	
Metronidazole			76%		
Mirtazapine	100%	100%	96%		
Nicotine	100%	100%	100%	95%	62%
Norethindrone	33%		4%		
Norgestrel	100%		22%	14%	
Norsertraline	100%	100%	96%	100%	76%
Omeprazole	100%	100%	78%		
Oxazepam	100%	100%	87%	90%	
Oxybenzone (Benzophenone-3)	100%	95%	78%	81%	85%
Oxycodone	100%	100%	52%		
Panthenol	95%	67%	74%		
Paroxetine		5%	30%		
PFBS	100%	100%	48%	100%	83%
PFDA			48%		
PFDoDA					
PFHpA	67%	100%	83%	62%	83%
PFHxA	100%	100%	96%	71%	33%

Compound	WW IN	WW OUT	Rivers	Lakes	DW
PFHxS	67%	100%	87%	95%	83%
PFNA	33%	67%	96%	67%	67%
PFOA	100%	100%	96%	100%	100%
PFOS_linear	33%	100%	52%	95%	100%
PFPeA					
PFTeDA					
PFUnDA					17%
Primidone	71%	81%	61%		
Progesterone	100%		4%		
Propranolol	100%	100%	91%		
Propylparaben	95%	81%	70%	57%	50%
Pyrimethamine		5%	26%		9%
Ramipril	100%	100%	74%		
Ranitidine	100%	100%	57%		
Ricinoleic acid	62%	5%			
Roxithromycin	19%	38%	13%		
Salicylic acid	100%	100%	83%		
Sertraline	100%	100%			
Simvastatin			39%		
Sotalol	90%	100%	61%		
Sucralose	100%	100%	100%	57%	62%
Sulfamethoxazole	100%	100%	65%	81%	
Sulisobenzone	100%	100%	96%	76%	
Tamoxifen					
Terbutaline	100%	90%			
Testosterone	100%	100%	9%	14%	
Thiabendazole	67%	100%			
Tolytriazole	100%	100%	83%	90%	74%
Tramadol	100%	100%	78%	90%	
Tributyl citrate acetate	100%	100%	100%	100%	97%
Triisopropanolamine	100%	100%	96%	100%	97%
Trimethoprim	100%	100%	87%		
Tris(2-butoxylethyl) phosphate	100%	100%	100%	81%	
Valproic acid	100%	71%	65%	100%	71%
Valsartan	100%	100%	91%		
Venlafaxine	100%	100%	83%		
β-Estradiol		33%	91%	100%	

Appendix D – Parameters for method performance

Table D1: Parameters for method performance for OMPs.

		Average LOQs, [ng/L]							
	Linearity R	**River**	**Drinking water**	**Lake**	**Wastewater influent**	**Wastewater effluent**	**Average absolute recovery_River**	**Average ME_River**	**STD**
Albuterol (Salbutamol)	0.9987	0.051	0.035	0.034	0.12	0.078	132%	-23%	1%
Atenolol	0.9984	0.19	0.22	0.21	0.75	0.49	8%	-91%	79%
Sotalol	0.9977	0.032	0.038	0.036	0.13	0.083	127%	60%	28%
Hydrochlorothiazide (HCTZ)	0.9986	0.29	0.56	0.54	1.9	1.2	69%	206%	15%
Nicotine	0.9997	0.052	0.025	0.024	0.084	0.055	105%	-53%	28%
Metoprolol	0.9995	0.21	0.07	0.067	0.24	0.16	97%	-45%	18%
Atovastatin (Lipitor)	0.9974	0.086	0.015	0.016	0.057	0.037	17%	-80%	1%
Carbamazepine	0.9959	0.073	0.019	0.02	0.07	0.045	100%	-58%	54%
Cetirizine	0.9978	0.028	0.016	0.017	0.058	0.037	115%	-31%	0%
Citalopram	0.9993	0.44	0.11	0.12	0.41	0.26	92%	-73%	19%
Mirtazapine	0.9994	0.053	0.018	0.02	0.069	0.044	98%	-63%	5%
Oxazepam	0.9995	0.13	0.017	0.018	0.062	0.04	110%	-82%	6%
Paroxetine	0.9996	0.16	0.078	0.084	0.29	0.19	39%	-51%	10%
Lamotrigine	0.9965	1.1	0.11	0.11	0.4	0.26	76%	-72%	89%
Metformin	0.9958	0.063	0.059	0.063	0.22	0.14	6%	-14%	66%
Valproic acid	0.9995	5.1	1.8	1.9	6.7	4.3	114%	-58%	0%
Oxybenzone (Benzophenone-3)	0.9999	0.22	0.17	0.18	0.62	0.4	28%	-38%	27%
Oxycodone	0.9996	0.043	0.021	0.022	0.077	0.049	120%	-9%	92%
Primidone	0.9996	2.9	1.7	1.8	6.1	4	95%	-38%	23%
Simvastatin	0.9989	0.72	0.77	0.82	2.8	1.8	48%	-98%	60%
DEET	0.9997	0.083	0.074	0.082	0.25	0.18	113%	-22%	5%
BAM (Dichlorobenzamide)	0.9977	0.8	0.81	0.89	2.7	1.9	46%	-88%	23%
Bezafibrate	0.9989	0.33	0.14	0.15	0.48	0.34	136%	-72%	9%
Bicalutamide	0.9998	0.018	0.021	0.023	0.062	0.045	101%	-6%	26%
Bisoprolol	0.9989	0.046	0.026	0.029	0.077	0.056	113%	-54%	13%

	Linearity R	Average LOQs, [ng/L]					Average absolute recovery_River	Average ME_River	STD
		River	Drinking water	Lake	Wastewater influent	Wastewater effluent			
Clarithromycin	0.9983	0.025	0.024	0.026	0.071	0.051	70%	-32%	29%
Climbazole	0.9964	0.059	0.031	0.034	0.091	0.066	107%	-59%	7%
Clindamycin	0.9999	0.036	0.019	0.02	0.055	0.04	99%	-60%	21%
Clozapine	0.9951	0.074	0.026	0.029	0.077	0.056	81%	-72%	0%
Diazepam	0.9922	0.096	0.025	0.027	0.072	0.052	111%	-78%	11%
Fexofenadine	0.9993	0.054	0.022	0.024	0.065	0.047	104%	-66%	19%
Loperamide	1.0000	0.03	0.019	0.02	0.055	0.04	37%	-57%	70%
Memantine	0.9995	0.28	0.47	0.51	1.4	1	106%	41%	18%
Propranolol	0.9998	0.042	0.02	0.021	0.058	0.042	100%	-67%	10%
Caffeine	0.9997	0.71	0.28	0.31	1.1	0.77	100%	-63%	23%
Ranitidine	0.9994	6.5	3.8	4.3	15	11	36%	27%	35%
Chloramphenicol	0.9996	2.4	0.13	0.14	0.81	0.39	112%	-76%	14%
Tramadol	0.9992	0.79	0.092	0.098	0.57	0.28	81%	-20%	72%
Valsartan	0.9990	0.24	0.19	0.2	1.1	0.55	119%	-34%	24%
Codeine	0.9998	0.76	0.11	0.11	0.66	0.32	111%	-82%	15%
Fluconazole	0.9995	0.21	0.045	0.048	0.28	0.13	106%	-75%	14%
Lidocaine	0.9990	0.32	0.017	0.019	0.11	0.052	103%	-49%	18%
Diclofenac	0.9993	0.76	0.46	0.45	1.4	0.88	92%	10%	48%
Aceclofenac	0.9558	NA	420	410	1200	800	NA	NA	NA
Mefenamic acid	0.9994	0.14	0.051	0.05	0.15	0.097	107%	-58%	21%
Meclofenamic acid	0.9996	1.5	0.53	0.52	1.6	1	98%	-61%	33%
Ibuprofen	0.9999	12	6.7	6.5	15	12	102%	-49%	17%
Ethylparaben	1.0000	0.13	0.13	0.14	0.43	0.28	114%	-99%	3%
Propylparaben	0.9999	0.24	0.033	0.035	0.1	0.068	108%	-86%	27%
Methylparaben	1.0000	0.14	0.056	0.06	0.18	0.12	111%	-50%	24%
Furosemide	1.0000	4.2	0.53	0.6	1.2	1.1	65%	-89%	17%
Gemfibrozil	0.9998	0.25	0.36	0.3	0.58	0.54	119%	-98%	32%
Diltiazem	0.9980	0.097	0.05	0.042	0.081	0.075	94%	-74%	8%

	Linearity R	Average LOQs, [ng/L]					Average absolute recovery_River	Average ME_River	STD
		River	Drinking water	Lake	Wastewater influent	Wastewater effluent			
Tamoxifen	0.9998	4.5	0.19	0.16	0.31	0.29	3%	-98%	12%
Losartan	0.0018	0.18	0.053	0.066	0.2	0.14	80%	-64%	87%
Omeprazole	0.9965	0.04	0.017	0.021	0.064	0.045	86%	-73%	17%
Acetaminophen	0.9982	2	1.4	1.5	4	2.3	47%	-45%	9%
Metronidazole	0.9839	3.9	1.8	1.8	4.9	2.8	40%	-77%	1%
Sulfamethoxazole	0.9976	0.17	0.06	0.067	0.37	0.2	131%	-75%	0%
Trimethoprim	0.9955	0.21	0.023	0.025	0.14	0.076	107%	-90%	18%
Amitriptyline	0.9978	2.2	0.52	0.58	0.6	0.52	68%	-60%	55%
Norsertraline	0.9977	20	1300	20	20	20	32%	-80%	25%
Sertraline	0.9989	1.7	0.49	0.55	0.57	0.5	32%	-65%	33%
Venlafaxine	0.9992	0.96	0.66	0.69	5.1	2	93%	-39%	55%
Desvenlafaxine	0.9997	0.035	0.022	0.023	0.17	0.067	99%	-43%	37%
Erythromycin	0.9989	0.58	0.017	0.019	0.1	0.057	85%	-37%	39%
Amoxicillin	NA	NA	NA	NA	NA	NA	NA	NA	NA
Azithromycin	0.9976	0.19	0.014	0.016	0.085	0.047	54%	-11%	38%
Ciprofloxacin	0.9779	5.7	0.014	0.016	0.086	0.047	17%	89%	141%
Roxithromycin	0.9996	0.2	0.008	0.009	0.049	0.027	58%	-16%	8%
Triisopropanolamine	1.0000	0.047	0.055	0.059	0.19	0.13	39%	-10%	95%
Tributyl citrate acetate	0.9999	0.13	0.11	0.12	0.37	0.27	44%	-34%	25%
Terbutaline	0.9868	0.053	0.086	0.092	0.3	0.21	155%	11%	4%
Pyrimethamine	0.9972	0.086	0.019	0.02	0.064	0.045	106%	-83%	15%
Sulisobenzone	0.9997	0.36	0.14	0.15	0.49	0.35	96%	-51%	88%
2,2'-Dimorpholinyldiethyl-ether	0.9999	2.7	1.1	1.2	3.8	2.7	96%	-84%	10%
Tolytriazole	0.9998	3.3	0.33	0.36	1.2	0.82	4%	-23%	141%
Ifosfamide	0.9990	0.25	0.05	0.054	0.17	0.12	123%	-85%	25%
Laurilsulfate	0.9989	13	9.7	10	33	24	114%	91%	44%
Chlorzoxazone	0.9999	0.12	1.5	1.6	5.1	3.6	108%	531%	18%
Panthenol	0.9991	0.3	0.11	0.12	0.38	0.27	4%	-65%	19%

	Linearity R	Average LOQs, [ng/L]					Average absolute recovery_River	Average ME_River	STD
		River	Drinking water	Lake	Wastewater influent	Wastewater effluent			
Ricinoleic acid	0.9999	54	7.6	8.2	26	19	61%	-87%	84%
Sucralose	0.9994	5.8	4.7	5	16	12	47%	289%	136%
Salicylic acid	0.9994	1.1	1.4	1.5	4.7	3.3	4%	-23%	30%
Thiabendazole	0.9922	0.54	0.078	0.083	0.27	0.19	111%	-87%	22%
4-Chloro-3-methylphenol	0.9996	3.7	5.7	6.1	20	14	102%	30%	33%
Ramipril	0.9995	0.038	0.042	0.045	0.14	0.1	126%	-23%	18%
Daidzein	0.9863	1	0.092	0.099	0.32	0.23	119%	-91%	9%
Carazolol	0.9972	0.25	0.017	0.018	0.057	0.041	82%	-95%	11%
Di-(2-ethylhexyl)phosphoric acid	0.9999	0.68	0.72	0.78	2.5	1.8	93%	-16%	29%
4-Chloro-2-isopropyl-5-methylphenol	0.9998	2	1.3	1.4	4.4	3.1	50%	-54%	11%
Tris(2-butoxylethyl) phosphate	0.9990	0.17	0.097	0.1	0.34	0.24	48%	22%	84%
3-(4-Methylbenzylidene)camphor	0.9999	NA	1.6	1.7	5.4	3.9	NA	NA	NA
Fluoxetine	0.9996	9	4.3	4	7.3	5.3	47%	-67%	28%
FOSA	0.9958	0.1	0.095	0.082	0.1	0.14	63%	-14%	13%
PFBS	0.9787	0.5	0.092	0.091	0.23	0.2	129%	-6%	25%
PFHxA	0.96	0.41	0.065	0.064	0.16	0.14	106%	-23%	19%
PFDA	0.9812	0.23	0.13	0.096	0.24	0.21	102%	-10%	22%
PFDoDA	0.9922	3.8	5.9	2.9	3.5	5	56%	-6%	30%
PFOS	0.9859	0.56	0.18	0.15	0.35	0.35	112%	-2%	16%
PFHpA	0.9766	0.4	0.092	0.075	0.18	0.18	125%	-22%	18%
PFNA	0.9852	0.19	0.076	0.062	0.16	0.14	117%	-12%	22%
PFPeA	0.9761	0.62	0.11	0.1	0.26	0.24	41%	-45%	29%
PFOA	0.9823	0.31	0.099	0.091	0.24	0.22	118%	-12%	21%
PFHxS	0.9785	0.18	0.044	0.039	0.1	0.09	127%	-4%	29%
PFUnDA	0.9873	1.5	1.8	0.87	1.7	2	84%	-4%	28%
PFTeDA	0.997	0.43	0.42	0.21	0.41	0.49	24%	-43%	17%
17α-Ethynylestradiol	0.9999	0.79	0.87	0.79	0.87	0.87	110%	−19%	1%
17α-Estradiol	0.9995	0.19	0.75	0.19	0.75	0.75	115%	157%	0%

		Average LOQs, ng/L							
	Linearity R	**River**	**Drinking water**	**Lake**	**Wastewater influent**	**Wastewater effluent**	**Average absolute recovery_River**	**Average ME_River**	**STD**
β-Estradiol	0.9998	0.46	0.97	0.46	0.97	0.97	118%	35%	1%
Estriol	0.9991	0.54	0.51	0.54	0.51	0.51	116%	−24%	3%
Estrone	0.9996	0.47	1.26	0.47	1.26	1.26	119%	97%	1%
Etonogestrel	0.9947	0.24	0.15	0.24	0.15	0.15	117%	−50%	6%
Dienogest	0.9919	0.21	1.2	0.21	1.7	1.7	128%	−65%	6%
Gestodene	0.9943	0.23	1.6	0.23	2.1	2.1	126%	−57%	5%
Norethindrone	0.9944	0.59	4.6	0.59	6.2	6.2	126%	−54%	5%
Norgestrel	0.9965	2	16	2	21	21	109%	−56%	7%
Progesterone	0.9966	0.18	1.4	0.18	1.9	1.9	95%	−54%	3%
Dihydrotestosterone	0.9969	17	10	17	13	13	140%	75%	1%
Testosterone	0.9953	0.07	0.47	0.07	0.62	0.62	113%	−56%	0%

Appendix E – Occurrence of OMPs in different water matrices from previous studies

Table E1: Organic micropollutants found in different water matrices in previous studies from Sweden and Europe.

Organic micropollutant	Category	Wastewater (ng/L)				Recipient of WW (ng/L)	Surface water (ng/L)		Drinking water (ng/L)	
		Sweden		Europe		Sweden	Sweden	Europe	Sweden	
		Influent	Effluent	Influent	Effluent				Raw	Treated
17-α-ethinylestradiol (EE2) *, **	Hormone			1 a	0,20-1,3 a	-	-	0,5-230 h		
17-β-estradiol (E2) *, **	Hormone			20 a	0,4-1,3 a	-	-	0,3-147 h		
2,2'-Dimorpholinyldiethyl-ether	Industrial chemical					-	-			
3-(4-Methylbenzylidene)camphor	Personal care product					-	-			
4-Chloro-2-isopropyl-5-methylphenol	Industrial chemical					-	-			
4-Chloro-3-methylphenol	Industrial chemical					-	-			
Aceclofenac	Pharmaceutical					-	-			
Acetaminophen (Paracetamol)	Pharmaceutical	21000-250000e	<100-<400e	6924-492340 a	<20-11733 a	55b	-	<1,5-1388a	≤6 e	≤2 e
Albuterol (Salbutamol)	Pharmaceutical					5b	-			
Amitriptyline	Pharmaceutical	15b	9.4b	106-2092 a	66-207 a	<5-18b	-	< 0,5-30a		
Amoxicillin *	Pharmaceutical			<87 g	31 g	35b	-	<2,5-245a		
Atenolol	Pharmaceutical	1600-43000e	270-65000e	12913-14223 a	2123-2870 a	170b	≤390c	<1-487a	≤7 e	≤3 e
Atorvastatin	Pharmaceutical	280b	45b			<50b	<50c	< 50a		
Azithromycin *	Pharmaceutical	14b	12b			<5b	≤27c	< 5.0-27a		

Organic micropollutant	Category	Wastewater (ng/L)				Recipient of WW (ng/L)	Surface water (ng/L)		Drinking water (ng/L)	
		Sweden		Europe		Sweden	Sweden	Europe	Sweden	
		Influent	Effluent	Influent	Effluent				Raw	Treated
BAM (Dichlorobenzamide)	Pesticide					22b	-			
Bezafibrate	Pharmaceutical		200b	420-971 a	117-418 a	14b		<10-60a		
Bicalutamide	Pharmaceutical					60b	-			
Bisoprolol	Pharmaceutical	200b	100b			40b	≤150c	<0.1-100a		
Caffeine	Stimulant			9902-25138 a	1744-2048 a	450b		163-743a	≤41 e	NC e
Carazolol	Pharmaceutical					<1.1b	-			
Carbamazepine	Pharmaceutical	890b	390b	950-2593 a	826-3117c	280b	4,9-760b	<0.5-251a	2 e	≤3 e
Cetirizine	Pharmaceutical					60b	-		≤1 e	≤1 e
Chloramphenicol	Pharmaceutical			<4-248 a	<6-21 a	<6.1b		<10a		
Chlorzoxazone	Pharmaceutical					3.4b	-			
Ciprofloxacin *,**	Pharmaceutical	90b	18b			65d	≤380c	<10-230a		
Citalopram	Pharmaceutical	23-290e	79-540e			80d	6,6-210c	6.6-190a		
Clarithromycin *	Pharmaceutical	260b	110b	40,1-54,4 g	NC g	80d	≤1100c	<1.0-330a		
Climbazole	Pharmaceutical					12b	-			
Clindamycin	Pharmaceutical	100b	140b			45d	≤140c	<1.0-87a		
Clozapine	Pharmaceutical					14b	-		≤0,4 e	NC e

Organic micropollutant	Category	Wastewater (ng/L)				Recipient of WW (ng/L)	Surface water (ng/L)		Drinking water (ng/L)	
		Sweden		Europe		Sweden	Sweden	Europe	Sweden	
		Influent	Effluent	Influent	Effluent				Raw	Treated
Codeine	Pharmaceutical	1240b	360b	1088-10321 a	372-5271 a	90d	≤340c	<1,5-347a		
Daidzein	Isoflavone					4.7b	-			
DEET (diethyltoluamide)	Pesticide					55b	-			
Desvenlafaxine	Pharmaceutical			5 g	4 g	-	-			
Di-(2-ethylhexyl)phosphoric acid	Industrial chemical					-	-			
Diazepam	Pharmaceutical			<0.9-7.6 a	1.6-5.1 a	<5b		0.6-0.9a		
Diclofenac *,**	Pharmaceutical	320-2700e	340-2500e	69-1500 a	58-599 a	230d	≤880c	<0.5-154 a	≤0,8 e	NC e
Diltiazem	Pharmaceutical	80b	40b	770-1559 a	95-357 a	8d	≤20c	<1-17a		
Erythromycin *	Pharmaceutical	85-480e	170-390e	71-2530 a	109-1385 a	<50d	≤65c	<0.5-159a	≤0,5 e	NC e
Estradiol *	Hormone	<10b	<5-13 f			<10d	<10c	<10a		
Estrone (E1)	Hormone			49 a	4,3-12 a	-		0,3-147 h	≤0,1 e	NC e
Ethylparaben	Paraben			589-2002 a	4-50 a	<0.057b		1,0-13a		
Etinylestradiol *	Hormone	<10b	<10b	2,5 g	NC g	<10d	<10c	<10a		
Fexofenadine	Pharmaceutical	290b	170b			50d	≤150c	<5.0-66a		
Fluconazole	Pharmaceutical	680b	400b			75d	1,8-290c	1.8-110a		
Fluoxetine	Pharmaceutical	50b	29b	14-86 a	16-29 a	<5d	≤32c	5,8-14a		

Organic micropollutant	Category	Wastewater (ng/L)				Recipient of WW (ng/L)	Surface water (ng/L)		Drinking water (ng/L)	
		Sweden		Europe		Sweden	Sweden	Europe	Sweden	
		Influent	Effluent	Influent	Effluent				Raw	Treated
FOSA (perfluorooctane sulfonamide)	PFAS		0.06-1.8b			-	0,032-0,46 ; 0,038c			
Furosemide	Pharmaceutical	460-2600e	560-4000e	1476-2789 a	629-1161 a	180b		<6-129a	≤5 e	NC e
Gemfibrozil	Pharmaceutical		17b	187-326 g	NC g	25b	-			
Hydrochlorothiazide	Pharmaceutical	480-1300e	1500-2600e	670 g	74 g	240b	-		≤4 e	≤2 e
Ibuprofen	Pharmaceutical	1000-18000e	>400-1600e	1681-33764 a	143-4239 a	90d	≤180c	1-2370a	≤2 e	≤1 e
		970b	245b				-	<0.5-140		
Ifosfamide	Pharmaceutical		23 f			14b	-			
Irbesartan	Pharmaceutical	770b	450b			110b	2,2-430c	2.2-130a		
Lamotrigine	Pharmaceutical					240b	-			
Laurilsulfate	Personal care product					-	-			
Lidocaine	Pharmaceutical					90b	-			
Loperamide	Pharmaceutical	6.23b	8.5b			2b	0,58-3,6c	0.58-3.6a		
Losartan	Pharmaceutical					230b	-		≤1 e	NC e
Meclofenamic acid	Pharmaceutical					-	-			
Mefenamic Acid	Pharmaceutical					2.2b	-			
Memantine	Pharmaceutical	28b	24b			4,9d	≤15c	<0.5-6.5a		

Organic micropollutant	Category	Wastewater (ng/L)				Recipient of WW (ng/L)	Surface water (ng/L)		Drinking water (ng/L)	
		Sweden		Europe		Sweden	Sweden	Europe	Sweden	
		Influent	Effluent	Influent	Effluent				Raw	Treated
Metformin	Pharmaceutical	730b	330b			<100d	<100c	<100a		
Methylparaben	Paraben			2642-11601 a	<3-50 a	<0.17b	-	<0,3-68a		
Metoprolol	Pharmaceutical	240-7600e	300-17000e	75-110 a	41-69 a	450d	950c	<0.5-10 a	≤3 e	≤2 e
Metronidazole	Pharmaceutical			569-2608 a	265-373 a	15b		<1.5-12a		
Mirtazapine	Pharmaceutical	230b	180b			90d	≤210c	<10-130a		
Nicotine	Stimulant			3919-9684 a	52 a	25b		12-86a		
Norsertraline	Pharmaceutical					75b	-			
Omeprazole	Pharmaceutical					-	-			
Oxazepam	Pharmaceutical	340-730e	400-960e	22-50 a	33-58 a	180d	≤580c	2,4-11a	≤2 e	NC e
Oxybenzone (Benzophenone-3)	Personal care product					-	-			
Oxycodone	Pharmaceutical			5,0-12 a	7,0-12 a	13b		0,5-3a		
Panthenol	Pharmaceutical					190b	-			
Paroxetine	Pharmaceutical	40b	10b			<10d		<10a		
PFBA (perfluorobutanoic acid)	PFAS		0.87-21b			-	0,47-3,7 ; 1,7c			
PFBS (perfluorobutanesulfonic acid)	PFAS		0.5-21b			-	0,030-19 ; 2,5c			

Organic micropollutant	Category	Wastewater (ng/L)				Recipient of WW (ng/L)	Surface water (ng/L)		Drinking water (ng/L)	
		Sweden		Europe		Sweden	Sweden	Europe	Sweden	
		Influent	Effluent	Influent	Effluent				Raw	Treated
PFDA (perfluorodecanoic acid)	PFAS	0.22-7.1b				<0.4b	0,024-4,4 ; 0,048c			
PFDoDA (perfluorododecanoic acid)	PFAS	0.15-4.2b				<17b	0,016-0,82 ; <0,19c			
PFHpA (perfluoroheptanoic acid)	PFAS	1-17b				2.6b	0,36-1,7 ; 1,6c			
PFHxA (perfluorohexanoic acid)	PFAS	0.55-22b				7.1b	0,51-4,2 ; 11c			
PFHxS (perfluorohexanesulfonic acid)	PFAS	0.58-10b				<5.4b	0,051-18 ; 34c			
PFNA (perfluorononanoic acid)	PFAS	0.24-706b				2.0b	0,090-5,8 ; 0,24c			
PFOA (perfluorooctanoic acid)	PFAS	2.5b				<3.6b	0,21-4,2 ; 4,4c			
PFOS (perfluorooctanesulfonic acid)	PFAS	0.78-79b				<6.4b	0,040-6,9 ; 19c			
PFPeA (perfluoropentanoic acid)	PFAS	2.4-14b				-	3,3c			
PFTeDA (perfluorotetradecanoic acid)	PFAS	<0.05b				-	0,093-1,5 ; <0,05c			
PFUnDA (perfluoroundecanoic acid)	PFAS	0.17-1.7b				2.9b	0,018-1,8 ; <0,16c			
Primidone	Pharmaceutical					8b				

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		Sweden		Europe		Sweden	Sweden	Europe	Sweden	
		Influent	Effluent	Influent	Effluent				Raw	Treated
Propranolol	Pharmaceutical		90b	60-638 a	93-388 a	20 b		<0.5-107 a		
Propylparaben	Paraben			598-3090 a	26-63 a	<0.077b		<0,2-7a		
Pyrimethamine	Pharmaceutical					-	-			
Ramipril	Pharmaceutical					3.4b	-			
Raniticine	Pharmaceutical	240b	240b	<12-5060 a	<9-425 a	30d	≤110c	<3-32a		
Ricinoleic acic	Pharmaceutical					-	-			
Roxithromycin	Pharmaceutical	400b	130b			<50d	≤1100c	<50-240a		
Salicylic acic	Pharmaceutical			5866-52000 a	75-209 a	20b		4-62 a		
Sertraline	Pharmaceutical	75b	14b			<10d	≤28c	<10-18a		
Simvastatin	Pharmaceutical	68000 f	<100 f	<7-115 a	<3-5 a	40b		<0,6a		
Sotalol	Pharmaceutical			100 g	53 g	20b	2,4-5c			
Sucralose	Artificial sweetener		1700-11000b			-	-			
Sulfamethoxazole	Pharmaceutical	500b	130b	<3-115 a	10,0-19 a	80d	≤620c	<0,5-2a		
Sulisobenzone	Personal care procuct					350b	-			
Tamoxifen	Pharmaceutical	210b	50b	143-215 a	<10-369 a	<5d	≤13c	<10-212a		
Terbutaline	Pharmaceutical					2.6b	-			

Organic micropollutant	Category	Wastewater (ng/L)				Recipient of WW (ng/L)	Surface water (ng/L)		Crinking water (ng/L)	
		Swecen		Europe		Swecen	Swecen	Europe	Swecen	
		Influent	Effluent	Influent	Effluent				Raw	Treatec
Thiabencazole	Pharmaceutical					4.1b	-			
Tolytriazole	Pharmaceutical					-	-			
Tramacol	Pharmaceutical	2000b	1700b	733-48488 a	739-59046 a	560d	≤1800c	<30-5970a	0,18-6 e	2,0-6 e
Tributyl citrate acetate	Incustrial chemical					75b	-			
Triisopropanolamine	Incustrial chemical					-	-			
Trimethoprim	Pharmaceutical	83-290e	130-310e	213-2925 a	128-1152 a	90d	6,8-210c	<1,5-108a	≤0,7 e	NC e
Tris(2-butoxylethyl) phosphate	Incustrial chemical		240-16000b			-	-			
Valproic acic	Pharmaceutical					-	-			
Valsartan	Pharmaceutical			342-1734 a	192-344 a	90b	-	<1-55a		
Venlafaxine	Pharmaceutical	620b	420b	120-249 a	95-188 a	130d	6-440c	1,1-35a		

***Watch list EU (WFC), ** CEC – Contaminants of emerging concern (from WFC)**

a. Petrie et al., (2015)
b. Malnes et al., (2021)
c. Fick et al., (2011)
d. Ahrens et al., (2016)
e. Helmfrid et al., (2010)
f. Helmfrid et al., (2006)
g. Couto et al., (2019)
h. Barbosa et al., (2016)