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Occurrence and removal of organic micropollutants in drinking water

Analytical approaches for wide-scope screening of contaminants of emerging concern

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Abstract

With the rapidly expanding global population, demand for clean drinking water is increasing. However, the widespread use of synthetic chemicals makes it challenging to produce safe and clean drinking water. A wide range of common chemicals can pose problems for drinking water producers, particularly pharmaceuticals, pesticides, per- and polyfluoroalkyl substances (PFASs), drugs, flame retardants, food additives, personal care products and industrial chemicals. Conventional drinking water treatment is not designed to effectively remove all these compound groups, and many organic compounds may slip through treatment barriers due to their high polarity and mobility. This thesis examined the removal efficiencies of unwanted substances at drinking water treatment plants (DWTPs) employing various treatment strategies, and sought to develop broad and accurate analytical techniques to measure a wide range of micropollutants. The aim was to improve understanding of the occurrence and removal of contaminants of emerging concern (CECs) in raw, process and drinking water in Sweden and internationally.

A broad target screening method based on large volume extraction and high-resolution mass spectrometry (HRMS) was developed to investigate the status of Sweden's most important water source and one major DWTP. The method was then refined using a semi-automated extraction method and a broader analytical method, which was used in a field study of several drinking water treatment plants along Sweden's second most important water source. The influence of operational age on the effectiveness of granular activated carbon (GAC) filters in removing CECs was studied in one full-scale DWTP. To extend the scope of the analytical method further, a tool for creating relevant suspect lists was developed. A suspect list created using this tool and an extensive target list were used in a large screening study of raw water and drinking water samples from 13 DWTPs located in 11 countries in Europe and Asia.

The novel findings in this thesis on the current status of CECs in raw water and drinking water, and on the suitability of current treatment techniques for efficient removal of CECs in drinking water production, can help improve drinking water quality worldwide.

Keywords: contaminants of emerging concern; organic micropollutants, drinking water; water treatment; mass spectrometry; screening methods

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Närvaron och borttagning av organiska mikroföroreningar i dricksvatten

Analytiska tillvägagångsätt för breda analyser av oönskade ämnen

Sammanfattning

På grund av världens ständigt växande befolkning ökar efterfrågan på dricksvatten. Samtidigt medför den ökande användningen av syntetiska kemikalier att svårigheterna med att producera säkert och rent dricksvatten ökar. Det finns ett flertal kemiska ämnesgrupper som kan utgöra ett problem för dricksvattensproducenter, men i denna avhandling har fokus legat på läkemedel, pesticider och per- and polyfluoroalkyl substanser (PFAS), men även på droger, flamskyddsmedel, livsmedelstillsatser, hygienkemikalier samt industrikemikalier har studerats. Traditionella barriärer inom dricksvattenproduktion är inte utvecklade för att effektivt avlägsna dessa oönskade organiska ämnen som riskerar att slinka igenom på grund av hög polaritet och mobilitet. Därför finns det ett behov av att studera borttagningseffektiviteten av oönskade ämnen vid vattenverk med olika strategier för rening, liksom ett behov av breda och noggranna analytiska tekniker för att mäta ett brett spektrum av miljöföroreningar.

Denna avhandling innehåller ett flertal screeningstudier för oönskade organiska ämnen i råvattenkällor och dricksvattenverk i både Sverige och andra delar av världen. En bred screeningmetod utvecklades för att med hjälp av högupplösande masspektrometri och högvolyms-extraktioner undersöka statusen i Sveriges viktigaste vattenkälla och största dricksvattenverk (Artikel I). Metoden blev sedan vidareutvecklad genom ett semi-automatiskt extraktionssystem och en utökad analysmetod för en studie av ett antal vattenverk som alla använde sig av samma vattenkälla (Artikel II). I samma studie undersöktes också hur operationell ålder på granulerat aktivt kol (GAC) påverkar reningseffektiviteten av oönskade organiska ämnen i ett fullskaligt vattenverk (Artikel II). För att ytterligare utöka mängden ämnen i den analytiska metoden togs ett verktyg fram för att skapa listor på relevanta kemikalier fram, så kallade suspect-listor (Artikel III). Ämnena i denna lista blev sedan tillsammans med ett stort antal utvalda miljöföroreningar analyserade genom en stor screeningstudie i Europa och Asien med rå- och dricksvattenprover från 13 vattenverk från 11 länder (Artikel IV).

Denna avhandling bidrar till en ökad förståelse av den rådande statusen för oönskade organiska ämnen i råvattenkällor, processvatten och dricksvatten, samt hur väl nuvarande reningstekniker är lämpliga för att effektivt avlägsna oönskade organiska ämnen vid dricksvattenproduktion.

Nyckelord: kommande föroreningar av bekymmer, dricksvatten, vattenrening, masspektrometri, screeningmetoder

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Dedication

To my loving family, to the ones we got and the one we lost.

“So long, and thanks for all the fish.”
Douglas Adams, The Hitchhiker's Guide to the Galaxy

Contents

List of publications

This thesis is based on the work contained in the following papers, referred to by Roman numerals in the text:

I. **Troger, R**., Klockner, P., Ahrens, L., Wiberg, K. (2018)
Micropollutants in drinking water from source to tap - Method development and application of a multiresidue screening method.
Science of the Total Environment 627, 1404-1432.

II. **Troger, R**., Kohler, S. J., Franke, V., Bergstedt, O., Wiberg, K. (2020)
A case study of organic micropollutants in a major Swedish water source - Removal efficiency in seven drinking water treatment plants and influence of operational age of granulated active carbon filters.
Science of the Total Environment 706, 135680.

III. Durig, W.*, **Troger, R.***, Andersson, P. L., Rybacka, A., Fischer, S., Wiberg, K., Ahrens, L. (2019)
Development of a suspect screening prioritization tool for organic compounds in water and biota. *Chemosphere* 222, 904-912.

IV. **Troger, R.,** Ren, H., Yin, D., Postigo, C., Nguyen, P., Baduel, C., Golovko, O., Been, F., Joerss, H., Rosa Boleda, M., Polesello, S., Roncoroni, M., Taniyasu, S., Menger, F., Ahrens, L., Yin Lai, F., Wiberg, K. (2020)
What's in the water? – Target and suspect screening of contaminants of emerging concern in raw water and drinking water from Europe and Asia
Manuscript.

*Shared first authorship

The contribution of Rikard Tröger (RT) to Papers I-IV was as follows:

I. RT was responsible for developing the analytical method, the general study design, collecting the samples, sample extraction, running the LC-MS analysis, data evaluation, and for writing the manuscript with the support of all co-authors. RT was also the supervisor for Master's student Philipp Klöckner, who helped with sample extraction.

II. RT was responsible for developing the analytical method, planning the sampling campaign, collecting samples, sample extraction, running the LC-MS analysis, data evaluation, and for writing the manuscript with the support of all co-authors.

III. RT and Wiebke Dürig shared equal responsibility for constructing the database, creating the prioritisation tool (SusTool) and evaluating the tool, with the support of all co-authors. RT was responsible for the final version of the manuscript and for handling the peer-review process.

IV. RT was responsible for the study design, planning the sampling campaign including all logistics, extracting the samples, running the LC-MS analysis, data evaluation and writing the manuscript with the support of all co-authors. RT was also the supervisor for the exchange Master's student Hanwei Ren, who helped with sample extraction.

Additional publications

In addition to the papers included in the thesis, RT contributed extracted samples and assisted in manuscript writing for the following peer-reviewed publications produced within the SafeDrink project:

Rosenmai, A. K., Lundqvist, J., le Godec, T., Ohlsson, A., **Troger, R**., Hellman, B., & Oskarsson, A. (2018). *In vitro* bioanalysis of drinking water from source to tap. *Water Research* 139, 272-280.

Oskarsson, A., Rosenmai, A. K., Mandava, G., Johannisson, A., Holmes, A., **Troger, R**., Lundqvist, J. (2020). Assessment of source and treated water quality in seven drinking water treatment plants by *in vitro* bioassays – oxidative stress and antiandrogenic effects after artificial infiltration. *Science of the Total Environment.* 2020, 144001

Abbreviations

CEC	Contaminants of emerging concern
DOC	Dissolved organic carbon
DL	Detection limit
DWTP	Drinking water treatment plant
GAC	Granular activated carbon
HLB	Hydrophilic lipophilic balanced
HRMS	High-resolution mass spectrometry
IS	Internal standard
LC	Liquid chromatography
MDL	Method detection limit
MS	Mass spectrometry
NF	Nanofiltration
OMP	Organic micropollutant
PFAS	Per- and polyfluoroalkyl substance
PMT	Persistent, mobile and toxic
POP	Persistent organic pollutant
RO	Reverse osmosis
RSD	Relative standard deviation
SMILES	Simplified molecular-input line-entry system
SPE	Solid-phase extraction
UPLC	Ultra-performance liquid chromatography
UV	Ultraviolet
WWTP	Wastewater treatment plant

1 Introduction

Clean and safe drinking water is essential for human life, and it is important to have access to raw water sources without pollution or to implement effective water treatment systems. The increasing use of synthetic chemicals poses a growing threat to raw water sources and the environment (aus der Beek et al. 2016; Sousa et al. 2018; Wilkinson et al. 2017; Yang et al. 2017). These widespread, often unregulated and potentially hazardous compounds are generally referred to as contaminants of emerging concern (CECs) and are currently not included in routine monitoring programmes (Schulze et al. 2018). For simplicity, in this thesis the term CECs also includes pesticides, even though they are regulated. The continuous release and widespread occurrence of CECs in the environment raise concerns, as they may have potential adverse effects on environmental and human health, but their properties are not yet fully understood (Webb et al. 2003). In aquatic environments, polar compounds that show environmental mobility and reach water bodies are a particular concern (Reemtsma et al. 2016; Schulze et al. 2018).

Although surface water is highly impacted by wastewater effluent and other point sources (Sousa et al. 2018), certain CECs can also be found in groundwater (Gaston et al. 2019; Lapworth et al. 2012; Stuart et al. 2012). Classical treatment processes employed by drinking water treatment plants (DWTPs), such as sedimentation, sand filtration and disinfection, have been shown to provide limited removal efficiency of CECs (Kot-Wasik, Jakimska, and Sliwka-Kaszynska 2016; Padhye et al. 2014b; Stackelberg et al. 2007). To combat this growing problem, advanced treatment techniques such as granular activated carbon (GAC), nanofiltration, ozonation and reverse osmosis have been shown to be more efficient in removing CECs (Stackelberg et al. 2007; Teodosiu et al. 2018). Awareness of potential problems with persistent, mobile and toxic (PMT) organic chemicals is increasing (Reemtsma et al. 2016), as barriers to distribution (*e.g.* wastewater treatment plants (WWTPs), subsurface

environments and DWTP processes) generally have inefficient removal process systems. Concerns about the occurrence and effects of a large number of CECs on aquatic environments are likely to increase in the future (Jin et al. 2020).

2 Objective and research questions

Drinking water producers are responsible for producing clean and safe drinking water. Removal of CECs can be challenging for drinking water producers, since many compounds are polar and mobile, and therefore not effectively removed by conventional drinking water treatment techniques. At present, GAC filtration is the most commonly used treatment for removal of organic pollutants in DWTPs, although these filters are not primarily intended for removal of CECs, but to remove odour and taste. Some DWTPs use advanced treatment techniques for better removal of CECs, such as filtration through membranes or advanced oxidation, which have been shown to efficiently remove a wide range of CECs. In order to detect and combat the occurrence of CECs in drinking water, reliable trace analysis methods are needed. Measurement of trace levels of CECs in raw and drinking water requires advanced analytical methods, which are costly and time-consuming to develop and apply. With the growing numbers and amounts of chemicals used in society worldwide, it is important to use wide-scope screening methods. The main objective of this thesis was to develop and apply broad-range and wide-scope screening methods for CECs in raw water and drinking water, in order to provide a better understanding of the current status of CEC occurrence in drinking water production.

The objective of the thesis were to address the following research questions:

1. How can CECs in raw water and drinking water be accurately and precisely quantified at trace levels and how can novel CECs be traced and identified (Papers I & III)?
2. What is the current occurrence of CECs in raw and drinking water in Sweden and internationally (Papers I, II & IV)?
3. How does the performance of GAC treatment vary with operational age of the GAC material (Papers I & II)?
4. How efficiently are CECs removed in current full-scale drinking water treatment plants (Papers I, II & IV)?

3 Background

3.1 Compound groups

Based on current knowledge, there are several important groups of CECs to research and monitor in raw water and drinking water (Petrovic et al. 2005; Caliman and Gavrilescu 2009; Lapworth et al. 2012; Stuart et al. 2012; Ivancev-Tumbas 2014; Wilkinson et al. 2017; Sousa et al. 2018; Gaston et al. 2019). The CECs include chemicals such as pharmaceuticals, pesticides and per- and polyfluoroalkyl substances (PFASs), flame retardants, food additives, personal care products and industrial chemicals (Sousa et al. 2018; Richardson and Ternes 2014; Menger et al. 2020). Pharmaceuticals and personal care products are widely discharged to the environment due to poor removal in WWTPs, and are mainly a problem in surface water (Bade et al. 2015; Gago-Ferrero et al. 2017), while PFASs have been shown to pose a threat to both surface water and groundwater sources (Gobelius et al. 2018; Lapworth et al. 2012). Pesticides impacts surrounding water bodies in agricultural areas (Mekonen et al. 2016; Badach, Nazimek, and Kaminska 2007; Bulut et al. 2010), but can also migrate to the groundwater (Fava et al. 2010).

3.2 Analytical approaches

To analyse a wide range of CECs, a variety of different screening methods have been developed (Gervais et al. 2008; Benotti et al. 2009b; Wode et al. 2012; Padhye et al. 2014a; Gago-Ferrero et al. 2017; Ren et al. 2020). These methods need to handle CECs with varying physio-chemical properties, such as polarity. To reach satisfactory method detection limits (MDLs), large water volumes may be needed for pre-concentration and analysis (Daniels et al. 2020; Troger et al. 2018), since the concentrations of CECs in raw water, but especially in drinking water, are usually in the ng L^{-1} range (Crone et al. 2019; Teodosiu et al. 2018; Yang et al. 2017; Furlong et al. 2017).

3.2.1 Extraction methods

When analysing CECs in water, solid phase extraction (SPE) is commonly used to achieve adequate sensitivity of the analysis (Pittertschatscher et al. 1999; Wode et al. 2012; Chen et al. 2010). To achieve low MDLs for as many compounds as possible, large water volumes (>1 L) are sometimes required (Troger et al. 2018; Daniels et al. 2020; Trenholm et al. 2006). During extraction, the CECs of interest in water samples are loaded and concentrated on an absorption material and subsequently eluted from the SPE material using an appropriate solvent (Figure 1). A commonly used absorption material is hydrophilic lipophilic balanced (HLB) sorbent (Daniels et al. 2020; Hennion 1999). The material is normally packed into a cartridge, but can also be packed into disks (with smaller particles), which improves the potential flow rate while retaining good extraction efficiency (Leandro et al. 2006).

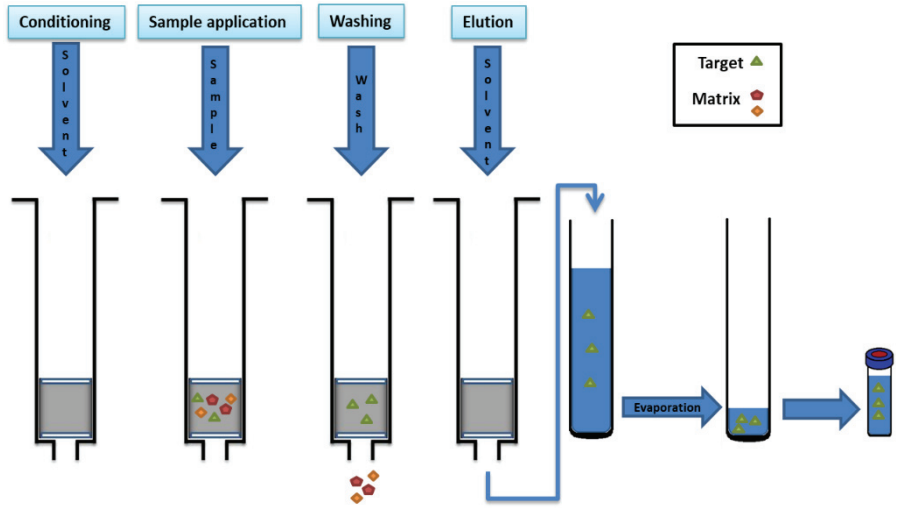

Figure 1. Schematic overview of a typical solid phase extraction (SPE) procedure for extraction of contaminants of emerging concern (CECs) in water.

3.2.2 Mass spectrometry

Quantitative and qualitative analysis of CECs is typically performed using a chromatographic system coupled to a mass analyser (Menger et al. 2020; Hernandez et al. 2012; Richardson 2012). When analysing legacy persistent organic pollutants (POPs), a gas chromatography (GC) system coupled to a mass spectrometer (MS) is often used (Richardson 2012). For polar contaminants, it is more feasible to use liquid chromatography (LC) coupled to MS (Richardson and Ternes 2014). Liquid chromatography enables separation of polar and thermally unstable compounds that could not be analysed using GC. The state-of-the-art screening method for polar CECs is ultra-performance liquid chromatography (UPLC) coupled to high-resolution mass spectrometry (HRMS) (Menger et al. 2020). This enables simultaneous analysis of thousands of compounds but also retrospective data analysis, which is valuable for the discovery of novel CECs (Lopez et al. 2016).

3.2.3 Target and suspect screening

There are three basic approaches to broad screening of CECs, target screening, suspect screening and non-target screening (Menger et al. 2020). Non-target screening (Krauss, Singer, and Hollender 2010; Menger et al. 2020) is not covered in this thesis and is therefore not further described. Target screening (Figure 2) is often used for monitoring of CECs (Gervais et al. 2008; Gago-Ferrero et al. 2017; Jansson and Kreuger 2010; Gobelius et al. 2018; Wode et al. 2012; Benotti et al. 2009b). It provides high certainty in the identification of a peak and also enables reliable quantification, which is essential in monitoring programmes. To increase the scope of target analytes and include less studied CECs, HRMS enables the possibility of suspect screening (Krauss, Singer, and Hollender 2010) Suspect screening (Figure 2) which can be performed for any number of compounds for which the molecular formula (and preferably also the structure) is available. This is done by searching for peaks with exact matching masses. A suspect list can be created in many different ways, *e.g*. by compiling information from relevant literature (Richardson and Ternes 2014; Gaston et al. 2019) or using databases (Gago-Ferrero et al. 2018; Durig et al. 2019; Mardal et al. 2019; Schymanski et al. 2015). After a suspect has been tentatively identified, it can be included in a target method for confirmation and quantification.

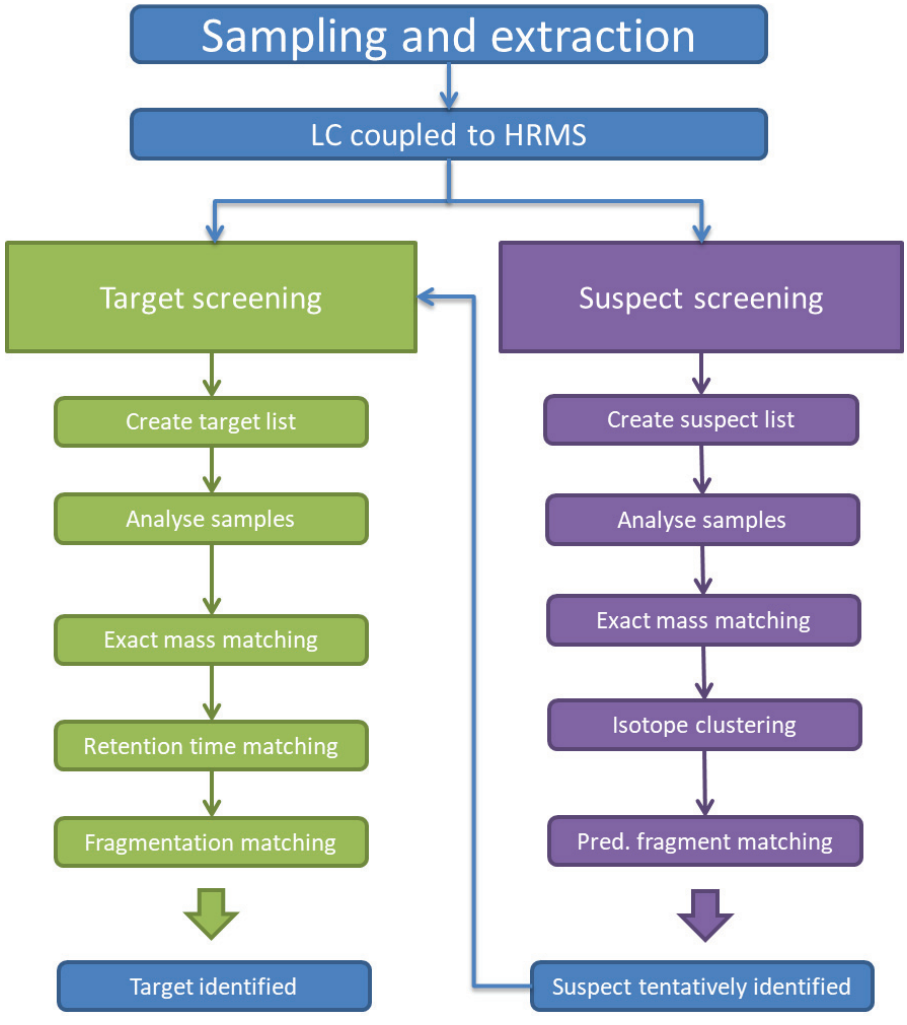

Figure 2. Schematic illustration of the workflow for target screening (left) and suspect screening (right). LC = liquid chromatography; HRMS = high-resolution mass spectrometry.

3.3 Drinking water treatment

To date, drinking water treatment has mostly involved the removal of particles, dissolved organic carbon (DOC) and harmful bacteria and viruses from the raw water. This is usually achieved with a combination of filtration, coagulation, sedimentation and disinfection. However, these treatment steps have been shown to be inefficient in removal of CECs (Stackelberg et al. 2007). Modern DWTPs treating raw water contaminated with CECs need to apply more advance treatment techniques to provide safe drinking water (Teodosiu et al. 2018).

3.3.1 Granular activated carbon (GAC)

Granular activated carbon filtration is one of the most commonly applied treatment techniques for removal of CECs (Stackelberg et al. 2007; Teodosiu et al. 2018; Ternes et al. 2002). It works on the principle of adsorption of CECs to the GAC material (Troger et al. 2020; Boleda, Galceran, and Ventura 2011) However, the removal efficiency of CECs by GAC filters decreases over time due to saturation of GAC material and it requires replacement or regeneration on a regular basis, which can be cost-intensive (Troger et al. 2018; Padhye et al. 2014b; Belkouteb et al. 2020).

3.3.2 Nanofiltration and reverse osmosis

Nanofiltration and reverse osmosis are very efficient treatment processes for removal of CECs (Boleda, Galceran, and Ventura 2011; Escher et al. 2011; Radjenovic et al. 2008). Both are high-pressure membrane techniques that prevent larger molecules from passing through the membranes depending on molecular cut-off point and type of membrane (Crone et al. 2019). Their effectiveness in removing CECs has been demonstrated both in pilot-scale treatment plants (Babi et al. 2007; Troger et al. 2018) and in full-scale DWTPs (Radjenovic et al. 2008; Boleda, Galceran, and Ventura 2011; Escher et al. 2011).

3.3.3 Ozonation

Ozonation treatment is used to remove CECs from both wastewater (Esplugas et al. 2007; Nakada et al. 2007; Margot et al. 2013) and from drinking water (Teodosiu et al. 2018; Kot-Wasik, Jakimska, and Sliwka-Kaszynska 2016; Boleda, Galceran, and Ventura 2011). The treatment employs ozone to oxidise CECs occurring in the water, transforming the substances to other substances or ultimately mineralising them (Adil et al. 2020; Broseus et al. 2009). Although ozonation has shown to be effective in the breakdown of CECs, there are concerns that transformation products can potentially be hazardous for humans and the environment (Adil et al. 2020; Zhang et al. 2020).

4 Materials and methods

4.1 Method development and selection of target compounds

A total of 123 different CECs were included in the initial method development in **Paper I**. These were selected from the following compound groups; pesticides (*n=75*), pharmaceuticals and personal care products (*n*=35), PFASs (*n*=12) and food additives (*n*=1). The selection was based on contaminants previously detected in water samples and the availability of reference standards (Petrovic, Gonzalez, and Barcelo 2003; Xindi C. Hu 2016; Ivancev-Tumbas 2014; Westerhoff et al. 2005; Webb et al. 2003; Mekonen et al. 2016; Benotti et al. 2009a; Kumar and Xagoraraki 2010; Segura et al. 2011; Padhye et al. 2014a).

Two different SPE sorbents, Oasis HLB (Waters) and Bond-Elut ENV (Agilent), were evaluated for extraction of 1-L and 5-L samples. The water used for this experiment was drinking water. Differences in recoveries, matrix effects and MDLs between the two different extraction volumes were studied and evaluated.

Eleven additional CECs were added in **Paper I** to increase the scope of the method before analysis of the samples, and thus a final total of 134 compounds were targeted. The target analyte range was further extended to 163 CECs in **Paper II** and 177 CECs in **Paper IV**. Recoveries, matrix effects and MDLs were calculated and evaluated separately in each of the papers for quality control. The full list of all compounds included and their CAS number, compound group, ion mode, neutral mass and detection limit, can be found in Table A1 in the Appendix to this thesis.

4.2 General layout of the case studies

A number of field studies, which included in total 20 full-scale DWTPs, were conducted as part of this thesis work. In **Paper I**, a "source to tap" approach was employed, with the focus on drinking water production, using raw water from Lake Mälaren, Sweden's most important (2 million people served) raw water source. Samples were collected upstream in the flow path of the river Fyris, downstream a large conventional municipal WWTP, in the lake itself, at the raw water intake to the DWTP and all the way out into the distribution system (Figure 3). The study also included sampling after several treatment steps inside the DWTP and sampling from a pilot-scale treatment system. In this study, 5-L samples were extracted and analysed using the target method as described in section 4.1.

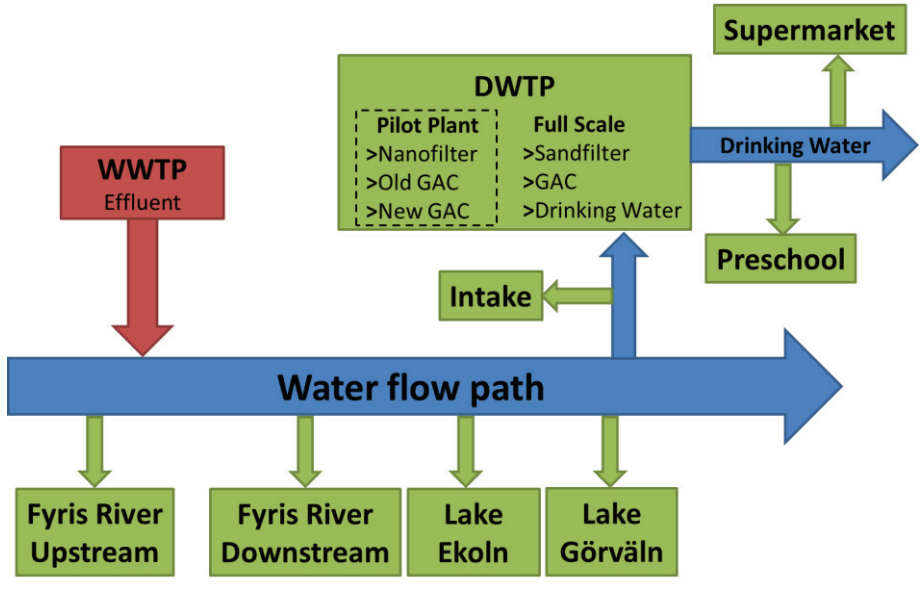

Figure 3. Schematic overview of the different water sampling locations along the natural flow path of surface water to Lake Mälaren, within a drinking water treatment plant (DWTP) (full-scale and pilot-scale, with a granular activated carbon (GAC) filter), and in the drinking water distribution network (modified from **Paper I**).

The case study described in **Paper II** investigated Sweden's second most important (0.7 million people served) raw water source, the river Göta Älv. Samples (5 L) were collected along the river's flow path, including from seven DWTPs using the river as their main water source, either directly or from a connected lake (Figure 4). In one DWTP, samples were also collected after individual GAC filters of varying operational age, to investigate the impact of deployment time on the CEC removal efficiency.

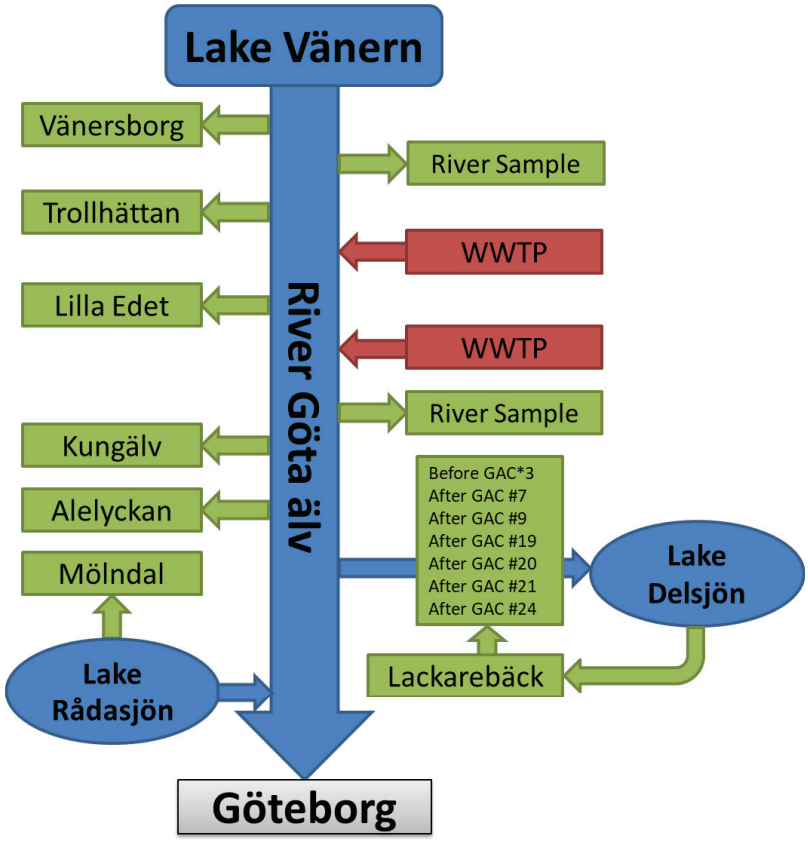

Figure 4. Schematic overview of sampling sites (green boxes) on the river Göta Älv. Raw water and drinking water were sampled at all drinking water treatment plants (DWTPs) (modified from **Paper II**). At Lackarebäck DWTP, six additional samples were collected after six different granular activated carbon (GAC) filters. Lake Delsjön receives its water mainly from Göta Älv.

In **Paper IV**, the scope of the screening was geographically wider, with raw water and drinking water samples from 13 different DWTPs located in 11 different countries in Europe and Asia (Belgium, China (*n*=2), Czech Republic, Germany, Italy (*n*=2), Japan, Spain, Sweden, Switzerland, The Netherlands and Vietnam). It should be noted that the selected DWTPs are not representative of all existing DWTPs in the respective countries in Europe and Asia. For logistical and redundancy reasons, triplicate 1-L samples were used in this study, instead of a single 5-L sample as in **Papers I & II**.

4.3 Chemical analysis

4.3.1 Sample collection and handling

In **Papers I & II**, all samples were collected as grab samples in 12-L stainless steel containers and stored at +4 °C until extraction, which was carried out within a maximum of one week after sampling. The water samples were transferred to 5-L amber glass bottles before extraction.

In **Paper IV**, the raw water and drinking water grab samples were collected in triplicate from each DWTP (2 x 3 samples from each plant) using 1-L poly-propylene bottles that were pre-cleaned with ethanol and Milli-Q water. The samples were packed in cooling boxes and shipped using the best available express shipment method to the laboratory at SLU, where they were stored at +4 °C until extraction, which was performed within a few days. The samples were transferred to 1-L glass bottles before extraction.

4.3.2 Filtration and extraction

A classical extraction method, where the samples were first filtered through a glass fibre filter (Whatman GF/F, 0.7 µm, 142 mm) and then extracted using cartridge-based SPEs, was applied In **Paper I**. One 5-L subsample was extracted using a 1 g Bond-Elut ENV cartridge and one subsample was extracted using a 1 g Oasis HLB cartridge. The preconditioning, application, and elution were identical for both types of SPE cartridge. The SPE cartridges were preconditioned with 30 mL methanol, followed by 20 mL Milli-Q water. The samples were applied directly from the 5-L glass bottles using a vacuum manifold at a rate of ~1 drop/s (~12 h). Each SPE cartridge was eluted three times, using 10 mL of methanol. The eluate was reduced using an evaporation system (N-Evap 112 Nitrogen Evaporator) (Organomation Associates Inc.) to ~0.5 mL in several steps. The extract was finally transferred to an amber glass LC/MS-vial and diluted to 1 mL using Milli-Q water. The vials were stored at -20 °C until instrumental analysis.

In **Papers II & IV**, a semi-automated extraction system was used. The samples were extracted using a 4790 SPE-DEX® (Horizon Technology, Salem, New Hampshire, USA) with 47 mm Atlantic HLB-M SPE disks (Horizon Technology). The samples were filtered through a 1-µm glass fibre filter (1 Micron - Fine, Fast Flow Sediment Pre-Filters Horizon Technology) placed in series with the SPE disk. The filter and the SPE disk were then extracted together. The SPE (and filter) were preconditioned using 1 × 25 mL Milli-Q

water, followed by 2 × 25 mL methanol and finally 2 × 25 mL Milli-Q water. The sample was then loaded onto the SPE through the filter. The filter and the SPE disk were washed with 2 × 25 mL 5% methanol. After the washing step, the system was air-dried for 10 minutes before elution. Elution of the SPE disk (and filter) was performed using 3 × 25 mL methanol in **Paper II** and 1 × 25 mL methanol followed by 1 × 25 mL acetonitrile in **Paper IV**. In both studies, the eluate was reduced to ~1 mL using a TurboVap Classic II system (Biotage, USA). The extract was transferred stepwise to an amber glass LC/MS-vial, reduced to ~0.5 mL and then diluted to 1 mL with Milli-Q water. The final extracts were stored at -20 °C until instrumental analysis.

4.3.3 Standards and internal standards

Papers I, II & IV included a similar number of target analytes, with small variations between the studies. The three main target groups in each study were pharmaceuticals, pesticides and PFASs, including internal standards (IS) from each group. In addition, flame retardants, phthalates, food additives, drugs, industrial chemicals, personal care products and benzos (benzotriazoles/benzothiazoles) were analysed. **Paper I** focused on 134 CECs (+11 IS), **Paper II** on 163 CECs (+27 IS) and **Paper IV** on 177 CECs (+37 IS).

4.3.4 Instrumental analysis

All samples in **Papers I, II & IV** were analysed using the same instrument and analytical method, although the number of target analytes varied between the studies. The analysis was performed using an ultra-performance liquid chromatography (UPLC) system (Acquity H-Class with FTN injector, Waters, Milford, USA). The MS device used was a quadrupole-time-of-flight (QToF) mass spectrometer (Xevo G2-S, Waters, Manchester, UK).

Two different columns were used, depending on the ion mode. The column used in negative ion mode was a Acquity UPLC BEH-C18 column (Waters, 2.1 x 100 mm, 1.7 µm particle size), and in positive ion mode an Acquity UPLC HSS T3-C18 (Waters, 2.1 x 100 mm, 1.8 µm particle size). The reason for having a different column for the positive ion mode analysis was because the T3 column improves the retention of polar compounds, especially charged compounds, due to secondary interaction with the silica particles. The T3 column could not be used in negative ion mode, due to higher pH in the mobile phase.

The mobile phase was Milli-Q water for phase A and acetonitrile for phase B. To improve the ionisation and sensitivity, a different pH was used in positive and negative ion modes. In positive mode, 0.01% of formic acid was added to both the water and acetonitrile, and 5 mM of ammonium formate were added to the water phase (pH ~3). In negative mode, 0.01% of ammonium hydroxide was added to both phases, and 5 mM ammonium acetate were added to the water phase (pH ~8). Both ion modes used the same linear gradient, with a flow rate of 0.5 mL min^{-1} and a total run time of 21 min, starting at 5% acetonitrile and going up to 99%. The gradient, expressed as %B, was 0.0 min: 5%B, 0.5 min: 5%B, 16.0 min: 95%B, 16.1 min: 99%B, 19.0 min: 99%B, 19.1 min: 5%B, and 21.0 min: 5%B. The injection volume was 5 µL in **Paper I** and 10 µL in **Papers II and IV**.

All data were collected in MS^E-mode, which is referred to as data-independent acquisition. The resolution was typically ~30 000 at 556.28 m/z, using leucine enkephalin for the lock spray. The software UNIFI v1.7.0 was used for method development and data collection in **Paper I**, and UNIFI v1.8.2 was used for data evaluation in **Paper I** and for both data collection and evaluation in **Papers II & IV.**

In **Paper II**, DOC concentration was analysed using a Shimadzu TOC-VCPH carbon analyser following the procedures set up by Lavonen *et al*. (Lavonen et al. 2015).

4.4 Quality assurance and quality control (QA/QC)

In the studies described in **Papers I, II & IV**, individual MDLs, absolute recoveries and matrix effect/suppression values were calculated. For the calculations, all spiked samples in **Papers I & II** were spiked at 20 ng L^{-1} (100 ng absolute) of each individual compound, while in **Paper IV** 50 ng L^{-1} (50 ng absolute) of each individual compound was used. All spiked samples used genuine drinking water as the matrix.

To calculate the absolute recovery, the average calculated concentration of a triplicate spiked before extraction was divided by the average calculated concentration of a triplicate spiked after extraction. Any concentration detected in the corresponding blank (unspiked) sample was subtracted before the division.

To calculate the matrix effect, the average calculated concentration of a triplicate spiked after extraction was divided by the average calculated concentration of an external calibration point (without matrix). Any concentration detected in the corresponding blank (unspiked) sample was subtracted before the division.

The MDLs was calculated from the detection limit (DL) as:

$$MDL = DL + (3 * RSD_{spiked} * DL) \quad (1)$$

where $DL = C_{spiked} * R_{cutoff} / (R_{spiked} - R_{blank})$, RSD_{spiked} is relative standard deviation, C_{spiked} is nominal added concentration in the spiked sample, R_{cutoff} is minimum detector counts used to not discard a peak, R_{spiked} is average detector counts in spiked sample, R_{blank} is average detector counts (if detected) in blank sample and RSD_{spiked} is relative standard deviation in the spiked sample

In all papers, the ±H adduct was used for quantification, and compounds were quantified with a linear calibration curve with a calibration curve ranging from 0 to 120 ng L^{-1}. All target and suspect compounds were identified using accurate mass screening with a 10 ppm mass error data extraction window and a one-minute time window. All compounds were paired with their corresponding IS, if available. If not, an appropriate IS was selected based on retention time and ionisation behaviour.

4.5 Suspect screening and SusTool

To expand the scope of the compounds selected for screening, a prioritisation tool for creating relevant suspect lists was developed in **Paper III**. The tool, called SusTool, employs a systematic approach, where all compounds are scored based on their physio-chemical properties.

The first step was to create a database consisting of large numbers of relevant chemicals. This was done by combining three different databases into one. Since this tool was developed for screening in the Swedish environment, one database used was the Swedish medical products list FASS (Farmaceutiska specialiteter i Sverige) containing 900 pharmaceuticals used in Sweden. The second database used was the Norman Network List #19 of emerging substances (920 compounds), which contains CECs detected in the environment. The last (and largest) database was a recent U.S. EPA database consisting of chemicals posing a potential health risk on human exposure (32 464 compounds) (Mansouri et al. 2016).

The final database was curated by removing compounds without CAS number, compounds considered as salts (compounds with metal counter-ions) and duplicates (based on CAS numbers). All compounds also included canonical simplified molecular-input line-entry system (SMILES) notations, which give the molecular structure, information needed to calculate their physio-chemical properties. The final database contained 31 832 compounds, spanning a wide range of compound classes and properties. The compounds in the database were characterised using 15 different parameters (Figure 5).

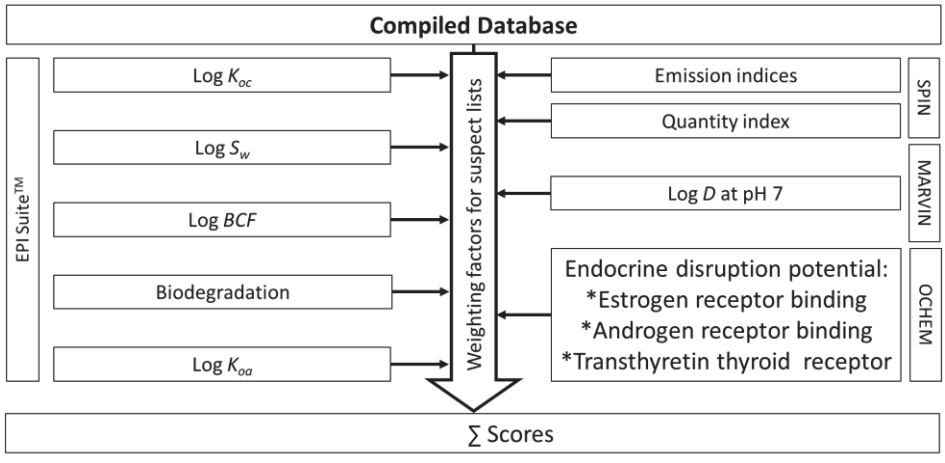

Figure 5. General overview of the structure of SusTool, a tool for producing relevant suspect screening lists for different matrices. K_{oc} = organic carbon-water partitioning coefficient; S_w = water solubility; BCF = bioconcentration factor; K_{oa} = octanol-air partitioning coefficient; D = octanol-water distribution coefficient assuming pH 7 (modified from **Paper III**).

The physio-chemical properties were calculated using EPI Suite™ 4.1 and ChemAxon/MarvinSketch. The selected physicochemical properties included the partitioning coefficient for organic carbon and water (K_{oc}), the octanol-air partitioning coefficient (K_{oa}), the aqueous solubility (S_w) and the octanol-water distribution coefficient (D) calculated assuming pH 7. Two other environmental fate characteristics were also considered, through the inclusion of ultimate biodegradation of organic compounds in the presence of mixed populations of environmental microorganisms and the bioconcentration factor (BCF), which were calculated using EPI Suite™ 4.1.

Estimates of potential exposure to specific environmental compartments/recipients were included in the database using data indices from the SPIN database compiled by the Nordic Council of Ministers Chemical Group (www.spin2000.net). The data used included compound-specific index values ranging from 0-5 for both chemical quantity (QI) and emissions (EI) to five different compartments (EI_{Air}, EI_{Water}, EI_{Soil}, $EI_{Sewage\ treatment}$, $EI_{Consumer}$), for air, surface water, soil, sewage treatment plants and consumers, respectively. The SPIN database covered 17% of the compounds in the final database for the EIs and 15% of the compounds for QI. Any missing index values were replaced with

average values of the same category to avoid over- or underestimation in the scoring of compounds with missing data.

In order to increase the relevance for human health impact, the potential to induce endocrine-related effects was included as one parameter in the scoring. Response data indicating interaction with estrogen and androgen receptors, or with the thyroid hormone transport protein transthyretin (TTR), were used to achieve this distinction. These values were calculated by the method developed by Rybacka *et al*. (Rybacka et al. 2015).

The final database compiled contained a total of 15 description parameters for each compound. In order to rank the substances individually, SusTool was developed. Step one was to introduce the ability to apply cut-off values for each parameter, in order to mitigate outliers with unrealistic values. Parameter values were converted into a relative value ranging from 0 to 1, with 1 representing a high rank for that parameter. This was done by applying minimum (PLLS) and maximum (PLMS) parameter score and vertex points (VP). These limits can easily be modified depending on the sample matrix that the suspect list is intended to be used for. For the parameters using PLLS and PLMS, linear scoring was applied, while the VP scoring was a bell curve-shaped model where the maximum score is achieved at the vertex. The values which gave a maximum score were derived from the literature (Kalberlah Fritz 2014; Schulze et al. 2018).

With all parameters scored between 0 and 1, an adjustable weighting factor was applied to each individual parameter so each score could be adjusted in accordance with its importance for the suspect list being created. The final score was calculated as:

$$Final\ Score = P_1 * W_1 + \ P_2 * W_2 + [\dots] + \left(\frac{EI_1 * WEI_1 + EI_2 * WEI_2 + [\dots]}{Sum\ WEI_x}\right) * QI * WQI$$

(2)

where P_X is the score (0-1) of each individual parameter and W_X is the weight assigned to that parameter, EI_x is the score of each emission index and WEI_x is the weight assigned to that parameter, QI is the score of the quantity index and WQI is the weight assigned to the quantity index.

Table 1. *Weighting factors used to create and apply a suspect list for screening of contaminants of emerging concern (CECs) in water (**Paper IV**). The weight ranged from 0 (no score) to 5 (highest score) and was used for all 15 descriptive parameters*

Parameter	Weight
log D	4
log K_{oc}	2
log S_w	5
Log BCF	1
Biodegradation	1
log K_{oa}	0
ED potential for ER	5
ED potential for AR	5
ED potential for TTR	5
EI_{Air}	0
EI_{Water}	4
EI_{Soil}	0
$EI_{Sewage\ treatment}$	2
$EI_{Consumer}$	3
QI	3

ED: endocrine disruptor, ER: oestrogen receptor, AR: androgen receptor, TTR: transthyretin transport protein

A suspect list with 500 compounds was created for screening CECs in water, by applying the weighting factors given in Table 1. Only the linear scoring, and not VP, was used. The suspect list created was used to perform suspect screening on all samples collected and analysed in **Paper IV**. For a suspect to be considered a detected feature during the suspect screening, a ±2 mDa (milli Dalton) mass error threshold was applied to all peaks. To further increase the confidence in the assigned suspects, only features that had at least one detected fragment from the *in silico* fragmentation were considered. All remaining peaks were manually checked to judge their peak shape. All features that passed the first steps were compiled into a subset suspect list. This subset suspect list contained retention times for all detected features and was run as a target list to re-confirm all detected features.

5 Results and discussion

The main findings in **Papers I-IV** are summarised and discussed in this chapter. For full details, see the individual papers.

5.1 Extraction method development

In **Paper I,** a sample extraction method for raw water and drinking water was developed. Two different sampling volumes (1 L and 5 L) and two different SPE sorbents (HLB and ENV) were tested, and recoveries and matrix effects (ion suppression) were evaluated (Figure 6).

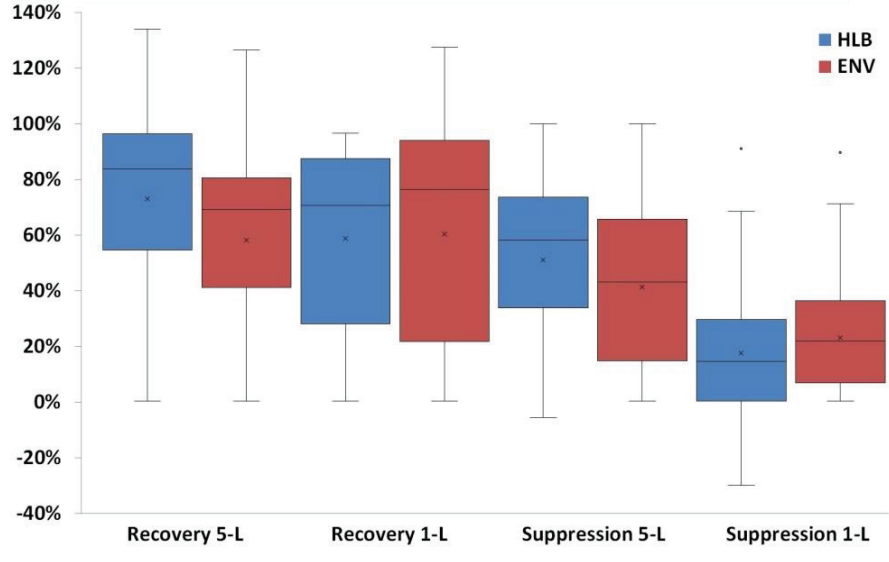

Figure 6. Box plots showing average recoveries (%) and matrix effects (suppression, %) in extraction tests using 5-L and 1-L drinking water samples and HLB and ENV sorbents in solid

phase extraction (SPE) (**Paper I**). Error bars represent the minimum and maximum value and the dots in the boxes represent the average value.

There were statistically significant differences (p<0.05, paired t-test) in recoveries and matrix effects between the HLB and ENV sorbents for all comparisons except the 1-L recoveries. Despite these differences observed, the method development test indicated that both SPE materials are suitable for a wide range of CECs, with acceptable recoveries (average>60%). The experiment also showed statistically significant increases (p<0.001) in matrix suppression on increasing from 1-L to 5-L samples for both the HLB and ENV sorbents, indicating that the gain in sensitivity for the method does not increase one to one with increased sample volume.

Method detection limit was calculated to compare the sensitivity between the 1-L and 5-L samples (Figure 7). The HLB and ENV sorbents performed similarly, with a median MDL of 0.24 ng L^{-1} for HLB and 0.26 ng L^{-1} for ENV, when using 5-L samples, compared with 0.69 ng L^{-1} and 1.0 ng L^{-1}, respectively, when using 1-L samples. Figure 7 shows the ratio between the MDLs for 1-L and 5-L samples when using HLB. If there were a proportional relationship between MDL and sample volume (*i.e*. 1-L *vs*. 5-L), the ratio would be 5 for all compounds. Compounds with MDL ratio >5 (marked in green in Figure 7) showed better than "expected" improvement in MDL going from a sample volume of 1 L to 5 L. Compounds with MDL ratio between 1 and 5 (marked in orange in Figure 7) showed an improvement in MDL on comparing 1-L with 5-L samples. The main explanation for a compound having MDL ratio below 5 is probably increased ion suppression from the extracted matrix in the 5-L samples. Another possible explanation is increased measurement uncertainty with lower concentrations in the extract, which may lead to higher MDLs since 3 x RSD is included in the MDL calculation (Equation 1). The median improvement in MDL when using 5-L compared with 1-L samples was 3.5 for HLB (and 3.3 for ENV). Therefore, in the case study, 5-L samples were used for extraction.

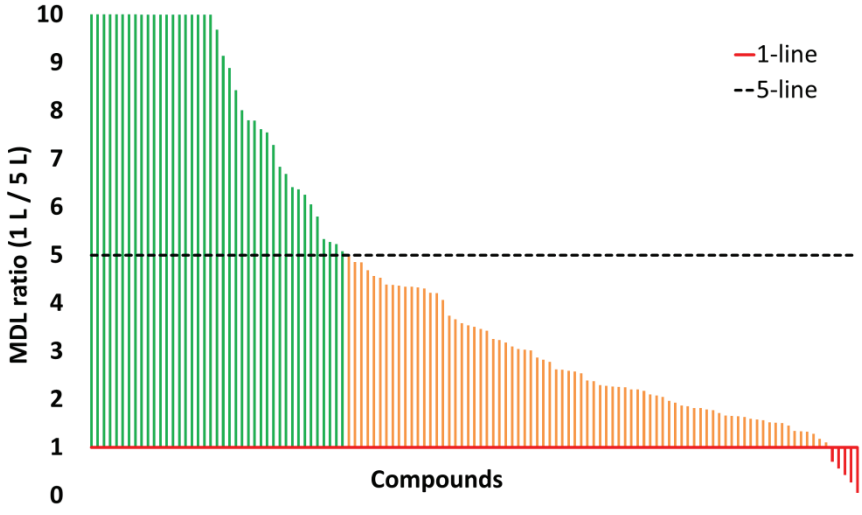

Figure 7. Ratio between method detection limit (MDL) for 1-L and 5-L samples for the detected target compounds (n=123) when using HLB solvent (modified from **Paper I**). The dotted black line indicates the "theoretical expected" ratio, and the red line marks the limit where a 5-L sample resulted in higher (worse) MDL than the 1-L sample.

5.2 Occurrence of CECs in Sweden's two main water sources and produced drinking water (Papers I & II)

In **Papers I & II**, the two main drinking source waters in Sweden, Lake Mälaren (**Paper I**) and the river Göta Älv (**Paper II**), were studied. Both water bodies are impacted by effluents from WWTPs, industrial areas, stormwater ponds and other polluted water.

The study in **Paper I** included sampling along the flow path of the source water, as well as sampling of the raw water, after each major treatment step inside the DWTP, and finally sampling of tap water from end users in the distribution network. The total concentrations of CECs detected and the concentration of each compound category are presented in Figure 8.

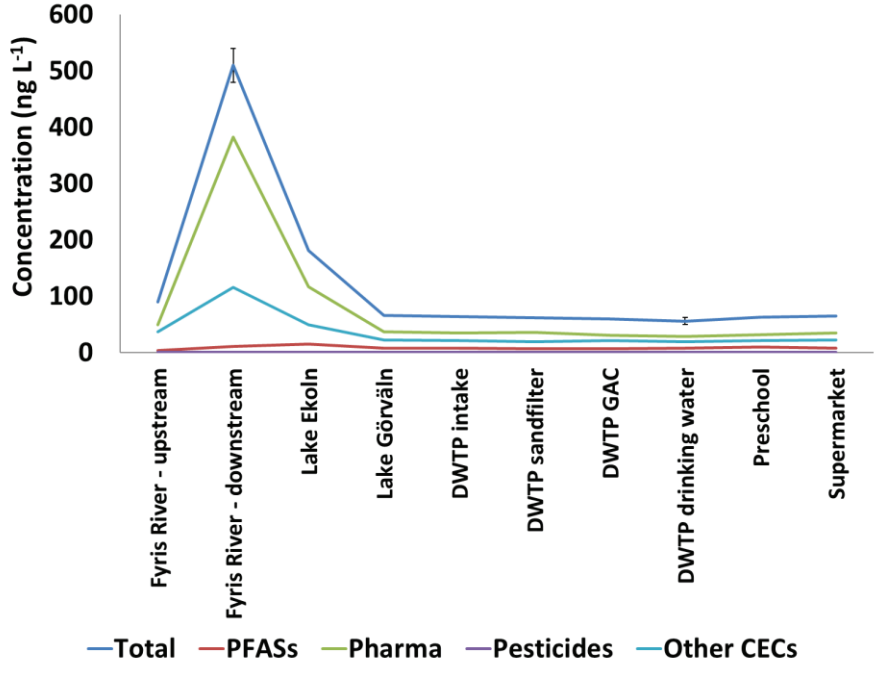

Figure 8. Total concentration (ng L^{-1}) of contaminants of emerging concern (CECs) and of the CEC subgroups PFASs, pharmaceuticals, pesticides and other CECs (modified from **Paper I**). The error bars for the total concentrations at "Fyris River – downstream" and "DWTP drinking water" represent the standard deviation calculated from multiple samples (n=3 and n=2, respectively) collected at those sampling points. The Fyris River upstream and downstream sites are related to Uppsala wastewater treatment plant.

There was a clear impact on the total CEC concentration level from the WWTP at Fyris River, with total concentrations ranging from 90 ng L^{-1} upstream to 510 ng L^{-1} downstream of the WWTP (Figure 8). The CEC concentration at the sampling points further down the flow path (Lake Görväln and DWTP intake) decreased to <90 ng L^{-1}. In the lakes, the pollutants were diluted with water from other sources in the catchment with lower CEC concentrations, and the total CEC concentrations decreased accordingly. After raw water intake, CEC concentrations stayed roughly the same throughout the treatment process in the DWTP and also in the distribution network. In total, 41 compounds were detected in the river water downstream of the WWTP, comprising 11 PFASs, 23 pharmaceuticals, two pesticides and five other CECs. This decreased to a total of 29 compounds in the finished drinking water and the tap water.

The study in **Paper II** was designed to follow the flow path of water in the river Göta Älv, which is the main water source for several DWTPs and Sweden's second most important source water. The total concentration of CECs detected and the concentration of each compound category are shown in Figure 9.

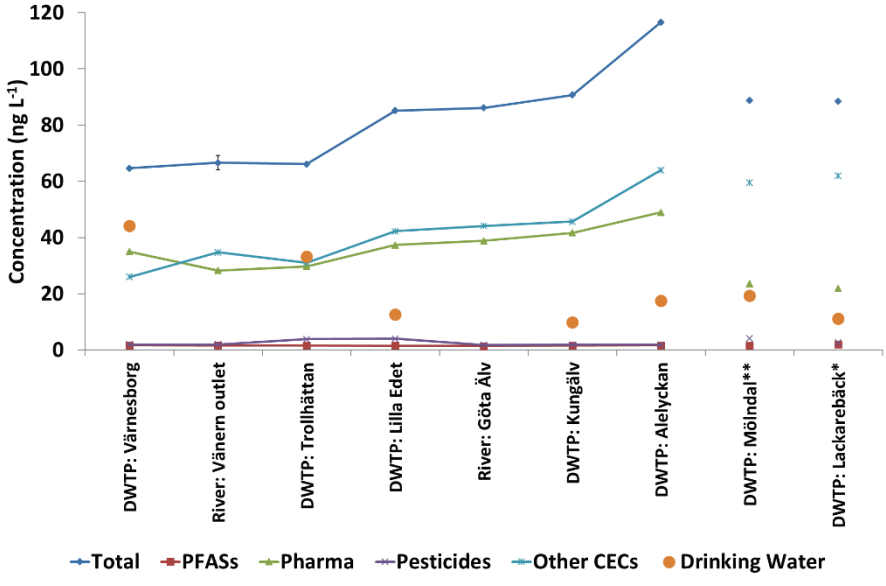

Figure 9. Total concentration (ng L^{-1}) of the 27 contaminants of emerging concern (CECs), and of the CEC subgroups PFASs, pharmaceuticals, pesticides, and other CECs, detected in river and raw water along (downstream, from left to right) the Göta Älv river (modified from **Paper II**). Total CEC concentrations (ng L^{-1}) in drinking water from corresponding drinking water treatment plants (DWTPs, n=7) are also shown (orange dots). Error bars for the total concentration at "River: Vänern outlet" indicate the standard deviation calculated from multiple samples (n=3) collected at that sampling point. *Not using Göta Älv as raw water directly; **not using Göta Älv as raw water at all.

As Figure 9 demonstrates, there was a similar trend of increasing CEC concentrations downstream of inputs of WWTP effluents as found in **Paper I**. In total, 27 different CECs were detected in the raw water, comprising seven PFASs, eight pharmaceuticals, seven pesticides and five other CECs. The number of detected CECs in the finished drinking water from the seven DWTPs studied varied from 17 to 22. In contrast to the study in **Paper I**, the total concentration of CECs found in the finished drinking water was lower than the corresponding raw water concentration from each DWTP ($p<0.001$, paired *t*-test).

5.3 Removal efficiency and influence of GAC operational age (Papers I & II)

The study in **Paper I** showed limited removal of CECs from the raw water, even though the DWTP was equipped with a GAC filter as part of the full-scale treatment process. This was likely due to the long deployment time (10+ years) of the GAC filter without any refill, replacement or regeneration. The study also included samples from a pilot plant that used the water after the sand filtration treatment step of the main treatment process. The pilot included a nanofiltration membrane (8" HFW 1000 filter, with a cut-off around 1000 Da), followed by GAC filtration. Samples were collected after a GAC filter employed for 5 months (old GAC in Figure 10) and a GAC filter only employed for one week (new GAC in Figure 10), both using water passed through the nanofiltration system. Figure 10 shows the total concentration of CECs for all compound groups and the total concentration of CECs after each treatment step.

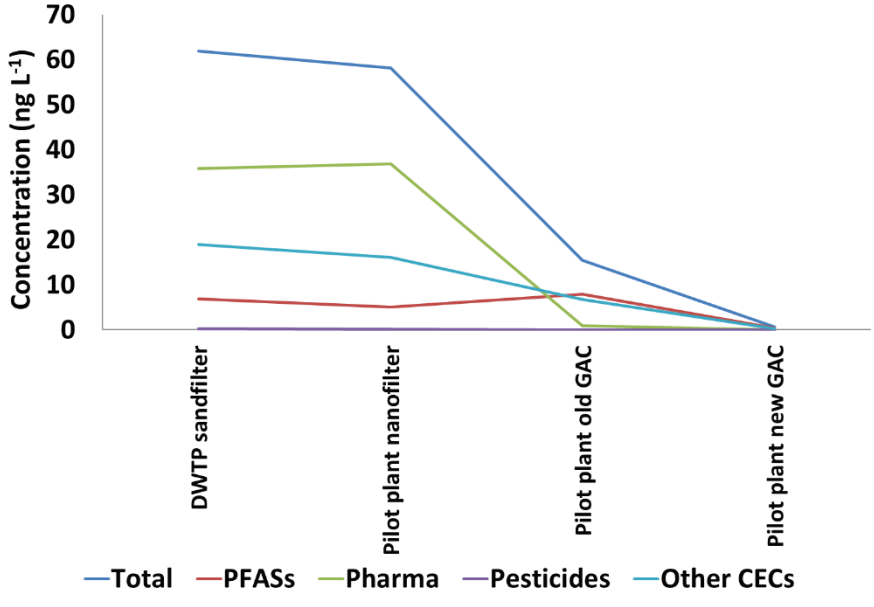

Figure 10. Total concentrations (ng L^{-1}) of contaminants of emerging concern (CECs), and of the CEC subgroups PFASs, pharmaceuticals, pesticides, and other CECs, in samples from the pilot-scale treatment plant (modified from **Paper I**).

In the pilot-scale plant, the total concentration of CECs decreased from 62 ng L^{-1} after the sand filtration and to 58 ng L^{-1} after the nanofiltration step. It further decreased to 16 ng L^{-1} after the old GAC and finally to 0.6 ng L^{-1} after the new

GAC. These findings show the importance of using fresh GAC for the removal of CECs from process water. The data in Figure 10 also suggest that PFASs are particularly challenging to remove from process water, unless a fresh GAC filter is employed.

To investigate the removal efficiency of different treatment techniques, raw water and drinking water samples from seven different full-scale DWTPs were analysed in the study in **Paper II**. Most of these DWTPs use the same river water (Göta Älv) as their main raw water. Thus, they typically have similar concentrations of CEC in their ingoing water. This permits comparison of the removal efficiencies across the DWTPs. Four of the seven DWTPs employ GAC filtration, one employs artificial infiltration and the two remaining plants employ only conventional treatment processes. When examining the removal efficiencies across the DWTPs, a clear distinction between PFASs and other compound groups was found. Therefore, PFASs were studied separately. Figure 11 presents a general overview of the treatment efficiency for each of the seven DWTPs.

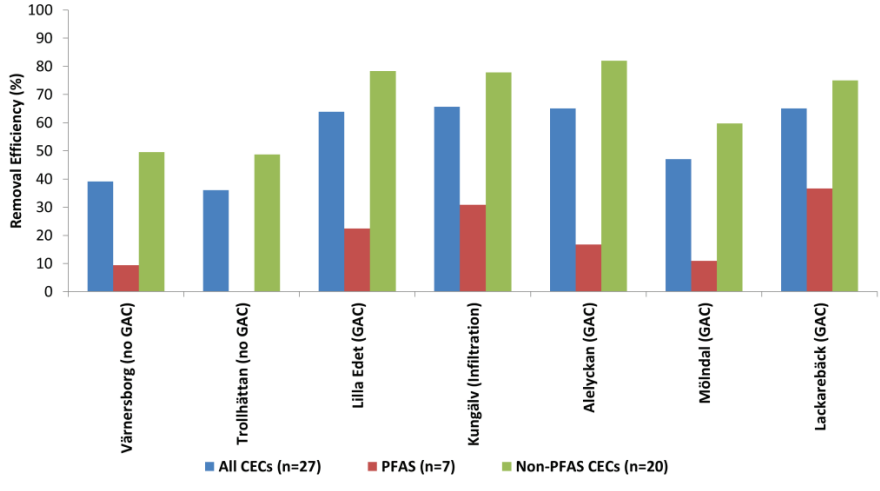

Figure 11. Removal efficiencies (%) for all contaminants of emerging concern (CECs), and for the two CEC subgroups PFASs and non-PFAS, at seven different drinking water treatment plants (DWTPs).

Total removal efficiency was lower for the two DWTPs without GAC or artificial infiltration (Vänersborg and Trollhättan). Vänersborg had an average (± standard deviation (SD)) total removal efficiency of 41% (±38%) and Trollhättan 35% (±37%) (Figure 11). These values are lower than the

corresponding average for Kungälv DWTP (using artificial infiltration), with an overall average removal efficiency of 67% (±37%) for all CECs. The four DWTPs that employed GAC filtration showed an average removal efficiency of 60% (range 49-63%, with SD varying from 34% to 37%. The DWTPs that employed GAC or artificial infiltration had significantly (p=0.014, one-sided t-test) higher removal efficiency than the two other DWTPs.

To further investigate the relationship between operational age and removal efficiency for GAC filters, samples from one of the DWTPs equipped with multiple GAC filters in parallel and with varying operational age were studied. Individual samples were collected after six different GAC filters. The results are presented in Figure 12.

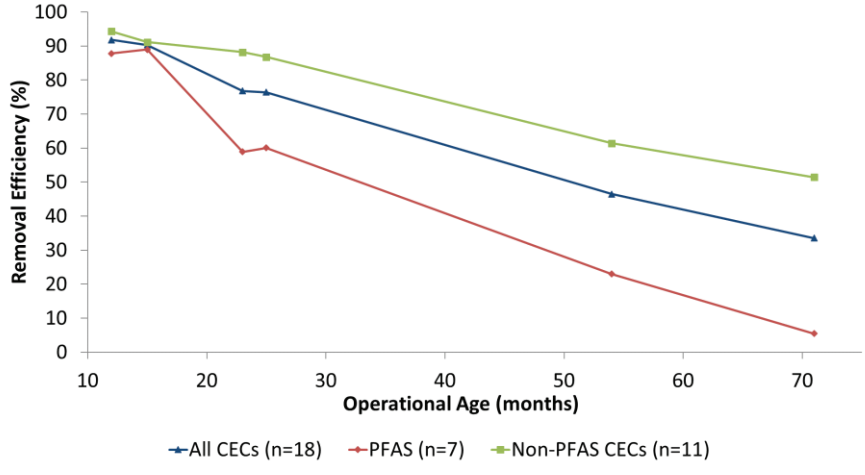

Figure 12. Removal efficiency (%) as a function of operational age of the granular activated carbon (GAC) filters for all contaminants of emerging concern (CECs), and for the two CEC subgroups PFASs and non-PFAS (modified from **Paper II**).

There was a clear decreasing trend in removal efficiency with increasing deployment time of the GAC. The average removal efficiency decreased from 92% and 90% after the youngest GAC filters (12 and 15 months, respectively) to only 46% for the 54-month-old filter, and the efficiency was even further decreased to 34% for the 71-month-old filter (Figure 12). PFASs decreased even more drastically than other (non-PFASs) compounds, going from 88-89% for the youngest filters down to only 5.4% for the oldest filter. The full-scale findings in **Paper II** were thus in good agreement with those in the pilot-scale study in **Paper I**.

5.4 International wide-scope screening of CECs in raw water and drinking water (Paper IV)

To expand the search for CECs of relevance in drinking water production, a multi-country study was conducted (**Paper IV**). The study included 13 DWTPs located in seven different European countries and four Asian countries (Figure 13). In total, 115 of 177 CECs analysed were detected in the raw water and 58 CECs in the drinking water, but with large variations between the different DWTPs.

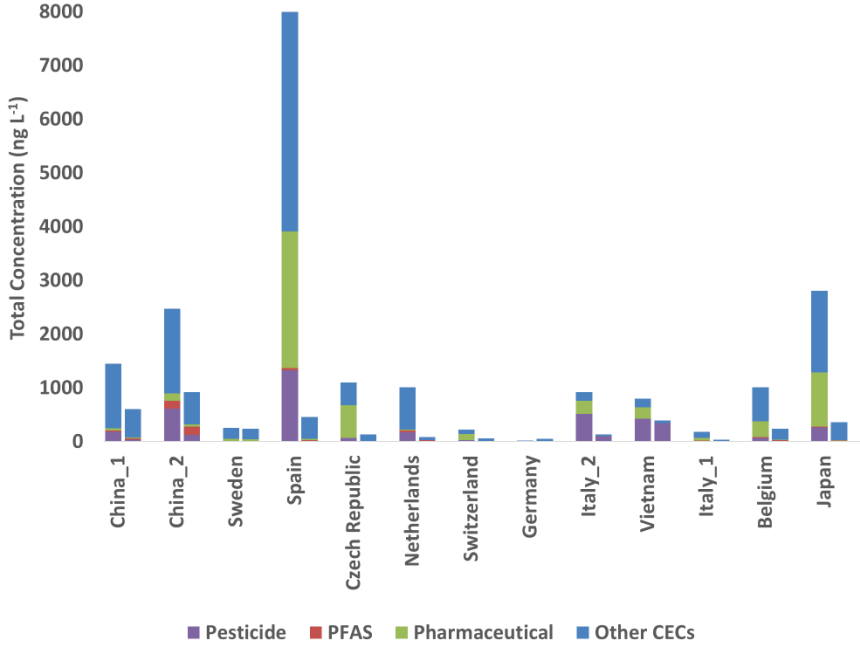

Figure 13. Total concentrations (ng L^{-1}) of all contaminants of emerging concern (CECs), and of the CEC subgroups pesticides, PFASs, pharmaceuticals and other CECs, in raw water (first bar) and drinking water (second bar) samples from the 13 selected drinking water treatment plants (DWTPs) in 11 European and Asian countries (modified from **Paper IV**).

As Figure 13 shows, there was a large spread in CEC concentrations in the raw water used by the different DWTPs. The number of CECs detected in the raw water varied from six (German DWTP) to 71 (Spanish DWTP). On average, 44 (±16) CECs were detected in the raw water from all 13 DWTPs. The number of CECs detected in the drinking water was lower, with an overall (all DWTPs) average of 19 (±8) for all DWTPs. The overall total concentration decreased from an average of 1500 ng L^{-1} (±2100 ng L^{-1}) in the raw water to 280 ng L^{-1} (±260 ng L^{-1}) in the drinking water.

The removal efficiencies for the different compound categories were also studied. Figure 14 shows the average removal efficiency for all CECs and for each individual compound group in the 13 different DWTPs.

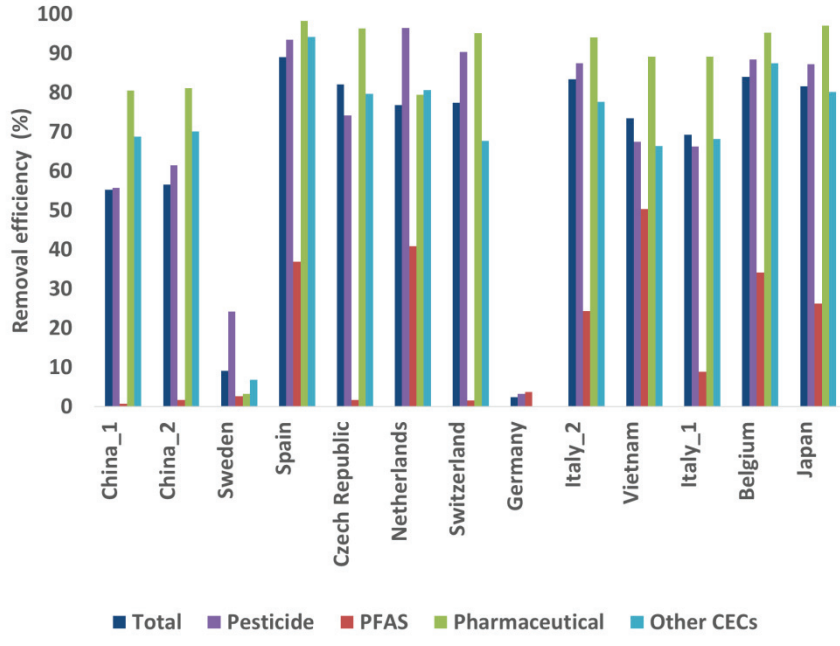

Figure 14. Average removal efficiency (%) for all contaminants of emerging concern (CECs) detected, and for the CEC subgroups pesticides, PFASs, pharmaceuticals and other CECs, in 13 drinking water treatment plants (DWTPs) in 11 European and Asian countries (modified from **Paper IV**).

The average total removal efficiency for all DWTPs was 65% (±28%), with removal efficiency ranging from 2.3% (Germany) to 89% (Spain). The high removal efficiency of the Spanish DWTP can likely be attributed to its implementation of reverse osmosis. As seen in Table 2, Germany and Vietnam had was the only DWTPs without GAC filtration, which in theory could lead to inefficient removal efficiency if no other advanced treatment steps are implemented. This was not the case for Vietnam, which showed total CEC removal of 73%. This was comparable to Italy_1 (69%), which has GAC filtration. The overall average removal of CECs in DWTPs with GAC treatment was 76% (±11%), with the Swedish DWTP (same as in **Paper I**) at the very low end (9.1%) because of high operational GAC age. In accordance with results in **Papers I & II**, PFASs showed the lowest removal efficiency among the compound categories, with an average of 18% (±18%) in the 13 different

DWTPs, while pharmaceuticals had the highest average removal of all the groups with 83% (±26%) (Figure 14).

Table 2. *Treatment steps in the 13 different drinking water treatment plants (DWTPs) in 11 European and Asian countries. Y = Yes, N = No (modified from* ***Paper IV****)*

Treatment Plant	Artificial infiltration	Pre-chlorination	Coagulation	Flocculation	Sedimentation	Rapid sand filtration	Slow sand filtration	GAC	Ultraviolet radiation	Chlorination	Ozonation	Ultrafiltration	Reverse osmosis
Belgium	N	N	Y	Y	Y	Y	N	Y	Y	Y	N	N	N
China #1	N	N	N	Y	Y	Y	N	Y	N	Y	Y	N	N
China #2	N	N	N	Y	Y	Y	N	Y	N	Y	Y	N	N
Czech Republic	N	N	Y	N	Y	Y	N	Y	Y	Y	Y	N	N
Germany	N	N	Y	Y	N	N	Y	N	N	Y	N	N	N
Italy #1	N	N	N	Y	N	Y	N	Y	N	N	Y	N	N
Italy #2	N	N	N	Y	Y	N	N	Y	N	Y	Y	N	N
Japan	N	N	Y	Y	Y	N	N	Y	N	Y	Y	N	N
Spain	N	Y	Y	N	Y	Y	N	Y	N	Y	Y	Y	Y
Sweden	N	N	Y	Y	Y	Y	N	Y	Y	Y	N	N	N
Switzerland	N	N	N	N	N	Y	Y	Y	N	N	Y	N	N
The Netherlands	Y	N	N	N	N	Y	N	Y	Y	N	N	N	N
Vietnam	N	Y	Y	Y	Y	Y	N	N	N	Y	N	N	N

5.5 Suspect screening and prediction of removal efficiency (Papers III & IV)

In total, 208 features were detected in the raw and drinking water samples from the study in **Paper IV** when using the suspect list with 500 suspects created with SusTool. Of these, 175 were unique suspects, meaning that some (n=33) had multiple possible detected peaks. To identify the suspect features representing the most relevant CECs for the selected DWTPs, the focus was on features occurring in drinking water, rather than in raw water. This is because humans are exposed to these compounds through drinking water, particularly in countries with high consumption of tap water without post-DWTP treatment. The exclusion of features only occurring in the raw water reduced the 208 features to 86. To maintain high relevance, only features detected in drinking water from at least two DWTPs were considered. This reduced the number of features to 39. These features were evaluated manually by judging whether the suspect feature was detected in the expected ion mode and had a realistic retention time, assessed from their polarity and active groups. This reduced the number of relevant features to 27. Of these, 19 had reference standards available for purchase. Two of the suspects (sucralose and tri-isopropanolamine) had already been analysed in the target method. In total, 17 reference compounds were purchased and used for confirmation. The standards consisted of: D-(−)-salicin, 4-hydroxyphenylpyruvic acid, serotonin, salidroside, ginkgolide A, ginkgolide J, ginkgolide C, helicin, chlorogenic acid, 5-amino-2-hydroxy-3-solfobenzoic acid, 7H-dodecafluoroheptanoic acid, DL-vanillactic acid lithium salt hydrate, dimidium bromide, dhurrin, asperuloside, γ-glu-cys and 4,4'-disulfanediylbis (2-aminobutanoic acid).

Most purchased reference compounds (16 out of 17) showed good ionisation and chromatography in the LC-HRMS analysis. Dhurrin did not ionise in either positive or negative ionisation mode and its corresponding feature was considered to be of unknown identity. The retention time of the reference compound did not match that of their corresponding suspected feature in 14 of the 16 other cases, and these features had to be classified as being of unknown identify. Vanillactic acid showed a similar retention time to the detected feature, but the fragmentation patterns did not match closely and confirmation was not possible. The feature corresponding to the 7H-dodecafluoroheptanoic acid standard was confirmed through both matching retention time and fragmentation. This compound has a similar structure to perfluoroheptanoic acid

(PFHpA), which was included in the target method and found in the raw water from all 13 DWTPs. The only difference between PFHpA and 7H-dodecafluoroheptanoic acid is that it is not fully fluorinated and one F atom is replaced with an H atom.

7H-dodecafluoroheptanoic was detected in both raw water and drinking water in the samples from China_1, China_2 and Italy_1, as well as in the drinking water samples from Spain, Czech Republic, Germany and Italy_2. The occurrence of a CEC in the drinking water, but not the raw water, could be explained *e.g.* by being formed during the treatment process or by desorbing from a GAC filter. 7H-dodecafluoroheptanoic acid has previously been tentatively identified using suspect screening in samples collected in China (Bade et al. 2015), but the study presented in **Paper IV** shows that this compound is fairly widespread.

An investigation of the behaviour of all 208 features detected in the DWTPs was performed. Even though the features were not confirmed, their removal from water is still of importance in the production of clean drinking water. The removal efficiency was estimated in a similar way as in the target analytes. Since no concentrations could be calculated, the response (area) of the features was used instead of quantities and, instead of substituting non-detected features in the drinking water with MDL/2, the cut-off for peak rejection in the data processing method (100) was used. The average removal efficiency of target analytes and the suspect features was then compared (Figure 15). To identify similarities in behaviour, the DWTPs were rearranged in order of decreasing average removal of the suspects. A trend line was added for the suspects and another for the targets. The two trend lines agreed relatively well, indicating that removal of a broad range of known compounds can be used as an indication of removal of unknown compounds. This observation may be of high value for drinking water producers globally in their planning for future treatment strategies to meet the increasing concern about human exposure to unknown CECs present in drinking water.

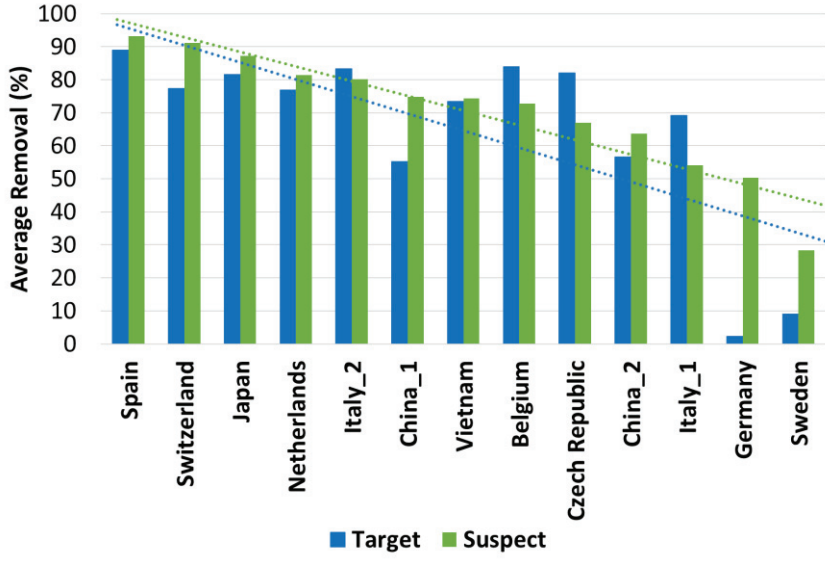

Figure 15. Comparison of the removal efficiency (%) of target compounds and suspect features in 13 drinking water treatment plants in 11 European and Asian countries (modified from **Paper IV**).

6 Conclusions and outlook

The main conclusions of this thesis are as follows:

- Internationally, there is large variation in raw water quality, with some waters containing orders of magnitude higher levels of CECs than others. This means that drinking water producers across the globe face different challenges and require access to accurate tools for identification and detection of relevant (potentially hazardous) CECs, as well as efficient treatment techniques. Current levels of known CECs in raw water from Sweden's two main sources are relatively low compared with those in other source waters studied.

- Current full-scale DWTPs show large variation in their CEC removal efficiency. This variation stems from the difference in treatment steps included in treatment process and the maintenance of treatment equipment (*e.g.* replacing or regenerating old GAC filters). However, new or unsaturated GAC filters are efficient in removing CECs. Promising alternative treatment techniques are nanofiltration and reverse osmosis, which appear to be efficient treatment steps for removing CECs.

- GAC treatment efficiency of CECs varies widely with deployment time and operational age, with an almost linear decrease in efficiency over time. Results from full-scale DWTPs agree well with pilot-scale data, including on a compound category basis, with PFASs shown to slip through more readily than other compound categories.

- Suspect screening and the subsequent confirmation process were successful in detection and identification of relevant, novel CECs previously not included in the target method. Thus, prioritisation by SusTool is useful for broad-scope screening of less well studied CECs.

The future outlook for drinking water producers across the globe is difficult and they face new challenging contaminants, so they require access to tools for identification and detection of relevant (potentially hazardous) CECs and efficient treatment techniques. The results presented in this thesis highlight the importance of wide-scope analytical methods in screening of CECs, in order to more comprehensively characterise water quality in terms of CEC occurrence. In the future, chemical analyses should be combined with broad toxicological methods to minimise the risk to humans from consumption of drinking water.

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Popular science summary

It is generally believed that tap water in developed countries, including Sweden, is safe to drink. Recognised problems with drinking water include bad odour or taste and contamination with pathogenic bacteria. This thesis showed that the levels of contaminants of emerging concern (CECs) are generally low in Swedish drinking water. No drinking water sample collected in Sweden showed concentrations of CECs above limit values. However, some CEC groups, such as perfluoroalkyl substances (PFASs), can pose a risk to humans due to their high persistency and bioaccumulative and potential toxic characteristics. PFASs are difficult to remove during drinking water treatment, and thus it is important to monitor their levels in the raw water and in drinking water.

Most compounds can be removed by using granulated activated carbon filters during drinking water treatment, but it is important that these filters are replaced or regenerated on a regular basis, since they lose their effectiveness with deployment time. Promising alternative treatment techniques are nanofiltration and reverse osmosis, which can efficiently reduce the levels of CECs during drinking water treatment.

Thousands of synthetic chemicals are currently in use worldwide and only a few of these are well studied and regulated, so it must be accepted that it is impossible to continuously monitor all synthetic chemicals at every drinking water production site across the globe. It is therefore crucial that researchers continue to develop and improve methods for screening for a broad range of CECs, to detect new potential threats to drinking water quality. The use of suspect screening, where compounds can be screened for without prior access to a reference standard, was shown to be a fruitful approach in this thesis, and enabled identification of a previously sparsely studied chemical compound (PFAS). In conclusion, drinking water producers are generally well aware of the occurrence of unwanted compounds in their raw water and have employed techniques to mitigate any unwanted substances. Based on current knowledge, it appears that drinking Swedish tap water in large quantities poses no risk to human health.

Populärvetenskaplig sammanfattning

Den allmänna uppfattningen i västvärlden, Sverige inkluderat, är att kranvatten är säkert att dricka, och att de problem som nu och då uppstår har att göra med dålig lukt eller smak och i vissa fall farliga bakterier. Denna avhandling bekräftar att nivåerna av oönskade kemiska föroreningar i allmänhet är låga i Svenskt dricksvatten. Inget dricksvatten från Sverige som analyserats inom ramen för den här avhandlingen hade föroreningshalter över de gränsvärden som finns. Vissa oönskade ämnen, såsom högfluorerade ämnen (PFAS) kan dock orsaka problem. De är långlivade, bioackumulera och kan ha hälsofarliga egenskaper. Förhöjda halter av PFAS i dricksvatten kan därför utgöra en risk för människors hälsa. Dessutom är det svårt att rena bort PFAS från dricksvatten och det är därför viktigt att övervaka deras förekomst i rå- och dricksvatten

De flesta oönskade ämnen kan renas bort genom att använda sig av granulerat aktivt kol som ett filter, men det är då viktigt att byta ut eller regenerera materialet regelbundet då det förlorar sin effektivitet med användningstid. Lovande alternativa reningstekniker är nanofiltrering och omvänd osmos, som har visat sig vara effektiva för att minska förekomst av oönskade ämnen i dricksvatten.

Tusentals kemikalier är i användning världen över, varav få är väl studerade och har gränsvärden. Vi måste vi acceptera att det är omöjligt att kontinuerligt övervaka alla ämnen vid all dricksvattenproduktion. Det är därför viktigt att forskningen fortsätter utveckla bättre metoder för att screena efter ett brett spektrum av oönskade ämnen. Genom så kallad ”suspect screening” kan man leta efter ämnen utan att ha tillgång till en referensstandard. Denna metod testades framgångsrikt i den här avhandlingen och resulterade i att ytterligare ett nytt PFAS ämne kunde identifieras. Sammanfattningsvis är dricksvattenproducenterna i allmänhet väl medvetna om förekomsten av oönskade ämnen i deras råvatten och använder tekniker för att rena det. Med nuvarande kunskap finns det inget som talar för att vi inte har ett säkert dricksvatten i Sverige. Vi kan därför fortsätta dricka vårt kranvatten utan med ro.

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Appendix

Table A1. *All compounds analysed in* ***Papers I, II & IV****. MDL = method detection limit, DA = Dalton*

Compound	CAS#	Compound Group	Ion Mode	Neutral Mass (Da)	MDL (ng/L)	Paper #
2.4-Dichlorophenoxyacetic acid	94-75-7	Pesticide	-	219.9694	25.64	Paper I
2.6-Dichlorbenzamid (BAM)	2008-58-4	Pesticide	+	188.97482	16.18	Paper I
Acetaminophen	103-90-2	PPCP	+	151.06333	17.52	Paper I
Acetamiprid	135410-20-7	Pesticide	+	222.06722	0.51	Paper I
Alachlor	15972-60-8	Pesticide	+	269.11826	1.07	Paper I
Albendazole sulfone	75184-71-3	PPCP	+	297.07833	0.55	Paper I
Amidosulfuron	120923-37-7	Pesticide	+	369.04129	0.55	Paper I
Amitryptiline	50-48-6	PPCP	+	277.18305	0.13	Paper I
Atenolol	29122-68-7	PPCP	+	266.16304	0.30	Paper I
Atrazine	1912-24-9	Pesticide	+	215.09377	0.40	Paper I
Atrazine-desethyl	6190-65-4	Pesticide	+	187.06247	3.02	Paper I
Atrazine-desisopropyl	1007-28-9	Pesticide	+	173.04682	1.77	Paper I
Azithromycin	83905-01-5	PPCP	+	748.50853	0.08	Paper I
Azoxystrobin	131860-33-8	Pesticide	+	403.11682	0.03	Paper I
Bentazon	25057-89-0	Pesticide	-	240.05686	0.17	Paper I
Benzoylecgonine	519-09-5	Drug	+	289.13141	0.09	Paper I
Bezafibrate	41859-67-0	PPCP	+	361.10809	0.25	Paper I
Bicalutamide	90357-06-5	PPCP	-	430.06104	0.02	Paper I
Bifenox-acid	53774-07-5	Pesticide	-	326.97013	8.12	Paper I
Bitertanol	55179-31-2	Pesticide	+	337.17903	4.24	Paper I

Caffeine	58-08-2	Food additive	+	194.08038	1.01	Paper I
Carbamazepine	298-46-4	PPCP	+	236.09496	0.14	Paper I
Carbendazim	10605-21-7	Pesticide	+	191.06948	0.84	Paper I
Carbofuran	1563-66-2	Pesticide	+	221.10519	8.25	Paper I
Carfentrazone-ethyl	128639-02-1	Pesticide	+	411.03643	2.89	Paper I
Chlorfenvinphos	470-90-6	Pesticide	+	357.96953	0.10	Paper I
Chloridazon (Pyrazon)	1698-60-8	Pesticide	+	221.03559	0.34	Paper I
Citalopram	59729-33-8	PPCP	+	324.16379	0.13	Paper I
Clarithromycin	81103-11-9	PPCP	+	747.47689	0.04	Paper I
Climbazole	38083-17-9	PPCP	+	292.09786	0.05	Paper I
Clomazone	81777-89-1	Pesticide	+	239.07131	2.28	Paper I
Clopidogrel	113665-84-2	PPCP	+	321.05903	0.04	Paper I
Codeine	76-57-3	PPCP	+	299.15214	0.22	Paper I
Cotinine	486-56-6	Drug	+	176.09496	0.23	Paper I
Cyanazine	21725-46-2	Pesticide	+	240.08902	0.51	Paper I
Cyprodinil	121552-61-2	Pesticide	+	225.12660	0.12	Paper I
Diazepam	439-14-5	PPCP	+	284.07164	0.06	Paper I
Dichlorprop	120-36-5	Pesticide	-	233.98505	16.54	Paper I
Diclofenac	15307-86-5	PPCP	-	295.01668	15.23	Paper I
Difenoconazole	119446-68-3	Pesticide	+	405.06470	0.08	Paper I
Diflufenican	83164-33-4	Pesticide	+	394.07407	1.08	Paper I
Diltiazem	42399-41-7	PPCP	+	414.16133	0.09	Paper I
Dimethoate	60-51-5	Pesticide	+	228.99962	9.55	Paper I
Diuron	330-54-1	Pesticide	+	232.01702	0.62	Paper I
Epoxiconazole	133855-98-8	Pesticide	+	658.14624	0.10	Paper I
Erythromycin	114-07-8	PPCP	+	733.46124	0.06	Paper I
Fenpropidin	67306-00-7	Pesticide	+	273.24565	0.07	Paper I
Fenpropimorph	67564-91-4	Pesticide	+	303.25621	0.05	Paper I
Flamprop	58667-63-3	Pesticide	-	321.05680	0.60	Paper I
Fluazinam	79622-59-6	Pesticide	-	463.95138	0.07	Paper I
Fluconazole	86386-73-4	PPCP	+	306.10407	0.54	Paper I
Fludioxonil	131341-86-1	Pesticide	-	248.03973	0.04	Paper I
Fluoxetine	54910-89-3	PPCP	+	309.13405	2.37	Paper I
Flurprimidol	56425-91-3	Pesticide	+	312.10856	0.39	Paper I
Flusilazole	85509-19-9	Pesticide	+	315.10033	0.08	Paper I
Flutriafol	76674-21-0	Pesticide	+	301.10267	0.27	Paper I

Foramsulfuron	173159-57-4	Pesticide	+	452.11142	15.61	Paper I
Fuberidazole	3878-19-1	Pesticide	+	184.06366	0.36	Paper I
Furosemide	54-31-9	PPCP	-	330.00772	85.52	Paper I
Hexazinone	51235-04-2	Pesticide	+	252.15863	0.28	Paper I
Hexythiazox	78587-05-0	Pesticide	+	352.10123	4.84	Paper I
Hydrochlorothiazide	58-93-5	PPCP	-	296.96447	2.55	Paper I
Imazalil	35554-44-0	Pesticide	+	296.04832	0.13	Paper I
Imidacloprid	138261-41-3	Pesticide	+	255.05230	0.95	Paper I
Irbesartan	138402-11-6	PPCP	-	428.23246	0.22	Paper I
Isoproturon	34123-59-6	Pesticide	+	206.14191	0.24	Paper I
Ketoprofen	22071-15-4	PPCP	+	254.09429	3.16	Paper I
Lamotrigine	84057-84-1	PPCP	+	255.00785	0.16	Paper I
Lidocaine	137-58-6	PPCP	+	234.17321	0.14	Paper I
Linuron	330-55-2	Pesticide	+	248.01193	4.19	Paper I
Losartan	114798-26-4	PPCP	-	422.16219	1.24	Paper I
Mandipropamid	374726-62-2	Pesticide	+	411.12374	0.05	Paper I
MCPA	94-74-6	Pesticide	-	200.02402	19.37	Paper I
Mecoprop	7085-19-0	Pesticide	-	214.03967	14.38	Paper I
Metalaxyl	57837-19-1	Pesticide	+	279.14706	0.10	Paper I
Metamitron	41394-05-2	Pesticide	+	202.08546	0.73	Paper I
Metazachlor	67129-08-2	Pesticide	+	277.09819	1.33	Paper I
Methabenzthiazuron	18691-97-9	Pesticide	+	221.06228	0.95	Paper I
Metolachlor	51218-45-2	Pesticide	+	283.13391	0.08	Paper I
Metoprolol	51384-51-1	PPCP	+	267.18344	0.23	Paper I
Metrafenone	220899-03-6	Pesticide	+	408.05724	0.08	Paper I
Metribuzin	21087-64-9	Pesticide	+	214.08883	0.79	Paper I
Metsulfuron methyl	74223-64-6	Pesticide	+	381.07430	0.16	Paper I
Naproxen	22204-53-1	PPCP	+	230.09429	1.14	Paper I
Nicotine	54-11-5	Drug	+	162.11570	0.68	Paper I
Ofloxacin	82419-36-1	PPCP	+	361.14378	0.90	Paper I
Oxazepam	604-75-1	PPCP	+	286.05091	0.52	Paper I
Oxycodone	76-42-6	PPCP	+	315.14706	0.43	Paper I
Penconazole	66246-88-6	Pesticide	+	283.06430	0.13	Paper I
Perfluorobutane sulfonic acid (PFBS)	375-73-5	PFAS	-	299.95027	0.01	Paper I
Perfluorodecanoic acid (PFDA)	335-76-2	PFAS	-	513.96732	0.02	Paper I
Perfluorododecanoic acid (PFDoDA)	307-55-1	PFAS	-	613.96093	0.14	Paper I

Perfluoroheptanoic acid (PFHpA)	375-85-9	PFAS	-	363.97690	0.04	Paper I
perfluorohexane sulfonic acid (PFHxS)	355-46-4	PFAS	-	399.94388	0.01	Paper I
Perfluorohexanoic acid (PFHxA)	307-24-4	PFAS	-	313.98009	0.13	Paper I
Perfluorononanoic acid (PFNA)	375-95-1	PFAS	-	463.97051	0.02	Paper I
Perfluorooctane sulfonamide (FOSA)	754-91-6	PFAS	-	498.95348	0.05	Paper I
Perfluorooctane sulfonic acid (PFOS)	1763-23-1	PFAS	-	499.93749	0.01	Paper I
Perfluorooctanoic acid (PFOA)	335-67-1	PFAS	-	413.97370	0.03	Paper I
Perfluoropentanoic acid (PFPeA)	2706-90-3	PFAS	-	263.98328	2.90	Paper I
Perfluoroundecanoic acid (PFUnDA)	2058-94-8	PFAS	-	563.96412	0.04	Paper I
Picoxystrobin	117428-22-5	Pesticide	+	367.10314	0.24	Paper I
Pirimicarb	23103-98-2	Pesticide	+	238.14298	0.20	Paper I
Prochloraz	67747-09-5	Pesticide	+	375.03081	0.13	Paper I
Propamocarb	24579-73-5	Pesticide	+	188.15248	0.72	Paper I
Propiconazole	60207-90-1	Pesticide	+	341.06978	0.07	Paper I
Propranolol	525-66-6	PPCP	+	259.15723	0.64	Paper I
Propyzamide	23950-58-5	Pesticide	+	255.02177	10.82	Paper I
Prosulfocarb	52888-80-9	Pesticide	+	251.13439	0.36	Paper I
Pyraclostrobin	175013-18-0	Pesticide	+	387.09858	0.04	Paper I
Pyroxsulam	422556-08-9	Pesticide	+	434.06202	0.04	Paper I
Quinmerac	90717-03-6	PPCP	+	221.02436	8.03	Paper I
Quinoxyfen	124495-18-7	Pesticide	+	306.99670	0.15	Paper I
Rimsulfuron	122931-48-0	Pesticide	+	431.05694	0.87	Paper I
Roxithromycin	80214-83-1	PPCP	+	836.52457	0.03	Paper I
Silthiofam	175217-20-6	Pesticide	+	267.11131	0.20	Paper I
Simazine	122-34-9	Pesticide	+	201.07812	0.60	Paper I
Sotalol	3930-20-9	PPCP	+	272.11946	5.14	Paper I
Spiroxamine	118134-30-8	Pesticide	+	297.26678	0.11	Paper I
Sucralose	56038-13-2	Food Additive	-	396.01455	6.59	Paper I
Sulfamethoxazole	723-46-6	PPCP	+	253.05211	2.66	Paper I
Sulfosulfuron	141776-32-1	Pesticide	+	470.06784	0.36	Paper I
Tamoxifen	10540-29-1	PPCP	+	371.22491	0.26	Paper I
Terbuthylazine	5915-41-3	Pesticide	+	229.10942	0.41	Paper I
Terbutryn	886-50-0	Pesticide	+	241.13612	0.05	Paper I
Thiacloprid	111988-49-9	Pesticide	+	252.02364	0.42	Paper I
Thiamethoxam	153719-23-4	Pesticide	+	291.01929	0.67	Paper I
Thifensulfuron methyl	79277-27-3	Pesticide	+	387.03072	0.19	Paper I

Tramadol	27203-92-5	PPCP	+	263.18853	0.23	Paper I
Trifloxystrobin	141517-21-7	Pesticide	+	408.12969	0.04	Paper I
Triflusulfuron-methyl	126535-15-7	Pesticide	+	492.10389	0.05	Paper I
Triticonazole	131983-72-7	Pesticide	+	317.12949	0.21	Paper I
Valsartan	137862-53-4	PPCP	-	435.22704	1.14	Paper I
Venlafaxine	93413-69-5	PPCP	+	277.20418	0.21	Paper I
1H-benzotriazole	95-14-7	Benzos	+	119.0484	0.13	Paper II
2.4.6-TBP	118-79-6	Flameretardant	-	327.7734	0.29	Paper II
2.4-Dichlorophenoxyacetic acid	94-75-7	Pesticide	-	219.9694	2.18	Paper II
4-Methyl-1H-benzotriazole	29385-43-1	Benzos	+	133.0640	0.06	Paper II
5.6-dimentyl-1H-benzotriazole hydrate	1354973-50-4	Benzos	-	147.0797	0.41	Paper II
5-chlorobenzotriazole (CBT)	94-97-3	Benzos	-	153.0094	0.10	Paper II
Acetaminophen	103-90-2	Pharmaceutical	+	151.0633	0.06	Paper II
Acetamiprid	135410-20-7	Pesticide	+	222.0672	0.01	Paper II
Alachlor	15972-60-8	Pesticide	+	269.1183	0.05	Paper II
Amidosulfuron	120923-37-7	Pesticide	+	369.0413	0.19	Paper II
Amitryptiline	50-48-6	Pharmaceutical	+	277.1831	0.01	Paper II
Atenolol	29122-68-7	Pharmaceutical	+	266.1630	0.06	Paper II
Atrazine	1912-24-9	Pesticide	+	215.0938	0.01	Paper II
Atrazine-desethyl	6190-65-4	Pesticide	+	187.0625	0.03	Paper II
Atrazine-desisopropyl	1007-28-9	Pesticide	+	173.0468	0.04	Paper II
Azithromycin	83905-01-5	Pharmaceutical	+	748.5085	0.04	Paper II
Azoxystrobin	131860-33-8	Pesticide	+	403.1168	0.004	Paper II
Bentazon	25057-89-0	Pesticide	-	240.0569	0.05	Paper II
Benzothiazole-2-sulfonic acid (BTSA)	941-57-1	Benzos	-	214.9711	0.41	Paper II
Bezafibrate	41859-67-0	Pharmaceutical	+	361.1081	0.02	Paper II
Bicalutamide	90357-06-5	Pharmaceutical	-	430.0610	0.003	Paper II
Bifenox-acid	53774-07-5	Pesticide	-	326.9701	1.16	Paper II
Bis(2-ethylhexyl) phthalate (DEHP)	117-81-7	Phthalate	+	390.2770	0.10	Paper II
Budesonide	51333-22-3	Pharmaceutical	+	430.2355	0.06	Paper II
Caffeine	58-08-2	Food Additive	+	194.0804	0.06	Paper II
Carbamazepine	298-46-4	Pharmaceutical	+	236.0950	0.57	Paper II
Carbendazim	10605-21-7	Pesticide	+	191.0695	0.03	Paper II
Carbofuran	1563-66-2	Pesticide	+	221.1052	0.48	Paper II
Carfentrazone-ethyl	128639-02-1	Pesticide	+	411.0364	5.09	Paper II
Cetirizine	83881-51-0	Pharmaceutical	+	388.1554	0.01	Paper II

Chloramphenicol	56-75-7	Pharmaceutical	-	322.0123	0.03	Paper II
Chlorfenvinphos	470-90-6	Pesticide	+	357.9695	0.01	Paper II
Chloridazon (Pyrazon)	1698-60-8	Pesticide	+	221.0356	0.01	Paper II
Citalopram	59729-33-8	Pharmaceutical	+	324.1638	0.01	Paper II
Clarithromycin	81103-11-9	Pharmaceutical	+	747.4769	0.01	Paper II
Climbazole	38083-17-9	Pharmaceutical	+	292.0979	0.003	Paper II
Clomazone	81777-89-1	Pesticide	+	239.0713	0.06	Paper II
Clopidogrel	113665-84-2	Pharmaceutical	+	321.0590	0.003	Paper II
Cocaine	50-36-2	Drug	+	303.1471	0.01	Paper II
Codeine	76-57-3	Pharmaceutical	+	299.1521	0.01	Paper II
Cresyl diphenyl phosphate (CDP)	945-730-9	Flameretardant	+	340.0865	0.01	Paper II
Cyanazine	21725-46-2	Pesticide	+	240.0890	0.02	Paper II
Cyazofamid	120116-88-3	Pesticide	+	324.0448	0.20	Paper II
Cybutryne	28159-98-0	Pesticide	+	253.1361	0.004	Paper II
Cyprodinil	121552-61-2	Pesticide	+	225.1266	0.01	Paper II
Diazepam	439-14-5	Pharmaceutical	+	284.0716	0.004	Paper II
Dichlorprop	120-36-5	Pesticide	-	233.9851	1.41	Paper II
Diclofenac	15307-86-5	Pharmaceutical	-	295.0167	0.48	Paper II
Difenoconazole	119446-68-3	Pesticide	+	405.0647	0.005	Paper II
Diflufenican	83164-33-4	Pesticide	-	394.0741	0.06	Paper II
Dimethoate	60-51-5	Pesticide	+	228.9996	0.63	Paper II
Diuron	330-54-1	Pesticide	+	232.0170	0.03	Paper II
Enalapril	75847-73-3	Pharmaceutical	+	376.1998	0.01	Paper II
Epoxiconazole	133855-98-8	Pesticide	+	658.1462	0.64	Paper II
Erythromycin	114-07-8	Pharmaceutical	+	733.4612	0.08	Paper II
Fenarimol	60168-88-9	Pesticide	+	330.0327	0.02	Paper II
Fenpropidin	67306-00-7	Pesticide	+	273.2457	0.01	Paper II
Fenpropimorph	67564-91-4	Pesticide	+	303.2562	0.01	Paper II
Fluazinam	79622-59-6	Pesticide	-	463.9514	0.004	Paper II
Fluconazole	86386-73-4	Pharmaceutical	+	306.1041	0.02	Paper II
Fludioxonil	131341-86-1	Pesticide	-	248.0397	0.01	Paper II
Flurprimidol	56425-91-3	Pesticide	+	312.1086	0.03	Paper II
Flusilazole	85509-19-9	Pesticide	+	315.1003	0.004	Paper II
Flutriafol	76674-21-0	Pesticide	+	301.1027	0.02	Paper II
Foramsulfuron	173159-57-4	Pesticide	+	452.1114	0.26	Paper II
Fuberidazole	3878-19-1	Pesticide	+	184.0637	0.01	Paper II

Gemfibrozil	25812-30-0	Pharmaceutical	-	250.1569	0.61	Paper II
Hexazinone	51235-04-2	Pesticide	+	252.1586	0.01	Paper II
Hexythiazox	78587-05-0	Pesticide	+	352.1012	0.12	Paper II
Ifosfamide	3778-73-2	Pharmaceutical	+	260.0248	0.01	Paper II
Imazalil	35554-44-0	Pesticide	+	296.0483	0.003	Paper II
Imidacloprid	138261-41-3	Pesticide	+	255.0523	0.06	Paper II
Irbesartan	138402-11-6	Pharmaceutical	+	428.2325	0.01	Paper II
Isoproturon	34123-59-6	Pesticide	+	206.1419	0.01	Paper II
Ketoprofen	22071-15-4	Pharmaceutical	+	254.0943	0.11	Paper II
Lamotrigine	84057-84-1	Pharmaceutical	+	255.0079	0.01	Paper II
Lidocaine	137-58-6	Pharmaceutical	+	234.1732	0.01	Paper II
Linuron	330-55-2	Pesticide	+	248.0119	0.15	Paper II
Losartan	114798-26-4	Pharmaceutical	-	422.1622	0.11	Paper II
Mandipropamid	374726-62-2	Pesticide	+	411.1237	0.01	Paper II
MCPA	94-74-6	Pesticide	-	200.0240	0.98	Paper II
Meclofenamic acid	644-62-2	Pharmaceutical	-	295.0167	0.44	Paper II
Mecoprop	7085-19-0	Pesticide	-	214.0397	0.84	Paper II
Metalaxyl	57837-19-1	Pesticide	+	279.1471	0.01	Paper II
Metamitron	41394-05-2	Pesticide	+	202.0855	0.01	Paper II
Metazachlor	67129-08-2	Pesticide	+	277.0982	0.11	Paper II
Methabenzthiazuron	18691-97-9	Pesticide	+	221.0623	0.02	Paper II
Metolachlor	51218-45-2	Pesticide	+	283.1339	0.01	Paper II
Metoprolol	51384-51-1	Pharmaceutical	+	267.1834	0.09	Paper II
Metrafenone	220899-03-6	Pesticide	+	408.0572	0.01	Paper II
Metribuzin	21087-64-9	Pesticide	+	214.0888	0.02	Paper II
Metronidazole	443-48-1	Pharmaceutical	+	171.0644	0.26	Paper II
Metsulfuron methyl	74223-64-6	Pesticide	+	381.0743	0.03	Paper II
Mirtazapine	61337-67-5	Pharmaceutical	+	265.1579	0.01	Paper II
Monobenzyl phthalate (MP)	2528-16-7	Phthalate	-	256.0736	0.25	Paper II
Monobutyl phthalate (MBP)	131-70-4	Phthalate	-	222.0892	0.77	Paper II
Morphine	57-27-2	Drug	+	285.1365	0.04	Paper II
Nicotine	54-11-5	Drug	+	162.1157	0.04	Paper II
Niflumic acid	4394-00-7	Pharmaceutical	-	282.0616	0.01	Paper II
Ofloxacin	82419-36-1	Pharmaceutical	+	361.1438	0.02	Paper II
Omeprazole	73590-58-6	Pharmaceutical	+	345.1147	1.38	Paper II
Oxazepam	604-75-1	Pharmaceutical	+	286.0509	0.04	Paper II

Oxazepam	604-75-1	Pharmaceutical	-	286.0509	0.29	Paper II
Oxycodone	76-42-6	Pharmaceutical	+	315.1471	0.02	Paper II
Penconazole	66246-88-6	Pesticide	+	283.0643	0.01	Paper II
Perfluorobutane sulfonic acid (PFBS)	375-73-5	PFAS	-	299.9503	0.004	Paper II
Perfluorodecanoic acid (PFDA)	335-76-2	PFAS	-	513.9673	0.005	Paper II
Perfluorododecanoic acid (PFDoDA)	307-55-1	PFAS	-	613.9609	0.004	Paper II
Perfluoroheptanoic acid (PFHpA)	375-85-9	PFAS	-	363.9769	0.02	Paper II
Perfluorohexane sulfonic acid (PFHxS)	355-46-4	PFAS	-	399.9439	0.004	Paper II
Perfluorohexanoic acid (PFHxA)	307-24-4	PFAS	-	313.9801	0.05	Paper II
Perfluorononanoic acid (PFNA)	375-95-1	PFAS	-	463.9705	0.01	Paper II
Perfluorooctane sulfonamide (FOSA)	754-91-6	PFAS	-	498.9535	0.01	Paper II
Perfluorooctane sulfonic acid (PFOS)	1763-23-1	PFAS	-	499.9375	0.003	Paper II
Perfluorooctanoic acid (PFOA)	335-67-1	PFAS	-	413.9737	0.01	Paper II
Perfluoropentanoic acid (PFPeA)	2706-90-3	PFAS	-	263.9833	0.65	Paper II
Perfluorotetradecanoic acid (PFTeDA)	376-06-7	PFAS	-	713.9545	0.003	Paper II
Perfluoroundecanoic acid (PFUnDA)	2058-94-8	PFAS	-	563.9641	0.004	Paper II
Picoxystrobin	117428-22-5	Pesticide	+	367.1031	0.15	Paper II
Pirimicarb	23103-98-2	Pesticide	+	238.1430	0.02	Paper II
Prochloraz	67747-09-5	Pesticide	+	375.0308	0.01	Paper II
Propamocarb	24579-73-5	Pesticide	+	188.1525	0.01	Paper II
Propiconazole	60207-90-1	Pesticide	+	341.0698	0.004	Paper II
Propoxycarbazone	145026-81-9	Pesticide	+	398.0896	0.09	Paper II
Propranolol	525-66-6	Pharmaceutical	+	259.1572	0.02	Paper II
Prosulfocarb	52888-80-9	Pesticide	+	251.1344	0.15	Paper II
Pyraclostrobin	175013-18-0	Pesticide	+	387.0986	0.003	Paper II
Pyrimethamine	58-14-0	Pharmaceutical	+	248.0829	0.01	Paper II
Pyroxsulam	422556-08-9	Pesticide	+	434.0620	0.01	Paper II
Quinoxyfen	124495-18-7	Pesticide	+	306.9967	0.005	Paper II
Ramipril	87333-19-5	Pharmaceutical	+	416.2311	0.004	Paper II
Rimsulfuron	122931-48-0	Pesticide	+	431.0569	0.44	Paper II
Roxithromycin	80214-83-1	Pharmaceutical	+	836.5246	0.01	Paper II
Silthiofam	175217-20-6	Pesticide	+	267.1113	0.01	Paper II
Simazine	122-34-9	Pesticide	+	201.0781	0.01	Paper II
Sotalol	3930-20-9	Pharmaceutical	+	272.1195	0.14	Paper II
Spiroxamine	118134-30-8	Pesticide	+	297.2668	0.01	Paper II
Sulfamethoxazole	723-46-6	Pharmaceutical	+	253.0521	2.26	Paper II

Sulfosulfuron	141776-32-1	Pesticide	+	470.0678	0.08	Paper II
Terbuthylazine	5915-41-3	Pesticide	+	229.1094	0.01	Paper II
Terbuthylazine-desethyl	30125-63-4	Pesticide	+	201.0781	0.08	Paper II
Terbutryn	886-50-0	Pesticide	+	241.1361	0.003	Paper II
Thiabendazole	148-79-8	Pharmaceutical	+	201.0361	0.01	Paper II
Thiacloprid	111988-49-9	Pesticide	+	252.0236	0.02	Paper II
Thiamethoxam	153719-23-4	Pesticide	+	291.0193	0.07	Paper II
Thifensulfuron methyl	79277-27-3	Pesticide	+	387.0307	0.05	Paper II
Tramadol	27203-92-5	Pharmaceutical	+	263.1885	0.01	Paper II
Tributyl phosphate (TNBP)	126-73-8	Flameretardant	+	266.1647	0.04	Paper II
Triethyl Phosphate (TEP)	78-40-0	Flameretardant	+	182.0708	0.15	Paper II
Trifloxystrobin	141517-21-7	Pesticide	+	408.1297	0.01	Paper II
Triflusulfuron-methyl	126535-15-7	Pesticide	-	492.1039	0.20	Paper II
Triflusulfuron-methyl	126535-15-7	Pesticide	+	492.1039	0.01	Paper II
Triisopropyl phosphate (TiPP)	513-02-0	Flameretardant	+	224.1178	0.09	Paper II
Trimethoprim	738-70-5	Pharmaceutical	+	290.1379	0.11	Paper II
Triphenyl phosphate (TPHP)	115-86-6	Flameretardant	+	326.0708	0.003	Paper II
Tris(2-chloroethyl) phosphate (TCEP)	115-96-8	Flameretardant	+	283.9539	0.17	Paper II
Tris(4-tertbutylphenyl) phosphate (TBPP)	78-33-1	Flameretardant	+	494.2586	0.002	Paper II
Triticonazole	131983-72-7	Pesticide	+	317.1295	0.01	Paper II
Valsartan	137862-53-4	Pharmaceutical	-	435.2270	0.10	Paper II
Venlafaxine	93413-69-5	Pharmaceutical	+	277.2042	0.01	Paper II
α-HBCD	134237-50-6	Flameretardant	-	641.6447	0.12	Paper II
β-HBCD	134237-51-7	Flameretardant	-	641.6447	0.03	Paper II
γ-HBCD	134237-52-8	Flameretardant	-	641.6447	0.05	Paper II
10.11-Dihydro-10-hydroxycarbamazepine	29331-92-8	Pharmaceutical	+	254.1055	0.97	Paper IV
10.11-dihydrocarbamazepine	3564-73-6	Pharmaceutical	+	238.1106	0.24	Paper IV
2.4-Dichlorophenoxyacetic acid	94-75-7	Pesticide	-	219.9694	20.07	Paper IV
2.6-Dichlorbenzamid (BAM)	2008-58-4	Pesticide	+	188.9748	2.97	Paper IV
4-(Trifluoromethyl)benzenesulfonamide	830-43-3	Industrial Chemical	-	225.0071	1.00	Paper IV
4-Amino-6-(trifluoromethyl)benzene-1.3-disulfonamide	654-62-6	Industrial Chemical	-	318.9908	2.82	Paper IV
4-Chloro-4'-fluorobutyrophenone	3874-54-2	Industrial Chemical	+	200.0404	0.45	Paper IV
5-Amino-2-chlorotoluene-4-sulfonic acid	88-53-9	Industrial Chemical	-	220.9913	6.50	Paper IV
Acetaminophen	103-90-2	Pharmaceutical	+	151.0633	1.83	Paper IV
Acetamiprid	135410-20-7	Pesticide	+	222.0672	0.10	Paper IV
Alachlor	15972-60-8	Pesticide	+	269.1183	0.56	Paper IV

Amidosulfuron	120923-37-7	Pesticide	+	369.0413	0.50	Paper IV
Amitryptiline	50-48-6	Pharmaceutical	+	277.1830	0.11	Paper IV
Atenolol	29122-68-7	Pharmaceutical	+	266.1630	0.22	Paper IV
Atrazine	1912-24-9	Pesticide	+	215.0938	0.07	Paper IV
Atrazine-desethyl	6190-65-4	Pesticide	+	187.0625	0.24	Paper IV
Atrazine-desisopropyl	1007-28-9	Pesticide	+	173.0468	0.38	Paper IV
Azithromycin	83905-01-5	Pharmaceutical	+	748.5085	0.13	Paper IV
Azoxystrobin	131860-33-8	Pesticide	+	403.1168	0.04	Paper IV
Bentazon	25057-89-0	Pesticide	-	240.0569	1.38	Paper IV
Benzyl butyl phthalate	85-68-7	Phthalate	+	312.1362	10.67	Paper IV
Bezafibrate	41859-67-0	Pharmaceutical	+	361.1081	0.16	Paper IV
Bicalutamide	90357-06-5	Pharmaceutical	-	430.0610	0.08	Paper IV
Bifenox-acid	53774-07-5	Pesticide	-	326.9701	10.02	Paper IV
Bis(2-ethylhexyl) phosphate	298-07-7	Industrial Chemical	-	322.2273	0.48	Paper IV
Bisoprolol	66722-44-9	Pharmaceutical	+	325.2253	0.05	Paper IV
Bitertanol	55179-31-2	Pesticide	+	337.1790	4.09	Paper IV
Boscalid	188425-85-6	Pesticide	+	342.0327	0.97	Paper IV
Caffeine	58-08-2	Food Additive	+	194.0804	0.66	Paper IV
Carbendazim	10605-21-7	Pesticide	+	191.0695	0.16	Paper IV
Cetirizine	83881-51-0	Pharmaceutical	+	388.1554	0.07	Paper IV
Chloramphenicol	56-75-7	Pharmaceutical	-	322.0123	0.61	Paper IV
Chlorfenvinphos	470-90-6	Pesticide	+	357.9695	0.10	Paper IV
Chloridazon	1698-60-8	Pesticide	+	221.0356	0.06	Paper IV
Chlorzoxazone	95-25-0	Pharmaceutical	-	168.9931	2.10	Paper IV
Citalopram	59729-33-8	Pharmaceutical	+	324.1638	0.05	Paper IV
Clarithromycin	81103-11-9	Pharmaceutical	+	747.4769	0.02	Paper IV
Climbazole	38083-17-9	Pharmaceutical	+	292.0979	0.03	Paper IV
Clomazone	81777-89-1	Pesticide	+	239.0713	0.77	Paper IV
Clopidogrel	113665-84-2	Pharmaceutical	+	321.0590	0.05	Paper IV
Clothianidin	210880-92-5	Pesticide	+	249.0087	2.97	Paper IV
Codeine	76-57-3	Pharmaceutical	+	299.1521	0.08	Paper IV
Cyanazine	21725-46-2	Pesticide	+	240.0890	0.39	Paper IV
Cyazofamid	120116-88-3	Pesticide	+	324.0448	4.60	Paper IV
Cybutryne	28159-98-0	Pesticide	+	253.1361	0.03	Paper IV
Cyflufenamid	180409-60-3	Pesticide	+	412.1210	0.73	Paper IV
Cyprodinil	121552-61-2	Pesticide	+	225.1266	0.08	Paper IV

DEET (N.N-Diethyl-3-methylbenzamide)	134-62-3	Pesticide	+	191.1310	0.03	Paper IV
Diazepam	439-14-5	Pharmaceutical	+	284.0716	0.03	Paper IV
Dibutyl phosphate	107-66-4	Industrial Chemical	-	210.1021	6.16	Paper IV
Dichlorprop	120-36-5	Pesticide	-	233.9850	27.26	Paper IV
Diclofenac	15307-86-5	Pharmaceutical	-	295.0167	10.99	Paper IV
Dienogest	65928-58-7	Hormone	+	311.1885	0.09	Paper IV
Difenoconazole	119446-68-3	Pesticide	+	405.0647	0.10	Paper IV
Diflufenican	83164-33-4	Pesticide	-	394.0741	2.63	Paper IV
Dimethoate	60-51-5	Pesticide	+	228.9996	0.81	Paper IV
Diuron	330-54-1	Pesticide	+	232.0170	0.19	Paper IV
Enalapril	75847-73-3	Pharmaceutical	+	376.1998	0.07	Paper IV
Fenofibrate	49562-28-9	Pharmaceutical	+	360.1128	6.07	Paper IV
Fenpiclonil	74738-17-3	Pesticide	-	235.9908	0.40	Paper IV
Fexofenadine	83799-24-0	Pharmaceutical	+	501.2879	0.02	Paper IV
Fluazinam	79622-59-6	Pesticide	-	463.9514	0.34	Paper IV
Fluconazole	86386-73-4	Pharmaceutical	+	306.1041	0.30	Paper IV
Fludioxonil	131341-86-1	Pesticide	-	248.0397	0.25	Paper IV
Flufenacet	142459-58-3	Pesticide	+	363.0665	0.70	Paper IV
Fluopicolide	239110-15-7	Pesticide	+	381.9654	0.11	Paper IV
Flusilazole	85509-19-9	Pesticide	+	315.1003	0.07	Paper IV
Flutriafol	76674-21-0	Pesticide	+	301.1027	0.12	Paper IV
Foramsulfuron	173159-57-4	Pesticide	+	452.1114	0.54	Paper IV
Fuberidazole	3878-19-1	Pesticide	+	184.0637	0.05	Paper IV
Furosemide	54-31-9	Pharmaceutical	-	330.0077	6.98	Paper IV
Gestodene	60282-87-3	Hormone	+	310.1933	0.53	Paper IV
Glibenclamide	10238-21-8	Pharmaceutical	+	493.1438	0.19	Paper IV
Glimepiride	93479-97-1	Pharmaceutical	+	490.2250	0.34	Paper IV
Hexamethylcyclotrisiloxane	541-05-9	Siloxane	+	222.0564	0.70	Paper IV
Hexazinone	51235-04-2	Pesticide	+	252.1586	0.05	Paper IV
Hydrochlorothiazide	58-93-5	Pharmaceutical	-	296.9645	12.44	Paper IV
Ifosfamide	3778-73-2	Pharmaceutical	+	260.0248	0.05	Paper IV
Imidacloprid	138261-41-3	Pesticide	+	255.0523	0.27	Paper IV
Irbesartan	138402-11-6	Pharmaceutical	+	428.2325	0.05	Paper IV
Isoproturon	34123-59-6	Pesticide	+	206.1419	0.05	Paper IV
Ivermectin	70288-86-7	Pharmaceutical	-	874.5079	30.51	Paper IV
Ketoprofen	22071-15-4	Pharmaceutical	+	254.0943	0.89	Paper IV

Lamotrigine	84057-84-1	Pharmaceutical	+	255.0079	0.06	Paper IV
Levamisole	14769-73-4	Pharmaceutical	+	204.0721	0.11	Paper IV
Levonorgestrel	17489-40-6	Hormone	+	312.2089	0.42	Paper IV
Linuron	330-55-2	Pesticide	+	248.0119	3.29	Paper IV
Loperamide	53179-11-6	Pharmaceutical	+	476.2231	0.03	Paper IV
Loratadine	79794-75-5	Pharmaceutical	+	382.1448	0.03	Paper IV
Losartan	114798-26-4	Pharmaceutical	+	422.1622	0.11	Paper IV
Mandipropamid	374726-62-2	Pesticide	+	411.1237	0.06	Paper IV
MCPA	94-74-6	Pesticide	-	200.0240	22.13	Paper IV
Mebendazole	31431-39-7	Pharmaceutical	+	295.0957	0.23	Paper IV
Meclofenamic acid	644-62-2	Pharmaceutical	-	295.0167	22.67	Paper IV
Mecoprop	7085-19-0	Pesticide	-	214.0397	31.71	Paper IV
Memantine	19982-08-2	Pharmaceutical	+	179.1674	4.63	Paper IV
Metalaxyl	57837-19-1	Pesticide	+	279.1471	0.05	Paper IV
Metazachlor	67129-08-2	Pesticide	+	277.0982	0.13	Paper IV
Methabenzthiazuron	18691-97-9	Pesticide	+	221.0623	0.11	Paper IV
Methadone	76-99-3	Pharmaceutical	+	309.2093	0.07	Paper IV
Metolachlor	51218-45-2	Pesticide	+	283.1339	0.07	Paper IV
Metoprolol	51384-51-1	Pharmaceutical	+	267.1834	0.08	Paper IV
Metribuzin	21087-64-9	Pesticide	+	214.0888	0.55	Paper IV
Metronidazole	443-48-1	Pharmaceutical	+	171.0644	0.85	Paper IV
Metsulfuron methyl	74223-64-6	Pesticide	+	381.0743	0.11	Paper IV
Mirtazapine	61337-67-5	Pharmaceutical	+	265.1579	0.07	Paper IV
Monobenzyl Phthalate	2528-16-7	Phthalate	-	256.0736	3.39	Paper IV
Monobutyl Phthalate	131-70-4	Phthalate	-	222.0892	14.04	Paper IV
N-Desmethylcitalopram	62498-67-3	Pharmaceutical	+	310.1481	0.09	Paper IV
Nicotine	54-11-5	Drug	+	162.1157	0.74	Paper IV
Niflumic acid	4394-00-7	Pharmaceutical	-	282.0616	0.15	Paper IV
Norethindrone	68-22-4	Hormone	+	298.1933	0.21	Paper IV
Norfloxacin	70458-96-7	Pharmaceutical	+	319.1332	6.64	Paper IV
Ofloxacin	82419-36-1	Pharmaceutical	+	361.1438	0.17	Paper IV
Omeprazole	73590-58-6	Pharmaceutical	+	345.1147	2.96	Paper IV
Oxazepam	604-75-1	Pharmaceutical	+	286.0509	0.27	Paper IV
Oxycodone	76-42-6	Pharmaceutical	+	315.1471	0.11	Paper IV
Penconazole	66246-88-6	Pesticide	+	283.0643	0.12	Paper IV
Perfluoro-2-propoxypropanoic acid (GenX)	13252-13-6	PFAS	-	329.9750	15.39	Paper IV

Perfluorobutane sulfonic acid (PFBS)	375-73-5	PFAS	-	299.9503	0.06	Paper IV
Perfluorodecanoic acid (PFDA)	335-76-2	PFAS	-	513.9673	0.14	Paper IV
Perfluorododecanoic acid (PFDoDA)	307-55-1	PFAS	-	613.9609	0.98	Paper IV
Perfluoroheptanoic acid (PFHpA)	375-85-9	PFAS	-	363.9769	0.16	Paper IV
Perfluorohexane sulfonic acid (PFHxS)	355-46-4	PFAS	-	399.9439	0.05	Paper IV
Perfluorohexanoic acid (PFHxA)	307-24-4	PFAS	-	313.9801	0.35	Paper IV
Perfluorononanoic acid (PFNA)	375-95-1	PFAS	-	463.9705	0.11	Paper IV
Perfluorooctane sulfonamide (FOSA)	754-91-6	PFAS	-	498.9535	0.55	Paper IV
Perfluorooctane sulfonic acid (PFOS)	1763-23-1	PFAS	-	499.9375	0.06	Paper IV
Perfluorooctanoic acid (PFOA)	335-67-1	PFAS	-	413.9737	0.14	Paper IV
Perfluoropentanoic acid (PFPeA)	2706-90-3	PFAS	-	263.9833	1.53	Paper IV
Perfluorotetradecanoic acid (PFTeDA)	376-06-7	PFAS	-	713.9545	1.13	Paper IV
Perfluoroundecanoic acid (PFUnDA)	2058-94-8	PFAS	-	563.9641	0.34	Paper IV
Picoxystrobin	117428-22-5	Pesticide	+	367.1031	0.47	Paper IV
Pirimicarb	23103-98-2	Pesticide	+	238.1430	0.06	Paper IV
Prochloraz	67747-09-5	Pesticide	+	375.0308	0.11	Paper IV
Progesterone	57-83-0	Hormone	+	314.2246	0.66	Paper IV
Propamocarb	24579-73-5	Pesticide	+	188.1525	0.21	Paper IV
Propiconazole	60207-90-1	Pesticide	+	341.0698	0.08	Paper IV
Propoxycarbazone	145026-81-9	Pesticide	+	398.0896	0.30	Paper IV
Propranolol	525-66-6	Pharmaceutical	+	259.1572	0.08	Paper IV
Propyzamide	23950-58-5	Pesticide	+	255.0218	5.10	Paper IV
Prothioconazole-desthio	120983-64-4	Pesticide	+	311.0592	0.10	Paper IV
Pyraclostrobin	175013-18-0	Pesticide	+	387.0986	0.09	Paper IV
Pyrimethamine	58-14-0	Pharmaceutical	+	248.0829	0.08	Paper IV
Pyroxsulam	422556-08-9	Pesticide	+	434.0620	0.03	Paper IV
Quinmerac	90717-03-6	Pesticide	+	221.0244	5.13	Paper IV
Quinoxyfen	124495-18-7	Pesticide	+	306.9967	0.23	Paper IV
Ramipril	87333-19-5	Pharmaceutical	+	416.2311	0.05	Paper IV
Roxithromycin	80214-83-1	Pharmaceutical	+	836.5246	0.04	Paper IV
Silthiofam	175217-20-6	Pesticide	+	267.1113	0.19	Paper IV
Sotalol	3930-20-9	Pharmaceutical	+	272.1195	0.79	Paper IV
Sucralose	56038-13-2	Food Additive	-	396.0146	18.15	Paper IV
Sulfaclozine	102-65-8	Pharmaceutical	-	284.0135	16.85	Paper IV
Sulfamethoxazole	723-46-6	Pharmaceutical	+	253.0521	0.69	Paper IV
Sulfosulfuron	141776-32-1	Pesticide	+	470.0678	0.30	Paper IV

Sulindac	38194-50-2	Pharmaceutical	+	356.0882	0.44	Paper IV
Telmisartan	144701-48-4	Pharmaceutical	+	514.2369	0.01	Paper IV
Terbuthylazine	5915-41-3	Pesticide	+	229.1094	0.08	Paper IV
Terbutryn	886-50-0	Pesticide	+	241.1361	0.04	Paper IV
Testosterone	58-22-0	Hormone	+	288.2089	0.47	Paper IV
Theobromine	83-67-0	Pharmaceutical	+	180.0647	4.32	Paper IV
Thiabendazole	148-79-8	Pharmaceutical	+	201.0361	0.54	Paper IV
Thiacloprid	111988-49-9	Pesticide	+	252.0236	0.08	Paper IV
Thiamethoxam	153719-23-4	Pesticide	+	291.0193	0.32	Paper IV
Thifensulfuron methyl	79277-27-3	Pesticide	+	387.0307	0.19	Paper IV
Tramadol	27203-92-5	Pharmaceutical	+	263.1885	0.09	Paper IV
Triadimefon	43121-43-3	Pesticide	+	293.0931	0.30	Paper IV
Triflusulfuron-methyl	126535-15-7	Pesticide	+	492.1039	0.11	Paper IV
Triisopropanolamine	122-20-3	Pharmaceutical	+	191.1521	0.32	Paper IV
Tris(2-chloroethyl) phosphate (TCEP)	115-96-8	Flameretardant	+	283.9539	1.65	Paper IV
Triticonazole	131983-72-7	Pesticide	+	317.1295	0.18	Paper IV
Valsartan	137862-53-4	Pharmaceutical	-	435.2270	0.78	Paper IV
Venlafaxine	93413-69-5	Pharmaceutical	+	277.2042	0.07	Paper IV
Verapamil	52-53-9	Pharmaceutical	+	454.2832	0.03	Paper IV
α-HBCD	134237-50-6	Flameretardant	-	641.6447	43.81	Paper IV
β-HBCD	134237-51-7	Flameretardant	-	641.6447	10.72	Paper IV
γ-HBCD	134237-52-8	Flameretardant	-	641.6447	14.03	Paper IV

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With the rapidly expanding global population, demand for clean drinking water is increasing. However, the widespread use of synthetic chemicals makes it challenging to produce safe and clean drinking water. A broad screening method based on large volume extraction and high- resolution mass spectrometry was developed to investigate the status of Sweden's most important water sources and drinking water. A large screening study of raw water and drinking water from 11 countries in Europe and Asia was also performed. The findings in this thesis can help improve drinking water quality worldwide.

Rikard Tröger received his doctoral education at the Department of Aquatic Sciences and Assessment at the Swedish University of Agricultural Sciences. He received his master's degree in analytical chemistry at Uppsala University and his bachelor's degree in chemistry at Uppsala University.

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