

ENVIRONMENT & HEALTH

# Micropollutants in Urban Wastewater

Literature Review concerning the sources of micropollutants in wastewater

### March 2025

Disclaimer: The review is based on the analysis of existing published research, which may be subject to updates, reinterpretation, or revision. The authors disclaim any liability for any loss or damage resulting from reliance on the information contained in this report. Readers are encouraged to conduct their own independent investigations and to consult the original sources cited herein for a more comprehensive understanding.

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### **Executive Summary**

### **OBJECTIVES**

Ramboll Deutschland GmbH (Ramboll) was commissioned by Clifford Chance to provide scientific, technical, regulatory and strategic consulting services in the field of data collection and assessment concerning so-called micropollutants (MP) in wastewater in the course of the planned recast of the EU Urban Wastewater Treatment Directive (UWWTD).

According to the Impact Assessment (IA) associated to the recast of the UWWTD, it was claimed that Pharmaceuticals and to a lesser extent Personal care products (PCP) represent a large share of the potentially harmful substances found in wastewater, hence their manufacturers would have to make a substantial contribution to the construction and operation of the 4<sup>th</sup> (quaternary) urban wastewater treatment stage in all EU Member States.

The project, finalised in March 2025, builds on previous work for Bundesverband der Arzneimittel Hersteller e.V. (now Pharma Deutschland), Bundesverband der Pharmazeutischen Industrie e.V., Pro Generika e.V. and Verband forschender Arzneimittelhersteller e.V. As part of the project, Ramboll conducted a literature search and reviewed relevant studies and publications regarding micropollutants in urban wastewater. For this project, the previous literature search was updated for the last two years and further extended. Therefore, Ramboll was complementing the previous approach to literature with additional scoping reviews (Task 1) and with an additional database (Task 2). Both tasks were focussing on information on other potential micropollutants that are no pharmaceuticals rather than on completeness.

### **KEY FINDINGS**

- There is clear and robust scientific evidence contained in the public literature that demonstrates that a number of different chemical substances fall within the scope of the Article 2(17) UWWTD definition of 'micropollutants' – and that these substances come from a wide variety of different sources including products, applications and other origins.
- According to the public literature, the sources of micropollutants come from, amongst others: pesticides, food ingredients or additives (e.g. sweetener, caffeine), pharma veterinary products, pharma human health, personal care, biocides, industrial chemicals (e.g. PFAS, flame retardants, plasticizers, corrosion inhibitors) and other sources.
- The concentration of detected micropollutants is mostly in the in the ppb to low ppm range and varies significantly depending on various factors like region, surrounding, weather, season, method employed etc. The concentration of detected substances of pharmaceutical origin seen in this study were lower, in the low ppb or even ppt (ng/l) range; however, also here the actual values differ significantly among the studies.
- Studies on (emerging) micropollutants in wastewater typically target defined substance groups, only covering a subset of micropollutants in the sample. Even wide-scope chemical target screening programs with >200 analytes do not necessary represent the full picture.

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- Publications on non-targeted screening of wastewater are still limited reflecting the analytical challenges concerning assessing the highly complex composition of micropollutants in wastewater matrix and concluding on their source. It is discussed in scientific literature that a further development of non-targeted methodology is still required, including: (i) harmonized protocols and quality requirements, (ii) infrastructures for efficient data management, data evaluation and data sharing and (iii) sufficient resources and appropriately trained personnel in the research and regulatory communities in Europe (Hollender et al., 2019).
- Based on the checked references and in particular the selection of target compounds in the individual studies, it can be concluded that pharmaceuticals represent the most intensely studied group of substances which may be classified as micropollutants meaning that there is a disproportionate and unequal focus on a subset of possible micropollutants in published literature. This could lead to an underrepresentation of other sources and micropollutants.
- To obtain a representative picture of a wastewater sample by identifying all known and unknown micropollutants of all sources, further research is needed using combined approaches of non-targeted, suspect screening and quantitative analysis (e.g. by targeted methods).
- There is clear and robust scientific evidence available in the public literature that sources of micropollutants found in urban wastewater are multiple and do vary. The focus on (human) health and cosmetics products alone as potential contributors is not supported by the available studies.
- The IA report from the EU Commission concluded that pharmaceuticals for human use represent 59% of input quantities to wastewater treatment plants and 66% of the total toxic load. These figures could neither be confirmed nor could definite, reliable figures be identified in the literature.

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### 1. Introduction

### 1.1 Background

In 2023, Ramboll assessed the data quality and assumptions in the Impact Assessment (IA) report by the European Commission, dated 26 October 2022 (EU COM, 2022a), on which the planned revision of the EU Urban Wastewater Treatment Directive (UWWTD) is based. The IA report concluded that pharmaceuticals for human use represent 59% of input quantities to wastewater treatment plants (14% for PCPs), 48% of the toxic chronic load (17% for PCPs) and 66% of the total toxic load Predicted No Effect Concentration (PNEC) (26% for PCPs), thus their manufacturers would have to make a substantial contribution to the construction and operation of the 4<sup>th</sup> treatment stage in all EU Member States.

Ramboll reviewed the IA report including the main sources cited therein. Ramboll furthermore conducted an independent literature search and reviewed relevant studies and publications regarding micropollutants in urban wastewater. Overall, Ramboll found the IA report being not transparent on how the share of the different sectors contributing micropollutants was calculated. Additional studies identified by Ramboll showed micropollutant concentrations related to the pharma industry in significantly smaller ratios than the data used in the IA report. Pharmaceuticals represent the beststudied group of micropollutants which may give them an unrepresentative share in the allocation of pollutant loads.

The present project, finalised in March 2025, aimed to update our first findings based on additional and more recent scientific literature.

'micropollutant' means a substance as defined in Article 3(1) of Regulation (EC) No 1907/2006 of the European Parliament and of

the Council (32), including its breakdown products, that is usually present in the aquatic environment, urban wastewater or sludge and that can be considered hazardous to the environment or human health on the basis of the relevant criteria set out in Parts 3 and 4 of Annex I to Regulation (EC) No 1272/2008, even in low concentrations. [Definition that it is used in the recast of the UWWTD]

### 1.2 Purpose and Objectives

Ramboll Deutschland GmbH (Ramboll) was commissioned by Clifford Chance to provide scientific, technical, regulatory and strategic consulting services in the field of data collection and assessment concerning so-called micropollutants (MP) in wastewater in the course of the planned recast of the EU Urban Wastewater Treatment Directive (UWWTD).

The project builds on previous work for Bundesverband der Arzneimittel Hersteller e.V. (now Pharma Deutschland), Bundesverband der Pharmazeutischen Industrie e.V., Pro Generika e.V. and Verband forschender Arzneimittelhersteller e.V. As part of the project, Ramboll conducted a literature search and reviewed relevant studies and publications regarding micropollutants in urban wastewater. For this project, the literature search was updated for the last two years and further extended. Therefore, Ramboll complemented the previous approach to literature search with additional scoping reviews (Task 1) and with an additional search database (Task 2). Both tasks prioritized gathering information on potential micropollutants other than pharmaceuticals, rather than aiming for completeness.

### 1.3 Limitations

Ramboll relied on publicly available information, data provided by the client, and its own expertise. The objective was not to conduct

a comprehensive systematic literature review but rather to identify additional studies deemed relevant to address the following key research questions. Given the vast amount of existing data and studies, Ramboll focused on research from EU countries published within the last five years. Publicly available sources were selected based on Ramboll's own criteria and professional judgment.

- What are potential sources according to the public scientific literature – of 'micropollutants' as defined in Article 2(17) of the UWWTD?
- Is there a bias/selective assessment in the public scientific literature – with the most intensely studied sources being pharma and cosmetics?
- 3. Is there evidence according to the public literature that other sources of micropollutants (i.e. non-pharma and noncosmetics) should also be held responsible for any relevant pollution that might justify applying a precautionary approach following only sources of micropollutants from pharma and cosmetic products should be subjected to the polluter-pays/extended producer responsibility requirements?
- 2. Literature search

### 2.1 Methodology

Ramboll had previously conducted a literature search using the following search term:

**Old search term:** ("Micropollutant\*" OR "Micro-pollutant\*") AND ("Urban Wastewater" OR "Domestic Wastewater" OR "Sewage Wastewater")

The search was done in the following databases and was focusing on literature published after 2018 (search was performed in January 2023):

- <u>PubMed</u>, by the National Library of Medicine by the U.S. Department of Health and Human Services (HHS),
- <u>Europe PubMed Central</u> (EuropePMC) by the European Molecular Biology Laboratory-European Bioinformatics Institute, and

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By this approach 37 relevant articles were identified and reviewed.

As recent information from the last two years (February 2023-December 2024) was not covered in the previous search, the literature search was updated and extended in this project.

Doing scoping tests, it was noticed that in scientific literature 'micropollutants' can be also found under different names like 'chemicals of emerging concern'. Therefore, also synonyms for micropollutants were included in the search term. In addition, the search term was broadened to wastewater in general without specific categories. Several search terms were tested; the most promising one was used for the further work.

**New search term:** ("Micropollutant\*" OR "Micro-pollutant\*" OR "Substances of concern" OR "chemicals of emerging concern" OR "contaminants of emerging concern" OR "emerging contaminants" OR impurities) AND (wastewater OR "waste-water" OR "waste water" OR effluent)

This new search term revealed in the database PubMed a total number of 3,426 hits (1,865 published since 2020). However, by screening through the titles it was noticed that the broader search had led to a significantly increased amount of not relevant findings.

SCOPUS was identified as a database more suitable for this research question. While PubMed and EuropePMC are primarily focusing on biomedical and life sciences literature, SCOPUS covers a broader range of relevant disciplines, including social sciences, engineering, and physical sciences, offering a more multidisciplinary perspective. Another big advantage with SCOPUS is that categories can be applied to the search already narrowing down the results to more suitable findings.

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Table 1: Number of hits for the old and new defined search term inSCOPUS.

SCOPUS	Old search term	New search term
Total hits	281	11,176
Hits for articles published since 2020	142	4,907
Applying relevant categories <sup>1</sup>	Not tested	1,163

The 1,163 hits were screened for relevant publications by title and abstract using the software <u>DistillerSR</u> which is a literature review software for easier screening. Relevance was assessed by personal judgement. As for the previous project, it was noted that a significant number of articles focused on technical aspects of different treatment technologies which were considered irrelevant for this review.

Next to the database SCOPUS, the following additional sources were used:

- General google search
- Focused searches in PubMed / EuropePMC
- Databases and publications from authorities (EU COM, ECHA, national authorities)

In total, 49 articles were identified in this project as being relevant to micropollutants in wastewater (with a focus on other micropollutants than the already wide studied pharmaceuticals). These articles were subsequently reviewed. Thereof, 13 were assumed to contain very relevant findings and are considered as key studies. Studies considered as key studies are discussed in more detail in chapter 3.

### 2.2 Review

Ramboll reviewed all identified studies that were considered as relevant, considering the following reviewing questions:

- Which micropollutants are considered?
- Is there an indication of quantity ratios (total share of micropollutants, subgroups of micropollutants, specific substances)?
- Is there an indication on the toxicity/hazard of the micropollutants?
- What is the source of the data (e.g. measurements, other studies)?
- Uncertainties / validity of the data
- Other relevant information and comments

In addition, the identified studies were used to extract exemplary information on selected substances for different groups of substances. The selection was done on a case-by-case decision and depending on how easy the data was accessible. The aim of this exercise was to collect some examples on individual substances found in wastewater that will potentially fall under the definition of micropollutants.

<sup>&</sup>lt;sup>1</sup> The following categories were used to narrow down the search: (A) Subject area: Environmental Science (B) Document type: Limited to Article/Review/Book Chapter, (C): Keywords: selected relevant keywords, e.g. micropollutants, wastewater, (D): Country: Excluding non-EU countries.



### 3. Results & Discussion

Micropollutants in wastewater represent a growing environmental concern with multi-faceted implications for ecosystem health and human safety (Eggen et al., 2014; Rogowska et al., 2020). They can enter wastewater through household discharges, agricultural runoff, industrial effluents, and improper disposal of chemicals.

The primary concern stems from their persistence and widespread distribution in the environment, as conventional wastewater treatment plants are often incapable of completely removing these compounds. In recent decades, there has been significant focus on analysing compounds like endocrine-disrupting chemicals (EDCs) and pharmaceutical substances (Rogowska et al., 2020), so that the awareness for micropollutants has increased.

The growing awareness of micropollutants' presence in water bodies has prompted increased research and efforts to develop advanced treatment technologies to address this challenge (Belete et al., 2023).

### 3.1 The definition of micropollutants

The definition of micropollutants as substances that can be considered hazardous to the environment or human health based on the criteria in Parts 3 and 4 of Annex I to Regulation (EC) No 1272/2008 represents a precautionary approach to environmental protection. This broader definition is significant because it does not limit the scope to only substances with a harmonised CLP classification (none of the addressed pharmaceuticals do have a harmonised classification see Appendix 1), as is often the case in other pieces of legislation. By including substances that might meet the relevant hazard criteria, even without an official harmonised classification, this approach allows for a more proactive stance in addressing potential environmental and health risks. It acknowledges that the process of officially classifying substances

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can be time-consuming and that emerging contaminants may pose risks before they are formally recognized. However, it also presents challenges in terms of implementation and monitoring, as it requires a more nuanced, uncertain and case-by-case evaluation of substances that may fall under this broader definition of micropollutants.

When applying the precautionary principle to address micropollutants, it seems crucial to consider a broad spectrum of substances across multiple sectors. This comprehensive approach is essential because micropollutants originate from diverse sources across multiple sectors as shown in many of the assessed studies. Research efforts acknowledge this fact and continue to progress in identifying the complex picture of wastewater contamination.

### 3.2 General concentration pattern

Trace quantities of micropollutants are detectable in environmental samples, with concentrations typically ranging from parts per billion (ppb) to parts per trillion (ppt) (Belete et al., 2023). These levels, expressed in micrograms per litre ( $\mu$ g/L) to nanograms per litre (ng/L), highlight the sensitivity required in analytical methods to accurately measure and monitor these substances in various environmental matrices. The current findings in literature correspond to those low concentration levels in wastewater samples, in the effluent samples the typical concentration is in the ppb to low parts per million (ppm) range.

Measurement Units and Concentration Analogies
1 part per billion (ppb) = 1,000 parts per trillion (ppt) 1 part per billion (ppb) = 0.001 parts per million (ppm)
1 ppm = 1 milligram/litre (mg/l) 1 ppb = 1 microgram/litre (μg/l) 1 ppt = 1 nanogram/litre (ng/l)

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#### Analogies

- I ppm is roughly one teaspoon substance in 50 litres of water
- 1 ppb is roughly one teaspoon of substance in 50,000 litres of water
- I ppt is roughly one teaspoon of substance dissolved in 50,000,000 litres of water

Directive 2020/2184 on the quality of water intended for human consumption foresees parametric values for drinking water as thresholds for certain substances. For organic pesticides this value is 0.1  $\mu$ g/L, the same is true for the sum of PFAS<sup>2</sup> and some other chemicals. The vast majority has significantly higher parametric values.

Considering as an example caffeine, EFSA indicates a safe level for human intake of 400 mg per day <sup>3</sup>. This concentration is present in 250 – 700 ml black and instant coffee, respectively (Petrović et al., 2020) (Petrović et al., 2020).

It should be noted that substitution and reduction of chemicals is possible in many industries, however, for some chemicals a scientifically derived dose-response curve indicates how far reduction in concentration is possible to ensure the envisaged effect. This is in particular valid for pharmaceuticals, for which the dose-response curve indicates that no further reduction in concentration is possible to ensure the envisaged effect.

### 3.3 Source of micropollutants

Even if the focus of the present study was not on identification of specific sources and additional efforts would be required to detail the sources of the substances identified in the present study, a non-exhaustive list may include the following micropollutant sources other than pharmaceuticals and personal care products:

### (1) Bona fide products/applications/uses

- veterinary and pet-care products
- biocides/treated articles
- pest control (e.g. pesticides, insecticides, rodenticides, etc.)
- detergents & bleaches
- domestic plant protection products, fertilizers, growth enhancers, fungicides, herbicides, weed killer, moss remover, etc.
- household cleaning products (kitchen cleaning products, bathroom cleaning products, floor cleaning products, carpet treatment products, fungicides etc.)
- dishwasher tablets, rinse aid, water softener, washing machine powder/tablets, fabric softeners, stain removers, colour enhancers, other textile cleaning products
- wastepaper, toilet paper, wet wipes, tissues, nappies, baby creams
- vape and tobacco products including residue e-liquids
- wax, resins, fragrances, flavourings

#### <sup>3</sup> Caffeine | EFSA

 $<sup>^2</sup>$  This is a subset of `PFAS Total' substances that contain a perfluoroalkyl moiety with three or more carbons (i.e. –CnF2n–, n  $\geq$  3) or a perfluoroalkylether moiety with two or more carbons (i. e. – CnF2nOCmF2m–, n and m  $\geq$  1)

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- food & feed (preservers, artificial sweeteners, food colourants, metabolites as well as residue pesticides in food and feed)
- household cleaning and care products (including shoe polish, silver polish, leather treatment products, window cleaning products, taxidermy care products, surfactants, fragrances, solvents etc.)
- automotive and bicycle cleaning and care products (including lubricants, polishes, muck-remover products, corrosion inhibitors etc.)
- inks, dyes, paints, coatings, adhesives, etc.
- plastic & rubber (polymer starting materials, flame retardants, colourants, UV protectors, tec.)
- preservatives
- textiles
- packaging
- medical devices and electronic equipment
- batteries
- water & wastewater transportation materials and infrastructure (e.g. plastics, cement, ceramics, metals, sealants, etc.)

### (2) Illicit and illegal products/waste

- illegal waste (including industrial, chemical, hazardous, etc.)
- illicit drugs and pharmaceuticals

### (3) Other sources

- use and disposal of cosmetic and pharma products bought outside the EU and used inside the EU/EEA e.g. Ireland.
- leaching from existing landfill sites
- 3.4 Approaches to measure micropollutants in wastewater

Historically, researchers have employed targeted screening approaches that focus on detecting pre-defined chemicals to identify organic micropollutants (Krauss et al., 2010) as cited in (Lai et al., 2021). In target analysis, substances are examined using reference standards to facilitate their identification and quantification. In many monitoring studies and campaigns, targeted screening is still a common technique, and most publications identified in this study are based on such targeted screening. It is essential to recognise that targeted analysis of water contaminants typically concentrates on a limited selection of chemicals, which may not fully reflect the actual pollution profile in water bodies. With this approach, there is also **a risk of biased results if the selection of analytes is not representative of the composition of the sample**.

In the recent years, non-target screening approaches were discussed as promising methods to help to close this knowledge gap in the future. Non-targeted screening is a technique used to identify unknown compounds in a sample without prior knowledge of their presence. There are still several challenges connected to nontargeted screening regarding successful qualification of analytes.

A recent Danish study observed 4094 unique substances (1482 thereof were filtered out as background), of which they could obtain the chemical structure for 785 compounds based on comparison of mass spectra with in-house experimental data as well as other libraries. Only 451 thereof could be assigned to one of the designated compound classes (e.g. pharmaceutical) in the scope of the project (Aggerbeck et al., 2024). A retrospective non-targeted analysis of

wastewater samples collected in Switzerland in 2018 resulted in one confirmed and 21 tentative substance identifications, indicating the presence of a diverse range of compounds, including manufacturing reagents, adhesives, pesticides, and pharmaceuticals in the samples (Lai et al., 2021).

Scientific literature highlights the need for further development of non-targeted methodologies, emphasizing the importance of (i) standardised protocols and quality requirements, (ii) infrastructures for efficient data management, evaluation and sharing and (iii) adequate resources and well trained personnel within the research and regulatory communities across Europe (Hollender et al., 2019).

High-resolution mass spectrometry (HRMS) combined with liquid chromatography (LC-HRMS) is increasingly being applied in environmental analysis through suspect and non-target screening techniques. These approaches enable a broad and detailed examination of sample composition without requiring prior knowledge of the substances present (Armin et al., 2025). Very recently researchers have developed a non-targeted method which they have optimised for industrial wastewater analysis (Armin et al., 2025; Purschke, 2020), but this method might be suitable for other matrices as well, e.g. rural wastewater..

While river water is not directly equivalent to wastewater, its micropollutant composition provides crucial insights into the broader environmental impact of these substances. A recent study on sources of chemical contamination of the Rhine River based on temporal high-frequency LC-HRMS monitoring data identified nearly 3,000 compounds as highly important for the management of water quality by a newly developed prioritization strategy (Chonova, 2025). In this study only 2.8 % of the prioritized profiles (corresponding to 83 profiles) are regularly monitored targets. The authors state that thousands of high-exposure compounds still have undefined chemical structure, origin, and

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environmental effects. They assumed that half of them originate from irregular emission sources, possibly industry.

It becomes even more challenging when it should come to quantification in a second step. In Japan, a recent study investigated wastewater treatment plant effluent and identified 734 profiles as frequently detected in selected WWTPs in Japan (Pandey et al., 2024). However, only five selected substances were quantified in a second step by targeted analysis in this study.

In this literature review only a few studies were found that used a combined approach including a target, suspect and non-target screening analysis of drinking and wastewater (for more details see section 3.6). In one study 51 substances were identified by a quantitative screening of the WWTP effluents (Hinnenkamp et al., 2022).

To obtain a representative picture of a wastewater sample by identifying all known and unknown micropollutants, further research is needed using combined approaches of non-targeted, suspect screening and quantitative analysis (e.g. by targeted methods).

#### 3.5 Substances identified in wastewater

Substances of the following substance groups were identified in wastewater from the literature among others:

- Pharmaceuticals
- Personal Care Products
- Pesticides
- PFAS
- Industrial chemicals
  - Surface modifiers
    - Surfactants
    - Siloxanes
  - Plastic additives

- Flame retardants
- Light stabiliser
- Process chemicals
  - Corrosion inhibitors
  - Cleaning agents
  - Adhesives
  - Solvents
- o Other
- Food ingredients/additives
  - o Sweeteners
  - o Caffeine

Substances were grouped to fit the purpose of this study; it is possible that some substances are relevant to more than one group. Examples of substances are discussed in the following for each substance group. A list of additional substances found in the studies can be found in Appendix 1.

### 3.5.1 Pharmaceuticals

Pharmaceuticals were not in focus of this review. However, in the following section selected pharmaceuticals will be discussed in more detail. As pharmaceuticals are still one of the widest studied substance groups in wastewater, there is a specific risk for biased results depending on the selection of analytes in targeted approaches. For example, in a critical review, *Quantitative and qualitative approaches for CEC prioritization when reusing reclaimed water for irrigation needs* (Verlicchi et al., 2023), the authors highlight key knowledge gaps and recommend that future research should expand monitoring investigations on polished effluent to include not only pharmaceuticals, but also other, less-explored

<sup>4</sup> This work was based on study data on 51 wastewater-borne substances (trace substances discharged from domestic and industrial connections) identified from analysing 151 trace

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classes of contaminants of emerging concern (CECs). In a fundbased solution proposed by BDEW (German Association of Energy and Water Industries) five APIs (Active Pharmaceutical Ingredients) were identified among the top 10 wastewater-born trace substances: Ibuprofen, diclofenac,  $17\beta$ -oestradiol, carbamazepine and clarithromycin (Czichy et al., 2020) (Table 2).<sup>4</sup> Based on this data the EU feasibility study on an EPR system for micropollutants gives a special focus to these substances (Bio Innovation Services & EU COM, 2022).

Table 2: List of pharmaceuticals identified by (Czichy et al., 2020)and corresponding environmental concentration thresholds.

Substance	CAS	Environmental concentration threshold			
		Value	Туре	Source	
Ibuprofen	15687- 27-1	0.022 μg/L	EQS-proposal	(SCHEER, 2022)	
Diclofenac	15307- 86-5	0.05 µg/L	EQS-proposal	(Finckh, Beckers, et al., 2022)	
17β-oestradiol	50-28-2	NA	NA	NA	
Carbamazepine	298-46- 4	0.5 μg/L	AA-EQS (freshwater)	(UBA, 2014)	
Clarithromycin	81103- 11-9	0.12 µg/L	EQS-proposal	(Finckh, Beckers, et al., 2022)	

Overall, while all the detected substances are present in very low ppb or even ppt levels, there are significant differences in concentrations between different studies for the five selected APIs

substances in the Ruhr region (Germany). Ramboll does not have access to the raw data therefore the representative of these results is unclear.

as shown in the following for the individual substances (in the selected studies investigated in more detail in this review, no data on  $17\beta$ -oestradiol was found).

### Ibuprofen

In one study conventional, low-loaded activated sludge treatment with carbon, nitrogen (nitrification and denitrification) removal and chemical phosphorus precipitation has already achieved efficient elimination of ibuprofen and levels were below LOQ in all effluent samples from three WWTPs in Austria (Reif et al., 2023). In another study, ibuprofen was found in the effluent of 8 WWTPs from the Danube River Basin with levels ranging from <LOQ to 624.63 ng/L, whereas in the same study maximum concentrations of ibuprofen measured in influent samples were much lower (maximum 1.3 ng/L), indicating negative removal (see also carbamazepine) (Ng et al., 2023). The highest ibuprofen concentration detected in effluent (624.63 ng/L) exceeds the EQS of 22 ng/L ((SCHEER, 2022)) by more than 28 times.

#### Carbamazepine

Negative removal was also observed for carbamazepine in one study that found the substance in all WWTP effluent samples investigated with concentrations ranging from 28-343 ng/L (for influent samples 21-181 ng/L) (Ng et al., 2023). The authors indicated that carbamazepine can form as a byproduct of its conjugated substances, which my revert to its free form (carbamazepine) during biological treatment. This can result in negative removal. Concentration of carbamazepine varies significantly among studies with values below and above the EQS of 0.5  $\mu$ g/L (500 ng/L), examples for other identified concentration of carbamazepine in effluent of WWTPs from other studies are as follows: 114.5 ng/L detected in WWTP from Netherlands (Narain-Ford, Van Wezel, et al., 2022), 395.7 ng/L (median concentration) detected in WWTP in Germany (Muschket et al., 2024).

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### Diclofenac

Diclofenac was found in one study of 52 WWTPs from 15 EU countries with median concentration of 1419.4 ng/L (Finckh, Beckers, et al., 2022). Diclofenac was found in effluents of WWTPs from the Danube River Basin, in concentrations ranging between 280 and 1312 ng/L (Ng et al., 2023). Both concentrations are well above EQS of 50 ng/L. Concentrations for diclofenac varied significantly among the studies, with values usually above EQS, for example 305 ng/L in a WWTP effluent in Serbia (Bogunović et al., 2021).

### Clarithromycin

Clarithromycin was measured in effluent of 7 WWTPs from the Danube River Basin with levels ranging from <LOQ to 3 ng/L and authors concluded efficient removal in these WWTPs (Ng et al., 2023). In a WWTP in Sweden clarithromycin was found in concentration of 36 ng/L in effluent prior to the 4<sup>th</sup> treatment step (Svahn & Borg, 2024). These values are below the EQS of 120 ng/L. Clarithromycin was found at different concentrations in 56 WWTP effluents from 15 European countries with concentrations ranging from <LOQ to 1174.7 ng/L (Finckh, Beckers, et al., 2022).

### 3.5.2 Personal Care Products

Personal Care Products (PCPs) is another already wider studied substance group in wastewater. As PCPs are used extensively all over the world, large amounts are released into sewage systems, making wastewater effluents the main pollution source into the environment (Posada-Ureta et al., 2012) as cited in (Tasselli et al., 2021). Three substances were exemplarily selected for further discussion, as they were part of several published analyses assessed in the current literature search and occurred in comparably high concentrations. The substances are summarized together with relevant environmental concentration thresholds in Table 3.

Table 3: List of selected substances associated to personal care products and corresponding environmental concentration thresholds.

Substance	CAS	Environmental concentration threshold			
		Value	Туре	Source	
Galaxolide (HHCB)	1222-05- 5	6.8 µg/L	PNEC	Brief Profile - ECHA	
Methylparaben	99-76-3	2.4 µg/L	PNEC	Brief Profile - ECHA	
Oxybenzone (BP-3)	131-57-7	0.67 µg/L	PNEC (freshwater)	<u>Brief Profile</u> - ECHA	

#### Galaxolide

Galaxolide is a polycyclic musk fragrance (PMF), which is only partially degradable and is therefore not removed by conventional WWTPs. Hence, synthetic musk compounds are present in various compartments such as rivers and agricultural fields fertilised with WWTP biosolids and have the capacity to bioaccumulate. For instance, (García-Galán et al., 2021) found galaxolide in an average concentration of  $191 \pm 27$  ng/L in a mixture of irrigation and rural drainage water. (Tasselli et al., 2021) found galaxolide and other PMFs in the water and sludge phase of a WWTP in Northern Italy.

#### Methylparaben

Methylparaben is used in a variety of personal care products such as shampoos, creams and cosmetics for its anti-fungal properties to prevent the growth of bacteria, mold and yeast. The substance is toxic to aquatic life with long-lasting effects. In a study conducted by (Ferreiro et al., 2020), samples were collected every

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hour for four hours in the influent of a WWTP in Biscay (Spain), showing concentrations between  $2.094 \pm 0.067 \mu g/L - 8.4 \pm 0.25 \mu g/L$  for methylparaben, which are lower (for the lower bound) and higher (for the upper bound) than PNEC. Another study by (Montes et al., 2023), investigating 93 samples of river water, coastal water and raw and treated wastewater from 33 sites in the North of Portugal and Galicia, Spain, showed that methyl-4hydroxybenzoate (methylparaben) was present in concentrations of  $0.025 - 1.15 \mu g/L$  in raw WWTP influent and  $0.006 - 0.48 \mu g/L$  in treated WWTP effluent. In the same study, methylparaben was assessed with an RQ of 1.39, which relates to moderate risk for aquatic species and correlates with levels below PNEC.

#### Oxybenzone

Oxybenzone (BP-3) is a chemical widely used in sunscreen formulations to provide broad-spectrum UV protection. In addition to its primary role in sunscreens, oxybenzone also has secondary applications in products such as coatings, plasters, modelling clay, finger paints, and other items designed to prevent UV degradation. However, concerns have arisen regarding its environmental impact, particularly in relation to coral bleaching. Due to these concerns, its use in sunscreens has been regulated in several countries. In 2022, the European Commission included oxybenzone in its watchlist, suggesting that it may pose a significant risk to the aquatic environment<sup>5</sup>. However, insufficient monitoring data prevent a definitive risk assessment.

In Italy, a study reported BP-3 concentrations of  $0.66\pm0.07 \ \mu$ g/L detected in water samples after primary sedimentation and  $0.30\pm0.03 \ \mu$ g/L detected in treated effluent collected at the end of the process from a municipal WWTP (Spina et al., 2020). Further, study by (Montes et al., 2023) conducted in Spain and Portugal sampled six WWTP sites and found BP-3 concentrations in raw

wastewater ranging from 0.157 to 2.162 µg/L and in treated wastewater from 0.023 to 1.385 µg/L. The risk assessment conducted in the report was based on the PNEC values from the NORMAN database, where the PNEC for freshwater is 1.54 µg/L and the marine PNEC is 0.154  $\mu$ g/L (Montes et al., 2023). Based on the measured BP-3 concentrations and these PNEC thresholds, the assessment indicated that BP-3 could pose a potential risk to coastal environments, but not to freshwater environments (Montes et al., 2023). In comparison, the ECHA database has set a lower PNEC of 0.67  $\mu$ g/L for freshwater and 0.067  $\mu$ g/L for marine environments. These values suggest that some of the maximum concentrations measured in WWTP effluents were more than twice the PNEC for freshwater, and up to 20 times higher than the PNEC for marine environments, particularly in coastal areas where some effluents are released into the sea. Therefore, BP-3 poses a potential risk to both freshwater and coastal environments, when all both PNEC values from ECHA and Montes et al. (2023) are considered.

Additionally, a study conducted in Spain assessed the maximum concentration of BP-3 in irrigation water, which is a mixture of reclaimed water from WWTP effluent and surface water. The concentrations ranged from 0.16 to 4.18  $\mu$ g/L, and a risk quotient of 6.24 was calculated, which was designated as a moderate environmental risk in the context of the report (García-Vara et al., 2023). This further highlights the environmental relevance of BP-3, particularly in aquatic systems where concentrations of the substance may pose risks to the ecosystem.

### 3.5.3 Pesticides

Several studies have identified pesticides in both influent and effluent wastewater samples, highlighting their insufficient removal in the WWTP.

One study quantified 18 pesticides in effluents and 6 in influents. Terburtryn, propiconazole, and tebuconazole, all commonly used as

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biocides, were the most frequently detected, appearing in over 85% of samples at concentrations ranging from 9 to 156 ng/L. In contrast, 14 out of the 18 pesticides were found in less than 20% of samples, and azoxystrobin, metconazole, and paclobutrazole were only detected at WWTP located in a small village of Otterup, suggesting a possible localized source (Kilpinen et al., 2023).

The study from (Montes et al., 2023) found six out of 8 investigated pesticides in wastewater (Detection frequency (DF)>80%), all of which were also present in river water, while only DEET and diuron were detected in coastal water, indicating decreasing pesticide prevalence. Lower average concentrations were observed in treated compared to raw samples. The study reported that diuron was found in both river and coastal waters, while tertbutryn and metolachlor appeared only in rivers. Further, it was reported that propanil had the highest concentrations across all water types but low detection in wastewater, suggesting localized contamination sources (Montes et al., 2023). Average concentrations of pesticides in raw and treated wastewater from this study are provided in Figure 4.

Below, key findings on pesticides detected at higher concentrations and potential human and ecological risks are discussed. List of selected pesticides can be found in Table 4.

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Carbendazim	10605- 21-7	0.15 µg/L	PNEC	(García- Vara et al., 2023)
Chlorotoluron	15545- 48-9	0.6 µg/L	Annual average EQS (AA EQS)	(Finckh, Beckers, et al., 2022)

# Table 4: List of selected pesticides identified and correspondingenvironmental concentration thresholds.

Substance	CAS	Environmental concentration threshold			
		Value	Туре	Source	
N,N-diethyl-m- toluamide (DEET)	134-62-3	88 µg/L	PNEC	(García- Vara et al., 2023)	
Diuron	330-54-1	0.32 µg/L	PNEC (freshwater)	Brief Profile - ECHA (date of access: 30.1.2025)	
Fenpropimorph	67564- 91-4	0.016 μg/L	PNEC (freshwater)	REACH Dossier (date of access: 30.1.2025)	
Imidacloprid	138261- 41-3	0 µg/l	PNEC (freshwater)	REACH Dossier (date of access: 30.1.2025)	
Propanil	709-98-8	0.2 µg/L	Annual average QS	(Finckh, Beckers, et al., 2022)	
Terbutryn	886-50-0	0.065 µg/L	PNEC	(García- Vara et al., 2023)	

### Carbendazim

Carbendazim, a fungicide, has been detected in treated wastewater and irrigation samples in both Spain and Germany, with notable concentration variations. In Spain, the maximum concentration in effluent wastewater reached 0.62  $\mu$ g/L (Lopez-Herguedas et al., 2022), while irrigation water containing reclaimed and surface water showed levels of 0.156  $\mu$ g/L (García-Vara et al., 2023). The concentration observed in effluent wastewater is significantly higher

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than the PNEC value while the one in irrigation water only slightly exceeds the PNEC value of 0.15  $\mu$ g/L and yields a relatively low RQ of 0.356, suggesting low ecological risk (García-Vara et al., 2023). In Germany, carbendazim was detected in treated wastewater samples in concentrations up to 0.012  $\mu$ g/L (Weitere et al., 2021) which is far below the PNEC value.

### Chlorotoluron

The study conducted by (López-Herguedas et al. 2022) reports a detection of chlorotoluron, an herbicide, in the effluent of 5 WWTPs in Spain with a maximum concentration of 7.45  $\mu$ g/L observed in one of the WWTPs during summer and winter. This value is significantly higher than the AA EQS value. Conducted risk assessment concluded that this herbicide is among the ones having the largest risks to algae. In contrast, chlorotoluron was not detected in any upstream and downstream WWTP samples in Germany (Weitere et al., 2021).

### Diethly toluamide (DEET)

The study by (Lopez-Herguedas et al., 2022) detected DEET, a common insect repellent, in the effluent of 5 WWTPs in Spain during summer and autumn, with a maximum concentration of 0.78  $\mu$ g/L. Their risk assessment identified DEET as one of the substances posing significant risk for fish, with an RQ>1 (López-Herguedas et al. 2022). In a similar campaign, (García-Vara et al., 2023) reported maximum DEET concentrations of 0.277  $\mu$ g/L during summer. Based on these findings, they calculated an RQ value of 0.003, concluding that the pesticide presented no toxicological risk.

### Diuron

Diuron, an herbicide with possible carcinogenic and endocrinedisrupting properties, had been detected in wastewater and environmental waters across Europe. In Spain and Portugal, influent average concentrations ranged from 0.017 to 0.461  $\mu$ g/L, with treated effluents between 0.050 to 0.309  $\mu$ g/L (Montes et al., 2023). In Spain, concentrations of diuron in wastewater samples collected

during summer and winter peaked at 0.090  $\mu$ g/L (Lopez-Herguedas et al., 2022). Garcia-Vara et al. detected a maximum concentration of 0.027  $\mu$ g/L in reclaimed irrigation water. Based on these findings they calculated an RQ value of 0.383, concluding that this herbicide presented low toxicological risk (García-Vara et al., 2023). In Austria, one study reported concentrations <LOD in WWTP effluents (Reif et al., 2023).

Values detected in wastewater effluents are typically lower than PNEC values for freshwater. However, due to variability in observed concentrations, caution is needed when interpretating results due to significant regional differences.

#### Fenpropimorph

The study by (Lopez-Herguedas et al., 2022) reported a maximum concentration of 1.860  $\mu g/L$  of fenpropimorph, a pesticide, in the effluent of 5 WWTPs in Spain during summer and autumn. This value is significantly higher than the PNEC value of 0.016  $\mu g/L$  for freshwater.

### Imidacloprid

Imidacloprid, a widely used pesticide, has been detected at varying concentrations in wastewater samples across different regions.

In Sweden, it was measured at 0.006  $\mu$ g/L in samples taken from WWTP prior to the 4<sup>th</sup> treatment step (Svahn & Borg, 2024), while in Spain, maximum concentrations in WWTP effluent reached 0.440  $\mu$ g/L during summer and autumn (Lopez-Herguedas et al., 2022). A study along the Danube River across 10 EU countries reported a peak concentration of 0.328  $\mu$ g/L (Ng et al 2023). All values are above the PNEC threshold value of 0  $\mu$ g/L for freshwater. Risks assessments showed very low human health risks (LoQ RQ <2) for treated wastewater but very high ecosystem health risks (log RQ >2) for both raw and treated wastewater, emphasizing environmental persistence of this pesticide and potential ecological impact (Neale et al., 2023).

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### Propanil

The study by (Montes et al., 2023) detected propanil, a pesticide, in both raw and treated wastewater samples in Spain and Portugal. In the influent, average propanil concentrations ranged from 0.167 to 1.109  $\mu$ g/L, while in treated wastewater, the levels varied between 0.088 and 1.196  $\mu$ g/L, indicating some values exceed also the QS value of 0.200  $\mu$ g/L. Despite the highest concentrations observed in all samples, it is important to note that DF was rather low, less than 25% in wastewater, indicating that the contamination may originate from sources other than WWTP itself (Montes et al., 2023).

### Terbutryn

Terbutryn was detected in various wastewater and environmental samples across Spain, Portugal, and Denmark. In Spain and Portugal, average influent concentrations ranged from 0.019 to 0.228 µg/L, while treated wastewater contained average concentrations from 0.002 to 0.361 µg/L (Montes et al., 2023). The maximum concentration in irrigation water, a mix of reclaimed and surface water, was 0.176 µg/L (García-Vara et al., 2023). This exceeds the PNEC of 0.065  $\mu$ g/L, yielding a RQ of 2.70, indicating ecological concern (García-Vara et al., 2023). (Kilpinen et al., 2023) reported terbutryn in all influent and effluent WWTPs samples in Denmark, with influent concentrations typically between 0.011 and 0.059  $\mu$ g/L, spiking at to 0.509  $\mu$ g/L in June 2020. Effluent levels correspondingly rose to 0.106  $\mu$ g/L in June and 0.156  $\mu$ g/L in July, compared to typical levels of 0.036 ng/L to 0.041 µg/L. RQ value for R. subcapitata ranged from 2.4 to 81, suggesting a significant ecological risk (Kilpinen et al., 2023). Terbutryn is primarily used as an herbicide for grass and weed control but also serves as an algicide in textile production and a biocide in building materials (Kilpinen et al., 2023).

### 3.5.4 PFAS

It is assumed that several thousands of per- and polyfluoroalkyl substances (PFAS) exist and it is therefore challenging to analytically determine a larger spectrum of these compounds simultaneously in one sample. In October 2022, the Commission suggested quality standards for the sum of 24 PFAS, including PFOS, in surface water and groundwater, derived from an opinion of the European Food Safety Authority (EFSA) and further backed up by opinions of the Scientific Committee on Health, Environment and Emerging Risks. The proposed standard for surface and groundwaters is 4.4 ng/l (as PFOA equivalents) (EU COM, 2022b).

The majority of wastewater analyses have primarily targeted a limited number of well-researched PFAS, with a particular emphasis on perfluoroalkyl acids (PFAA) (Thompson et al., 2022) as cited in (Ruyle et al., 2025). The TOP assay transforms precursor compounds - many of which lack commercially available analytical standards needed for quantification - into PFAA, that can be quantified. In a study by (Kaiser et al., 2021), which used the TOP assay, an estimated total PFAS content of 840 ng/L was measured in effluent samples of a WWTP in Austria, which was 91.1% higher than the results of the target PFAS analysis. According to the authors this suggests the presence of unknown precursors which are not commonly monitored. The study shows the complexity of PFAS in wastewater and its different sources.

In the following, some concentration levels found for selected wellknown PFAS are presented.

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Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Perfluorooctane sulfonic acid (PFOS)	1763- 23-1	0.65 ng/L	AA-EQS	(EU COM, 2011)
Pentafluorobutanoic acid (PFBA)	375- 73-5	0.4 μg/L	PNEC (freshwater)	Norman Ecotox Database as cited in (Montes et al., 2023)

Table 5: List of selected PFAS identified and correspondingenvironmental concentration thresholds.

### Perfluorooctane sulfonic acid (PFOS)

In Spain and Portugal, influent average concentrations ranged from <LOQ-233 ng/L, with treated effluents between <LOQ-44 ng/L in one study (Montes et al., 2023). PFOS was also detected in river in France near to WWTP with levels as high as 34 ng/L (well above the above the EU Environmental Quality Standards (EQS) of 0.65 ng/L) (Ayoub et al., 2022). In another study from Austria, PFOS was found in effluent in concentration of 2.77 ng/L (Kaiser et al., 2021).

### Pentafluorobutanoic acid (PFBA)

For PFBA, average concentration of <LOQ-115 ng/L in treated effluent were found in Spain and Portugal (concentration in influent ranged from <LOQ-87 ng/L) (Montes et al., 2023). In Germany, concentration of <LOD-719 ng/L in treated wastewater were reported in one study (Weitere et al., 2021).

Relatively high concentrations were also reported for other still less investigated PFAS in wastewater in scientific literature. For example,

(Finckh, Beckers, et al., 2022) found 6:2 fluorotelomer sulfonic acid with a median concentration of 283.85 ng/L from 56 effluent samples from 52 European WWTP. In another study perfluorobutane sulfonic acid (PFBS) was found in WWTP effluents in river basin from Spain with extraordinary high concentration of up to 936.1 ng/L in one WWTP (Beltrán De Heredia et al., 2024).

#### 3.5.5 Industrial chemicals

Industrial chemicals are frequently detected in wastewater, reflecting their widespread use in manufacturing, consumer products, and industrial processes. These substances enter WWTPs through industrial discharges, household wastewater, and runoff, often persisting in effluent even after treatment.

Effluent samples collected from 26 wastewater sources across 8 WWTPs detected various industrial chemicals at trace concentrations, including butylated hydroxytoluene, a synthetic antioxidant used as a preservative in foods, cosmetics, and industrial products, ranged from 0.0001 µg/L to 0.0006 µg/L. Aniline, an aromatic amine used in the production of dyes, rubber chemicals, and pesticides, ranged from 0.0004 µg/L to 0.0007 µg/L. 3-Methylphenol, used in the synthesis of pharmaceuticals, fragrances, and as an intermediate in chemical manufacturing, had a concentration of 0.0004 µg/L. 9-Methylacridine, used in organic synthesis, ranged from 0.0002 µg/L to 0.0006 µg/L. 1,2,3-Benzotriazole, a corrosion inhibitor and organic synthesis intermediate, varied from 0.0003 µg/L to 0.003 µg/L. 1,3-Diphenylquanidine, used as a vulcanisation accelerator in rubber production and as an intermediate in organic synthesis, ranged from 0.00007  $\mu$ g/L to 0.0009  $\mu$ g/L. 1,7-Dimethylxanthine, a caffeine metabolite with use as an intermediate in organic synthesis, ranged from 0.003  $\mu$ g/L to 0.006  $\mu$ g/L. Finally, 2-phenoxyethanol, a glycol ether solvent and preservative, ranged from 0.0007 µg/L to 0.001  $\mu$ q/L (Kilpinen et al., 2023).

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This section explores the presence and impact of key industrial chemicals in wastewater, focusing on their detection in effluent streams.

### 3.5.5.1 Surface modifiers

#### 3.5.5.1.1 Surfactants

Surfactants, commonly found in household and industrial detergents, cleaning agents, and various industrial applications, are contributors to wastewater contamination. Due to their widespread use, these chemicals often end up in effluents, where they can persist.

Table 6: List of selected surfactants identified and correspondingenvironmental concentration thresholds.

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (representative of alkylbenzene sulfonates)	85536- 14-7	268 µg/L	PNEC (Freshwater)	<u>Brief</u> Profile - ECHA
2,4,7,9-Tetramethyl- 5-decine-4,7-diol (TMDD)	126- 86-3	1000 µg/L	PNEC (Freshwater)	<u>Brief</u> <u>Profile -</u> <u>ECHA</u>

#### Alkylbenzene sulfonates

Alkylbenzene sulfonates are a group of anionic surfactants, known as some of the earliest and most used synthetic detergents. They are present in a variety of personal care and household cleaning products. Commercial linear alkylbenzene sulfonates (LAS) are a mixture with varying alkyl chain lengths. In these commercial

mixtures, the alkyl chain lengths typically range from 10 to 14 carbon atoms (C10–C14).

LAS surfactants were found in the highest concentrations in both influent and effluent samples from WWTPs in Greece (Gago-Ferrero et al., 2020). In the influent, C11-LAS reached the highest concentration of 431  $\mu$ g/L, while in the treated wastewater, the highest concentration of 17  $\mu$ g/L was measured for C12-LAS.

In wastewater samples from the Middle Danube Basin, LAS surfactants were detected at concentrations exceeding 2000  $\mu$ g/L (Terzić et al., 2008) as cited in (Đurišić-Mladenović et al., 2024). The original study from Terzic et al 2008 did not attribute these high levels to any specific source but noted that they were consistently present across all examined municipal wastewater samples.

### 2,4,7,9-Tetramethyl-5-decine-4,7-diol (TMDD)

Another surfactant and anti-foaming agent, TMDD, was detected in WWTP effluent samples in Spain at concentrations ranging from 205 ng/L to 325 ng/L (García-Galán et al., 2021). TMDD is classified as hazardous to the aquatic environment, with potential to cause longlasting harmful effects on aquatic life. TMDD is commonly used in the industry to lower the surface tension of coatings, adhesives, paints, and printing inks as well as in pesticide formulations and in household products such as toilet and kitchen paper (Guedez & Püttmann, 2014) as cited in (García-Galán et al., 2021).

### 3.5.5.1.2 Siloxanes

Siloxanes are commonly used in personal care products, industrial applications, and manufacturing processes. Similar to surfactants, which are widespread in household and industrial uses, siloxanes can contribute to wastewater contamination due to their extensive use. Once released into the environment, they are known to be persistent and bioaccumulative raising concerns about their potential impact on water quality and ecosystems. Due to these environmental risks,

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regulatory measures are increasingly being introduced to limit the use and discharge of certain siloxanes, particularly in consumer products and industrial processes, to mitigate their long-term effects. This section presents examples of siloxanes detected in wastewater systems.

 Table 7: List of selected siloxanes identified and corresponding

 environmental concentration thresholds.

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Hexa- methylcyclotrisiloxane (D3)	541-05-9	78 μg/L	PNEC (freshwater)	Brief Profile - ECHA (date of access: 30.1.2025)
Octamethylcyclotetras iloxane (D4)	556-67-2	1.5 μg/L	PNEC (freshwater)	Brief Profile - ECHA (date of access: 30.1.2025)
Decamethylcyclopenta siloxane (D5)	541-02-6	1.2 μg/L	PNEC (freshwater)	Brief Profile - ECHA (date of access: 30.1.2025)
Dodecamethylcyclohe xasiloxane (D6)	540-97-6	NA	NA	NA
Octamethyltrisiloxane (L3)	107-51-7	NA	NA	NĀ
Decamethyltetrasiloxa ne (L4)	141-62-8	NA	NA	NA
Dodecamethylpentasil oxane (L5)	141-63-9	NA	NA	NA

The study by (Salgado et al., 2022) provides concentration of various siloxanes in wastewater effluents in Portugal, specifically analysing primary and secondary effluents, both raw and filtered.

Decamethylcyclopentasiloxane (D5) and Dodecamethylcyclohexasiloxane (D6) were the most prevalent siloxanes, with the highest average concentration of D5 peaking at 0.954  $\mu$ g/L in filtered primary effluent. Both compounds showed reduced concentrations in secondary and filtered effluents. Hexamethylcyclotrisiloxane (D3) and Octamethylcyclotetrasiloxane (D4) were detected at moderate average concentrations (0.127-0.246  $\mu$ g/L), while Dodecamethylpentasiloxane (L5) was detected at low average concentrations (<LOD-0.016  $\mu$ g/L). Octamethyltrisiloxane (L3) and Decamethyltetrasiloxane (L4) were <LOD across all samples (Salgado et al., 2022).

#### 3.5.5.2 Plastic additives

#### 3.5.5.2.1 Flame retardants

Flame retardants are chemicals added to materials to prevent or slow the spread of fire. They are widely used in products such as furniture, electronics, and construction materials to improve fire safety. This section highlights examples of flame retardants that have been detected in wastewater systems.

Flame retardants were found in measured concentrations in effluent samples from wastewater treatment plants in both Spain and Germany.

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Table 8: List of selected flame retardants identified andcorresponding environmental concentration thresholds.

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Tributyl phosphate (TBP)	126-73- 8	35 - 82 µg/L	PNEC (freshwater)	Brief Profile - ECHA (date of access: 30.1.2025)
Tris(2-chloroethyl) phosphate (TCEP)	115-96- 8	4 µg/L	Lowest PNEC (freshwater)	(Finckh, Buchinger, et al., 2022)
Tris(2-butoxyethyl) phosphate (TBEP)	78-51-3	24 µg/L	PNEC (freshwater)	Brief Profile - ECHA (date of access: 30.1.2025)
Tris(1-chloro-2- propyl) phosphate (TCPP)	13674- 84-5	420 - 640 µg/L	PNEC (freshwater)	Brief Profile - ECHA (date of access: 30.1.2025)

In Spain, tributyl phosphate (TBP) was detected at a concentration of  $54 \pm 4$  ng/L, while tris(2-chloroethyl) phosphate (TCEP) was found at  $284 \pm 29$  ng/L (García-Galán et al., 2021). In Germany, treated WWTP effluent showed higher levels of flame retardants, including tris(2-butoxyethyl) phosphate (TBEP) at 336 ng/L and tris(1-chloro-2-propyl) phosphate (TCPP) at 864 ng/L, which were being released into the Ammer River (Müller et al., 2020). All flame retardants are below PNEC values (freshwater). Other flame retardants, such as melamine and bisphenol A have also been detected, however, these

are addressed under other sections as these substances also have other functions.

### 3.5.5.2.2 Light stabilisers

Light stabilisers are commonly used as additives in plastics and various industrial applications to protect materials from degradation caused by UV radiation. However, these substances have been reported to exhibit environmental persistence, bioaccumulation, and toxicity (PBT), which can pose significant environmental risks. In May 2023, UV-328 was added to the Stockholm Convention on Persistent Organic Pollutants as a persistent organic pollutant (POP) because of its PBT characteristics. Additionally, several light stabilisers have been added to the SVHC Candidate and Authorisation lists because of their environmental impact. For example, UV-329 was added to the SVHC list in 2024 due to its vPvB properties.

# Table 9: List of selected light stabilisers identified andcorresponding environmental concentration thresholds.

Substance	CAS	Environmental threshold		concentration
		Value	Туре	Source
UV-328	25973- 55-1	10 µg/L	PNEC (Freshwater)	<u>Brief Profile -</u> ECHA
UV-329	3147- 75-9	NA	NA	NA

A study measured the presence of light stabilisers in various aquatic systems (WWTP, seawater, and fish samples). All targeted light stabilisers (UV P, UV 326, UV 327, UV 328, UV 329, UV 360) were detected in all wastewater treatment samples (both influent and effluent), with concentrations ranging from 0.01 to 1.9  $\mu$ g/L. The study reported that concentrations were higher in influents rather

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than in effluents, likely due to the adsorption of compounds onto suspended solids during the treatment. UV-329 was the most commonly detected compound, found in 33% of influent samples (0.1–1.9  $\mu$ g/L) and 10% of effluent samples (0.05–0.57  $\mu$ g/L), suggesting incomplete removal (Torres-Padrón et al., 2020).

### 3.5.5.3 Process chemicals

#### 3.5.5.3.1 Corrosion inhibitors

This section focuses on corrosion inhibitors, which are chemical substances used to prevent or slow down the corrosion process in various materials, particularly metals. Due to their widespread use, corrosion inhibitors often end up in wastewater streams. The presence – especially of old inhibitors - in wastewater raised environmental concerns. Some organic inhibitors can be toxic to aquatic life and may persist in the environment (Ahmed et al., 2024).

The present literature searches revealed data mainly of the most common and widely used **benzotriazole derivatives** (e.g., BTA, 4-methylbenzotriazole, 5-methylbenzotriazole) and **triazoles** (e.g., 1,2,3-Benzotriazole, 1,2,4-Triazole), which are frequently used for metal protection, especially copper and its alloys.

# Table 10: List of selected corrosion inhibitors identified andcorresponding environmental concentration thresholds.

Substance	CAS	Environmental threshold		concentration
		Value	Туре	Source
5- Methylbenzo- triazole	29385- 43-1	8 µg/L	PNEC (Freshwater)	<u>Brief Profile -</u> <u>ECHA</u>
5-Methyl-1H- benzotriazole				
Tolyltriazole				

Benzotriazole	95-14- 7	97 μg/L	PNEC (Freshwater)	<u>Brief Profile -</u> ECHA
1H- Benzotriazole				

### 5- Methylbenzo-triazole

In samples from WWTP effluent of the secondary clarifier from Germany, tolyltriazole was found in concentrations up to 16.8  $\mu$ g/L (Neef et al., 2022), which exceeds the predicted no effect level indicated in the REACH registration dossier. (Finckh, Buchinger, et al., 2022) reported a median concentration value of 1.8  $\mu$ g/L in 56 effluent samples from 52 European WWTPs.

### 1H-Benzotriazole

A very recent study from Sweden reported average levels of benzotriazole of 386 ng/L in wastewater from a WWTP before the 4<sup>th</sup> treatment step (Svahn & Borg, 2024). In samples from WWTP effluent of the secondary clarifier from Germany, benzotriazole was found in concentrations up to 15.8 µg/L (Neef et al., 2022). (Kaiser et al., 2021) reported 1.31 µg/L in effluent of a WWTP in Austria. (Finckh, Buchinger, et al., 2022) measured 56 effluent samples from 52 European WWTPs and reported a median value of 3.59 µg/L for 1H-Benzotriazole.

### 3.5.5.3.2 Cleaning agents

Cleaning agents, commonly used in household and industrial settings, often contain substances that can persist in wastewater

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systems. This section includes studies identifying the types and concentrations of cleaning agents found in wastewater.

# Table 11: List of selected cleaning agents identified andcorresponding environmental concentration thresholds.

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Sulfamate	5329- 14-6	70 µg/L	PNEC (Derived)	(Freeling et al., 2020)

### Sulfamate

Sulfamic acid is a high production volume chemical, which is widely used for scale removal operations and chemical cleaning. It is also a common precursor to the manufacture of sweeteners. Sulfamate, the anion of sulfamic acid, was measured in the influent and effluent of 5 WWTPs in Germany, the concentrations ranged from 520 µg/L to 1900 µg/L and from 490 µg/L to 1600 µg/L, respectively (Freeling et al., 2020). It was also identified that WWTP effluent was the dominant source of sulfamate in the surface water. Approximately 30% of the reported sulfamate concentrations in groundwater and surface water exceed the PNEC. A conservative risk-quotient based analysis suggests that potential effects of sulfamate on aquatic organisms in wastewater-impacted waterbodies in Germany cannot yet be ruled out (Freeling et al., 2020). Additionally, the typical sulfamate concentrations in WWTP effluent in Germany were more than 1000 times higher than the effluent concentrations of the common pharmaceuticals carbamazepine and diclofenac, which are generally detected in the 0.05 to 0.5  $\mu$ g/L range (Freeling et al., 2020).



### 3.5.5.3.3 Adhesives

Adhesives, which are widely used in industries such as construction, packaging, and automotive, can release various chemical components into wastewater. This section reviews studies that have detected adhesives or their residues in wastewater.

# Table 12: List of selected adhesives identified and correspondingenvironmental concentration thresholds.

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Isophorone	2855-	60	PNEC	<u>Brief Profile</u>
diamine	13-2	µg/L	(Freshwater)	- ECHA
Melamine	108-78-	510	PNEC	Brief Profile
	1	µg/L	(Freshwater)	- ECHA

### Isophorone diamine

Isophorone diamine is widely employed in the production of coatings, adhesives, and paints due to its ability to enhance the durability and chemical resistance of epoxy formulations. The effluents from 6 municipal WWTPs in Germany (n = 38) were analysed for 127 suspected persistent and mobile chemicals. One of the chemicals detected, isophorone diamine, a substance commonly used as a hardener in heat-cured epoxies, was found with a median concentration of 0.192 µg/L in river samples. No data for WWTP effluent is provided. (Muschket et al., 2024)

### 3.5.5.4 Other

Table 13: List of selected other industrial chemicals identified andcorresponding environmental concentration thresholds.

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
2- Benzothiazolesulfonic acid	941- 57-1	NA	NA	NA
Bisphenol A	80-05- 7	23 µg/L	PNEC (Freshwater)	<u>Brief</u> Profile - ECHA

### 2-Benzothiazolesulfonic acid

Benzothiazole derivatives are primarily used as vulcanisation accelerators in tire production. In an aqueous medium, some of these substances convert to 2-Benzothiazolesulfonic acid<sup>6</sup>. 2-Benzothiazolesulfonic acid was detected in effluent samples from 15 EU countries, with a median concentration of 0.92  $\mu$ g/L in 56 samples collected from 52 wastewater treatment plants (Finckh, Buchinger, et al., 2022). Additionally, a maximum concentration of 0.15  $\mu$ g/L of 2-Benzothiazolesulfonic acid was found in effluent samples from 11 wastewater treatment plants along the Danube River, spanning 10 EU countries (Ng et al., 2023). This finding highlights the widespread presence of this substance in European wastewater.

#### Bisphenol A

Bisphenol A (BPA) is primarily used as a plastic monomer and in the production of epoxy resins. It is also present in smaller quantities in various materials, including flame retardants.

BPA has been detected in wastewater and surface waters across Europe, with concentrations varying by location. The lowest reported levels were found in treated effluents from two municipal WWTPs in Romania, ranging from 0.006 to 0.075  $\mu$ g/L, with an assessment concluding that at these concentrations, BPA posed a low risk to the aquatic environment (Chiriac et al., 2020). In a river near a WWTP in France, levels ranged from 0.08 to 0.24  $\mu$ g/L (Ayoub et al., 2022). In 10 EU countries along the Danube River, concentrations of up to 0.12  $\mu$ g/L were recorded in wastewater treatment effluents measured as part of the Joint Danube Survey 4 (JDS4) (Ng et al., 2023).

The levels of Bisphenol A (BPA) observed in wastewater treatment plants (WWTPs) exhibited significant variation. Influent concentrations spanned a wide range, with the lowest recorded at 0.33  $\mu$ g/L and the highest reaching 910  $\mu$ g/L. In contrast, effluent concentrations were generally lower, ranging from below the detection limit of 0.01  $\mu$ g/L to a maximum of 0.65  $\mu$ g/L (Tappert et al., 2024). A municipal WWTP in Italy reported 0.51  $\mu$ g/L in wastewater treatment plant effluents collected at the end of the process, with findings suggesting that even extremely low BPA concentrations (< 0.000001  $\mu$ g/L) could disrupt hormonal metabolism in amphibians and fish at various developmental stages. (Spina et al., 2020)

A representative concentration ( $C_{rep}$ ) of 0.63 µg/L was estimated based on three recent literature sources from different geographical regions. This value was determined by averaging the three highest reported concentrations, using the maximum values between influent and effluent for each source. (Manetti & Tomei, 2024)

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The highest recorded concentration was found in Spain, where 9.98  $\mu$ g/L was measured in primary effluent from a municipal WWTP in the Basque Country (Lopez-Herguedas et al., 2024)

While some studies indicated a low environmental risk, others raise concerns, especially regarding the potential effects on aquatic organisms at very low concentrations. However, all measured BPA concentrations in treated effluents reported in this section were below the PNEC values for freshwater, suggesting minimal immediate risk in those cases.

#### 3.5.6 Food ingredients / additives

Food ingredients are generally not classified as micropollutants but can contribute to water pollution and interfere with wastewater treatment processes. However, the ecological risk of sweeteners as one group is still under discussion as shown in the following chapter. Also, caffeine will be discussed in the course of this chapter.

#### 3.5.6.1 Sweeteners

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Acesulfam (K)	55589- 62-3	2.2 mg/L	PNEC (freshwater)	<u>Brief Profile</u> <u>- ECHA</u>
		0.724 mg/L		Norman Ecotox Database as cited in (Montes et al., 2023)
Sucralose	56038- 13-2	0.93 mg/L	PNEC (aquatic)	(Tollefsen et al., 2012)

### Sucralose

A study by Kilpinen et al. quantified four food additives in both influent and effluent wastewaters from WWTPs in Denmark. Sucralose was measured with a concentration range of 21.3-63.1  $\mu$ g/L in effluent wastewater. (Kilpinen et al., 2023)

A study measuring 232 chemicals in influent and effluent of wastewater treatment plants in Australia revealed a median level of 38.339 mg/L in effluent of WWTP in Australia (non-EU) (Linge et al., 2021). It might be questioned how far the Australian technology is comparable with the EU one, but we wanted to show these findings in order to complement the picture.

(Finckh, Beckers, et al., 2022) measured 56 effluent samples from 52 European WWTPs and ranked the sucralose median concentration of 15.3  $\mu$ g/L within the top 30 median concentrations.

(Lewis & Tzilivakis, 2021) concluded that since sucralose is not significantly metabolized by the human body, its potential to contaminate the aquatic environment is high, particularly because wastewater treatment facilities do not efficiently remove it. Sucralose is not readily biodegradable, is considered persistent in aquatic systems, and does not appear to generate significant transformation products or metabolites. Numerous studies have documented the widespread presence of sucralose in surface waters, marine and coastal waters, groundwater, and even drinking water. Available data suggest that sucralose is not highly toxic to aquatic organisms. Further research is needed to assess the potential toxicity of sucralose in terrestrial environments and to better understand its overall environmental risks.

#### Acesulfame

(Finckh, Beckers, et al., 2022) measured 56 effluent samples from 52 European WWTPs and ranked the acesulfame median concentration of  $1.9 \mu g/L$  within the top 30 median concentrations.

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Although acesulfame-K does not appear to be highly toxic to aquatic organisms, concerns exist regarding long-term exposure, as studies indicate it may increase oxidative stress in aquatic life. Additionally, research has shown that acesulfame-K undergoes transformation through various degradation processes. Studies investigating these transformation products in aquatic environments have confirmed their presence, with many of these byproducts considered more toxic than the parent compound (Lewis & Tzilivakis, 2021).

In 2021, (Lewis & Tzilivakis, 2021) contracted by the European Food Safety Authority (EFSA) assessed the environmental impact of artificial sweeteners using a systematic literature review. The authors conclude that multiple studies have been identified demonstrating the widespread presence of acesulfame-K, sucralose, cyclamates, and saccharin in surface waters, groundwater, coastal, and marine environments. Often the argument is used, that any measured levels are far below the established PNEC (as confirmed in our present review), it is important to highlight that EFSA also indicated further research needs to assess the potential toxicity of sucralose in terrestrial environments and to better understand its overall environmental risks. For acesulfame, the paper states that its persistence and high global consumption suggest that environmental concentrations are likely to increase over time. This is considered a significant concern by EFSA, although the limited available data on its ecological toxicity and impact on biodiversity provide some uncertainty. As concluded by EFSA, there is currently no strong evidence indicating harm to ecosystems or biodiversity at present concentration levels but it cannot be assumed that this will remain the case in the future.

### 3.5.6.2 Caffeine

Caffeine (CAF) and its metabolite theophylline are considered as indicators of anthropogenic contamination of aquatic environments.

#### Table 14: Environmental concentration threshold for caffeine

Substance	CAS	Environmental concentration threshold		
		Value	Туре	Source
Caffeine (CAF)	58-08-2	87 µg/L	PNEC (freshwater)	<u>Brief Profile</u> - ECHA

(Diogo et al., 2023) summarised CAF concentrations from different water samples around the world. In Europe, the highest concentration was reported for the influent of a WWTP in UK with 150 µg/L. In rivers and lakes, concentrations ranged from <0.004 to 1.27 µg/, while for seawater, concentrations from 0.016 to 0.058 µg/L were reported. Further studies investigated CAF concentrations at WWTPs in Sweden, observing concentrations of 22±3.8 ng/L at various stages of the WWTP (Ullberg et al., 2021) and 64,000 ng/L in influent samples (Golovko et al., 2021).

(Diogo et al., 2023) further investigated the chronic effects of sublethal concentrations (between 0.16 – 50  $\mu$ g/L) of CAF in a 28-day study in *Danio rerio*. The authors concluded that the exposure to CAF induces significant disruption in antioxidant defence pathways (superoxide dismutase, SOD; glutathione reductase, GRed and glutathione content, GSH); somewhat affected cellular energy allocation mechanisms (lactate dehydrogenase, LDH activity and lipids content) and were responsible for neuro-oxidative disturbances at the highest concentration.

### 3.6 Bias of categorisation

While in the above chapter substances have been allocated to certain categories it needs to be stressed, that the categorisation can

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introduce another level of bias as a number of substances can be allocated not just to one category. As an example, we would like to selectively indicate benzotriazole (CAS no. 95-14-7), which has an active REACH registration and thus has also other uses than in the pharma sector. Another prominent example is caffein, which is a pharmaceutical substance but also a well-known food ingredients. It is further known to be used in cosmetic products.

Furthermore, it should be highlighted that none of the assessed studies differentiate between veterinary and human pharmacological substances, similarly to the Pistocchi study, explained in more detail in the following. Therein, both kind of pharmaceutical substances are addressed, whereas, the (new) UWWTD only included products in Annex III relating to human health.

### 3.7 Key studies from scientific literature

The following chapter summarises selected key studies of particular interest when it comes to identifying micropollutants in wastewater, more information on all studies investigated in this literature review is provided in Appendix 3. The key studies have been selected on the basis of the information they provide. A lot of available studies focus on different treatment technologies and do not provide a comprehensive picture of the chemicals present in wastewater. The key studies mostly provide a broader picture on chemicals and potential sectoral distribution than other studies.

The study by Pistocchi et al 2022, often referenced in the Feasibility study<sup>7</sup> and Impact assessment<sup>8</sup>, and used as baseline for the envisaged polluter pay principle distribution evaluates the potential reduction of wastewater effluent toxicity through advanced treatment solutions in European plants. Given the lack of a comprehensive reference dataset for monitored substances, the researchers developed a so-called list of "total pollution proxy

substances" (TPPS) comprising of 1,337 substances regularly found in wastewater effluents. This list was compiled using several different datasets, including European monitoring campaigns (e.g., Finkch et al 2022), the Dutch WATSON database, expert judgement and substances identified as PMT by the German Environment Agency or regulated under EU water legislation. Since the substances are not categorized into specific groups and the list is extensive, it is challenging to draw conclusions about the distribution and prevalence of particular substance groups. The study states based on ((Alygizakis et al., 2018; Menger et al., 2021; Muir et al., 2019; Schulze et al., 2019) as cited in (Pistocchi et al., 2022)) that there is no simple way to determine if a given list of substances adequately represents all chemicals of concern. Awareness is limited to the substances one actively measures, while numerous other chemicals within the technosphere remain unidentified, posing potential future concern as "unknown unknowns". The Pistocchi study does not provide a percentage distribution across the substances for each sector, it merely notes that "the list includes several pharmaceuticals and personal care products, substances used in households, metabolites and transformation products, and inorganic substances including metals" (Pistocchi et al., 2022). Moreover, the study authors themselves highlight data gaps such as: it covers about 90% TPPS in terms of physicochemical properties, although usually estimated indirectly, attribution to an influent concentration could only be achieved for 688 TPPS (out of 1,337), and toxicity threshold range from 419 (31.3%) for chronic HC50 to 602 (45.0%) for PNEC.

# 3.7.1 Selected studies on wastewater analysis using targeted approaches

A study conducted by (Finckh, Beckers, et al., 2022) examined 56 effluent samples from 52 wastewater treatment plants (WWTPs) across Europe to assess the presence of 499 emerging chemicals (ECs) and their associated potential risks to the environment. Using solid-phase extraction followed by wide-scope chemical target

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screening, researchers identified 366 compounds, with concentrations ranging from < 1 ng/L to > 100  $\mu$ g/L. The detected substances included pharmaceuticals, pesticides, surfactants, food, plastic and rubber additives, per- and polyfluoroalkyl substances (PFAS), UV filters and corrosion inhibitors, collectively categorized as "others". In total, 111 pharmaceuticals, 96 pesticides and 98 other parent compounds were detected, along with 12, 39 and 10 transformation products (TPs), respectively (Figure 1, right). The detection rates compared to the number of analysed compounds show relatively constant findings within the three categories pharmaceuticals (79%), pesticides (69%) and others (73%) (Figure 1, left).

Very high maximum concentrations were retrieved for several industrial chemicals, including hexa(methoxymethyl)melamine (HMMM) (461  $\mu$ g/L), tetrapropyl ammonium (117  $\mu$ g/L), triethylphosphate (88  $\mu$ g/L), cyclohexylamine (70  $\mu$ g/L), 2,4-dichlorobenzoic acid (20  $\mu$ g/L), m-xylene-4-sulfonic acid (19  $\mu$ g/L), tetraglyme (19  $\mu$ g/L), and aminoacetanilide (12  $\mu$ g/L). The second-highest maximum concentration could be allocated to the hypnotic and anaesthetic drug secobarbital (150  $\mu$ g/L); also pentobarbital (14  $\mu$ g/L) could be detected in the same effluent.



Figure 1. Quantitative LC-HRMS screening results. Left: number of analysed (light coloured bar) versus detected (dark coloured bar) target compounds per use group category. Right: pie-chart of the detected target compounds per use group category: pharmaceuticals (blue), pesticides & biocides (green), others (purple) (Finckh, Beckers, et al., 2022).

The study "The Joint Danube Survey (JDS4)", conducted in 2019, has been focused on the occurrence of several hundred newly identified CEC in waters of the Danube River basin, including wastewater from selected wastewater treatment plants. A total of 419 CECs found in wastewater during JDS4 were included in the analysis from which, 311 CECs in treated wastewater discharged from WWTPs, and 306 CECs in wastewater entering WWTPs were detected. Only 198 substances were found both in the influents and effluents to/from WWTPs. Pharmaceuticals accounted for the largest proportion of detected CECs, with a total of 165 substances representing 39.4% of all detected CECs in wastewater (Figure 2) (Ansorge et al., 2024).



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### Figure 2. Group of emerging contaminants detected in wastewater within JDS4 (concentration of detected CECs were published as supplementary material to an article (Ng et al., 2023))

(Montes et al., 2023) studied 52 CECs over a year in transnational river basins, coastal areas of northern Portugal and Galicia (NW Spain), and the WWTPs discharging into them. Each of the facilities implemented initial and subsequent treatment phases utilizing activated sludge methods. Furthermore, one WWTP included an additional chlorination step as the final step in its treatment sequence. Investigated CECs included PPCP<sup>9</sup>s and their metabolites (n=22), pesticides (n=8), food additives (n=2), industrial chemicals (n=18), and cleaning agents (2). The study revealed widespread contamination and found that conventional WWTPs failed to fully remove over 60% of these substances. Despite high removal rates, compounds such as caffeine and xylene sulfonate were frequently detected in water at significant concentrations.

Average concentration (ng/L) and detection frequency (DF) (%) of PPCPs in the analysed samples of treated and raw wastewater is

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shown in Figure 3, of industrial and cleaning agents in Figure 4, and of pesticides in Figure 5.



# Figure 3. Average concentration and DF of PCPPs in treated and raw wastewater.

In addition to some pharmaceuticals and PCPs, both food additives, caffeine and acesulfame, reached concentrations up to 30 µg/L in raw wastewater, decreasing to ~1 µg/L in treated effluent, reflecting high removal but continued environmental discharge. Six pesticides were detected in raw wastewater at average concentrations of 0.3 µg/L, with diuron and DEET showing notable presence. Compounds like xylenesulfonate and CAP showed significant concentrations in raw wastewater, with CAP ranging from 0.59-1.9 µg/L and remaining persistent in treated effluent. Naphthalene sulfonic acid was detected at 77 ng/L in treated wastewater, indicating partial removal.







# Figure 5. Average concentration of industrial chemicals and cleaning agents in treated and raw wastewater.

(Golovko et al., 2021) studied the occurrence of 164 pre-defined target CECs (96 pharmaceuticals, 34 pesticides, 10 PFASs, 3 parabens, 9 industrial chemicals, 4 personal care products, 3 stimulants, 2 vitamins and other CECs) in influent and effluent

wastewater samples from 15 WWTPs in Sweden. Out of 164 CECs, 119 were detected in at least one sample. Mean concentrations in wastewater influent and effluent ranged from 0.11 ng/L for propylparaben to 64,000 ng/L for caffeine in wastewater samples and the highest concentration, as well as highest frequency of detection were found for 15 pharmaceuticals, three industrial chemicals and the stimulants caffeine (64,000 ng/L) and nicotine (9,600 ng/L). Overall, the most frequently detected CECs in wastewater treatment plants influent and effluent, sludge and surface water, included industrial chemicals like tetraethylene glycol, laureth-5 and DEHPA. Additionally, a personal care product (sulibenzone), several pharmaceuticals (diclofenac, losartan, venlafaxine, lamotrigine, carbamazepine, tramadol, fexofenadine, citalopram bicalutamide, metformin) as well as the stimulants caffeine and nicotine were also commonly identified.

(Ofrydopoulou et al., 2022) evaluated the contamination profile, removal efficiencies, and potential risks associated with a wide array of emerging contaminants (ECs) in two wastewater treatment plants (WWTPs) in Thessaloniki, Greece. A total of 172 ECs, including pharmaceuticals and personal care products (PPCPs), illicit drugs, perfluorinated compounds (PFCs), and organophosphate flame retardants (OPFRs), were investigated. Out of these, 80 compounds were identified corresponding to the 46% of the total scope of the method. The mean concentrations varied, ranging from  $ng^{-1}$  to  $\mu g^{-1}$ . The influent concentrations were generally higher than those in effluents, with compounds such as caffeine, acetaminophen, and antihypertensive drugs being the most prevalent. Removal efficiencies varied significantly, with some compounds like UV filters showing almost complete removal, while others, like lamotrigine, exhibited negative removal efficiencies. The ecotoxicological risk was assessed for both individual compounds and mixtures, revealing that some contaminants posed a high ecological risk, particularly in aquatic environments.

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# 3.7.2 Selected studies on wastewater analysis using combined targeted and non-targeted approaches

A recent Danish study (Aggerbeck et al., 2024) investigated unknown contaminants in the wastewater effluent samples from three WWTPs in the Greater Copenhagen area, with different distances to city, hospitals, industry, and rural areas. The authors observed 4094 unique substances, of which they could confirm the chemical structure for 785 compounds, 451 thereof could be assigned to a compound class (a confirmed substance with in-house experimental data on retention time and fragmentation spectra). **It is stated that therapeutics and drugs, make up 37 - 45% of the annotated compounds.** Figure 6 shows the composition and shares of different classes relative to the total number of compounds in the sample. Each bar represents an individual sample. In total nine samples across three sites were investigated. The detected molecules in each sample are stacked and categorised by compound class, using distinct colours.



### Figure 6. composition of compound area of particular classes, relative to the total number of compounds in the sample. Source: (Aggerbeck et al., 2024)

The study by (Hinnenkamp et al., 2022) investigated micropollutants in water samples from different stages of drinking water production impacted by wastewater treatment plant effluents. The study employed a combined approach including a target, suspect and nontarget screening analysis for a more comprehensive screening of organic micropollutants. A quantitative screening of WWTP effluents identified a total of 51 substances, with 19 of them also being found in the drinking water sample. Concentrations of detected compounds varied, with the highest levels found in WWTP effluents. Substances (excluding pharmaceuticals) with concentration ranges from 100 ng/L to > 1000 ng/L in WWTPs were 1H-Benzotriazole, 4-Methyl-1H-Benzotriazole, 2-Amino-1H-benzimidazole, and Diethyltoluamide (DEET) (industrial chemical). The research highlighted the importance of combining different screening methodologies to enhance identification confidence, underscoring the need for thorough monitoring to manage micropollutants effectively in water

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treatment systems. 65% (15 out of 23) of the detected compounds in the drinking water sample consisted of pharmaceuticals and their transformation products. Health risk assessments indicated no immediate threat from the concentrations detected.

The study by (Lopez-Herguedas et al., 2022) identified the contamination profile of wastewater treatment plant (WWTP) effluents in the Henares River Basin, with target and suspect screening analysis. It is clearly stated that "The number of CECs in WWTPs effluents is often so large that complementary approaches to the conventional target analysis need to be implemented." (Lopez-Herguedas et al., 2022). Samples from five WWTPs were collected in summer and autumn. In all samples a set of 162 predefined substances was measured by targeted approaches. The predefined set of substances consisted of 6 industrial chemicals, 51 pesticides (i.e., 10 insecticides, 26 herbicides, 15 fungicides), 2 personal care product related chemicals as well as 103 pharmaceuticals. 82 out of 162 emerging pollutants were detected through target analysis. The following table indicates the number of targeted substances per product category compared to the number of found substances in this category.

Category	No. of targeted substances	No of confirmed /found substances thereof	Percentage
Industrial chemicals	6	3	50%
Pesticides	51	17	33%
Personal care products	2	0	0%
Pharmaceuticals	103	62	60%

The study indicates that among the 82 targeted analytes, 76% of the compounds quantified corresponded to pharmaceuticals, 21% to

pesticides and 3% to industrial chemicals. However, if one considers the fact that pharmaceuticals made up  $\sim$ 63% of the substances that were targeted those figures are misleading and needs to be set in relation to this overrepresentation.

The complementary suspect screening annotated additional 215 chemicals (176 tentatively identified as probably structures and 39 as tentative candidates according to the classification by (Schymanski et al., 2014) from a list of over 40,000 compounds (based on the NORMAN database<sup>10</sup>) summing up to 297 "identified" substances. Apart from frequently detected pharmaceuticals, pesticides (herbicides and fungicides), PCPs and industrial chemicals could be detected in WWTP effluents by suspect screening as well. The study's risk quotient (RQ) assessments indicated that pharmaceuticals and pesticides posed a significant ecological risk in the area.

The study by (Lopez-Herguedas et al., 2024) investigated polar contaminants in the effluents from the Galindo wastewater treatment plant (WWTP) in the Basque Country, Spain. Over a nineweek period, 24-hour composite effluent samples from primary treatment, conventional activated sludge (CAS) secondary treatment, and a membrane bioreactor (MBR) pilot plant were collected and analysed. The study utilized advanced analytical methods to identify and quantify a range of contaminants of emerging concern (CECs). By combining a suspect screening approach (LC-HRMS) and multitarget analysis (GC-MS) approximately 200 compounds could be detected in the WWTP effluents. For the suspect screening the NORMAN SusDat database was used as suspect list of which 184 compounds could be annotated (82 guantified, 92 tentatively identified and 10 as tentative candidates following categorisation by (Schymanski et al., 2014)). Additional 14 substances were quantified by targeted analysis.

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Unfortunately, the authors did not provide a categorisation of the quantified substances (82 suspect screening + 14 targeted substances) but a Ramboll internal high-level analysis revealed 60 pharmaceuticals, 9 personal care product related chemicals, 12 pesticides and 15 industrial chemicals. The multi target analysis revealed additional 16 compounds – 3 pesticides, 10 industrial chemicals and 3 personal care product related substances. This means that the study confirmed presence of 112 substances, which can be categorised as follows: 60 pharmaceuticals ( $\sim$ 53%), 12 personal care products related substances ( $\sim$ 11%), 15 pesticides ( $\sim$ 13%) and 25 industrial chemicals ( $\sim$ 22%).

The supplementary documentation lists 113<sup>11</sup> tentatively identified or tentative candidates and can - according to a Ramboll internal high-level analysis - categorised as follows: 57 pharmaceuticals (50%), 2 pesticides (2%), 48 industrial chemicals (42%) and 6 PPC related substances (5%). The chemicals with the highest concentrations measured in the study, other than pharmaceutical chemicals, were as follows: industrial chemicals including caprolactam (29248 ng/L), Bisphenol A (9979 ng/L), Bisphenol S (2196 ng/L), 1H-Benzotriazole (5879 ng/L), 2-Hydroxybenzothiazole (2252 ng/L), and benzophenone (1685 ng/L); pesticides such as lindane (4342 ng/L) and its by-product beta-hexachlorocyclohexane (36702 ng/L). Additionally, a group of PAHs including Acenaphthylene (4398 ng/L), Phenanthrene (2749 ng/L), Acenaphthene (2291 ng/L), and Anthracene (893 ng/L) were found. Lastly, significant concentrations of food supplements like caffeine (35537 ng/L) and cotinine (3894 ng/L) were also measured.

The study by (Kilpinen et al., 2024) examined the temporal trends and sources of 150 organic micropollutants in effluent wastewater over three months analysing 168 effluent and 10 influent samples. Both targeted and suspect screening approaches were employed,

allowing for the full quantification of 64 micropollutants and the identification of 90 additional compounds through suspect screening. The study found that key events such as rain and industrial discharges impact micropollutant composition and concentrations in effluent wastewater. It was noted that PFAS compounds, tire-wear chemicals, and biocides correlated with rain events. Industrial discharges were linked to elevated levels of pharmaceuticals, such as amitriptyline and citalopram, affecting effluent quality over extended periods. The highest concentrations were measured for sweeteners and food ingredients (sucralose 34590.02 ng/L and caffeine 6169.10 ng/L) followed by the pharmaceuticals (e.g. furosemide 4898.74 ng/L) and industrial chemicals (1,2,3-Benzotriazole 1330.58 ng/L). PFAS ranged from 8.51 ng/L (PFHxA) to 0.75 ng/L (PFNA).

The study by (Kizgin et al., 2024) tested and identified various chemicals in the wastewater treatment plant (WWTP) effluent (Switzerland) using Biological Early Warning Systems (BEWS) and high-resolution mass spectrometry. Among the target compounds were lidocaine (a local anaesthetic), xylazine (a veterinary sedative), and aminoantipyrine (an analgetic drug). These compounds were detected but at concentrations too low to cause significant behavioral effects in test organisms. The study also identified a non-target compound, carbofuran, an insecticide banned in Switzerland and the EU. Carbofuran was detected at approximately 1.4  $\mu$ g/L. Additionally, herbicides such as 2,4-dichlorophenoxyacetic acid (2,4-D) and its metabolite 2,4-dichlorophenol (2,4-DCP) were present. The study highlighted the need for both target and non-target chemical monitoring, as unexpected compounds like carbofuran were significant contributors to observed toxicity responses.

(García-Vara et al., 2023) studied the contamination of irrigation water by CECs in the Baix Llobregat Agrarian Park (Spain). The

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investigation identified and semi-guantified 158 CECs in water used for irrigation, sourced from reclaimed wastewater that had undergone various treatments but still contained numerous contaminants. The CECs identified includes pharmaceuticals (covering more than 50% of the CECs tentatively identified), industrial chemicals, and pesticides, among others. CEC concentrations ranged from 0.3 ng/L for 2-(3,4-dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile to 97 µg/L for caprolactam. The environmental risk of each tentatively identified compound was assessed by calculating its risk quotient (RQ) by comparing the highest concentration found with predicted no-effect concentration (PNEC) values. Regarding their ecotoxicological risk, 14 out of 119 identified CECs showed an individual RQ over 1 and, therefore, presented a concentration potentially toxic for the aquatic environment. The highest risk (RO > 10) was allocated to two pharmaceuticals (O-desmethyl-venlafaxine and venlafaxine) and galaxolidone (a metabolite of the personal care product galaxolide). Moderate risk was predicted (1 < RQ < 10) for several industrial chemicals (2-ethylhexyl diphenyl phosphate, N-phenyl-1naphthylamine, and caprolactam), pharmaceuticals (carbamazepine, sulfamethoxazole, and temazepam), tire wear compounds (N,N'-diphenylguanidine), the UV filter oxybenzone, and caffeine and its metabolite theophylline.

### 3.8 Micropollutants in the focus of authorities

The German Centre for Micropollutants<sup>12</sup> is identifying and assessing relevant micropollutants in water bodies. The relevant micropollutants are compiled in brief dossiers and assessed according to the current state of the knowledge. To the relevant micropollutants belong so far 14 substances (2 food additives, 5 pharmaceuticals, 6 industrial chemicals, and 1 pesticide).

<sup>&</sup>lt;sup>12</sup> <u>Relevant Micropollutants | Umweltbundesamt</u>

The European Environment Agency's recent assessment on Europe's state of water 2024, based on data reporting by 19 Member States mentions that: "*a large range of micropollutants, such as metals, biocides and pharmaceuticals, can be found in urban wastewater with 92% of the residual toxicity in urban wastewater coming from the pharmaceutical and cosmetics sectors*" (as cited in (European Environment Agency, 2024). There is no reflection or justification for the 92% in this report. Following the cited references in the EEA's report, no proof of this statement was found, nor supporting background data (or calculations).

It is understood that this figure is taken from the EU Commission impact assessment. As communicated by the European Commission the calculations that led to the figure of 92% are mainly based on (Pistocchi et al., 2022), which is also referenced in the EEA report. Please refer to section 3.4.1 for more details and limitations of this study when used as basis for legal actions.

### 4. Conclusion

The present report presents a critical review, of available literature complementing the findings of a project from 2023. It shows a large variety of substances that was found in wastewater and large differences in the approaches to analyse and monitor micropollutants.

The IA report from the Commission concluded that pharmaceuticals for human use represent 59% of input quantities to wastewater treatment plants and 66% of the total toxic load. These figures could neither be confirmed nor could definite, reliable figures be identified in the literature.

However, the danger of a potential misallocation of shares to different sectors can be underlined by the fact that the vast majority of literature screened in this project focussed on selective

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measurement of micropollutants, which tends to focus often on substances from pharmaceuticals and personal care products with a risk of overlooking other potential contributors.

It is assumed that this selective approach is driven by several factors, including different status of scientific knowledge, regulatory and research priorities, the availability of analytical methods, and public and political attention. Pharmaceuticals have historically received significant attention in research on micropollutants in wastewater, partly due to their potential impacts on human health and aquatic ecosystems, as well as the extensive regulatory oversight and availability of monitoring data. This focus has sometimes led to a prioritization of pharmaceutical compounds over other contaminants, not necessarily because they pose greater risks, but because they are more frequently studied and better documented. The presence of pharmaceuticals in the environment has been widely discussed, what potentially could influence the research focus. Due to these factors, many other micropollutants, such as industrial chemicals, pesticides, and household chemicals, seem to receive less attention. However, it needs to be stressed that a systematic assessment of all available literature is missing in order to confirm the conclusions and findings in our projects. Nevertheless, it could be shown that many publications are available that confirm the risk of over- or underrepresentation of substances, which were not considered in the IA of the EU Commission.

Projects in which water bodies are screened for micropollutants without predefining the substances that should be investigated underscore the high number of substances that can be found in water bodies and that are less investigated in most wastewater measurement projects. Attempts for suspect screening in wastewater samples are in line with these findings and shows the plethora of different substances present. This underlines the perception of a misconception.

While no precise allocation of micropollutants to specific industry sectors can be retrieved in the scope of our projects, it could be confirmed that a wide variety of non-pharmaceutical substances contribute to the micropollutant loads in wastewater like industrial chemicals like corrosion inhibitors, flame retardants used in manufacturing processes, pesticides and herbicides from agricultural runoff and urban use, and household chemicals such as detergents, cleaning agents, and plastic additives. Thus, relying on currently available data for wastewater to determine cost-sharing responsibilities may overlook the complexity of micropollutant contamination in aquatic environments.

No data could be identified that allow making absolute statements about the percentage of micropollutants in urban wastewater. This is due to the fact that different analytical approaches are studied all having different focus areas and limitation but also due to the significant influence of external factors. The concentration of micropollutants in urban wastewater is highly variable and subject to numerous influences. Rainfall events and associated combined sewer overflows can significantly alter the composition and concentration of pollutants (Gooré Bi et al., 2015; Mutzner et al., 2022). Additionally, industrial production cycles and seasonal variations in substance use patterns contribute to the variability of micropollutant levels. The complex interplay of these factors makes it challenging to establish consistent, absolute percentages for micropollutants in urban wastewater. Expanded monitoring programs and suspect screening in wastewater could be a potential solution to gain a realistic picture of the micropollutants present in wastewater on which subsequent legal measures could build.

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Appendices

#### **APPENDIX 1 - SUBSTANCES IDENTIFIED IN WASTEWATER WITHIN THE PRESENT PROJECT**

Figure 7: Substances that were investigated in wastewater in the reviewed studies (non-exhaustive list) and their corresponding legal status (if available from ECHA webpage). The selection is not intended to be exhaustive; more comprehensive data on concentration of substances can be found in some databases (some examples for available databases presented in the following).

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP
Pharmaceuticals	Acetaminophen	103-90-2	-	-	-	-
Pharmaceuticals	10,11-Dihydro-10,11- dihydroxycarbamazepine	35079-97-1	-	-	-	-
Pharmaceuticals	Hydrochlorothiazide	58-93-5	-	-	-	-
Pharmaceuticals	Lamotrigine	84057-84-1	-	-	-	-
Pharmaceuticals	Acetaminophen	103-90-2	-	-	-	-
Pharmaceuticals	Losartan	114798-26-4	-	-	-	-
Pharmaceuticals	Diatrizoic acid	117-96-4	-	-	-	-
Pharmaceuticals	Primidon	125-33-7	-	-	-	-
Pharmaceuticals	Atorvastatin	134523-00-5	-	-	-	-
Pharmaceuticals	Lidocaine	137-58-6	-	-	-	-
Pharmaceuticals	Valsartan	137862-53-4	-	-	-	-
Pharmaceuticals	Irbesartan	138402-11-6	-	-	-	-
Pharmaceuticals	Candesartan	139481-59-7	-	-	-	-
Pharmaceuticals	Eprosartanmesylate	144143-96-4	-	-	-	-
Pharmaceuticals	Olmesartan	144689-24-7	-	-	-	-
Pharmaceuticals	Telmisartan	144701-48-4	-	-	-	-
Pharmaceuticals	Diclofenac	15307-86-5	-	-	-	-

<sup>13</sup> Harmonized classifications are only available for specific substances. Harmonised classifications are listed in Annex VI to the CLP Regulation and should be applied by all manufacturers, importers or downstream users of such substances and of mixtures containing such substances. Please note that if there is no harmonized classification available this does not necessary mean that the substance does not have a CLP classification. Manufacturers, importers or downstream users have to (self)classify and label hazardous substances and the resulting notified CLP classifications are available from ECHA website but often show a great variety for individual substances.

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP
						classification
Pharmaceuticals	Sulpiride	15676-16-1	-	-	-	-
Pharmaceuticals	N-Formyl-4-aminoantipyrine	1672-58-8	-	-	-	-
Pharmaceuticals	Ketoprofen	22071-15-4	-	-	-	-
Pharmaceuticals	Naproxen	22204-53-1	-	-	-	-
Pharmaceuticals	Oxypurinol	2465-59-0	-	-	-	-
Pharmaceuticals	Tramadol	27203-92-5	-	-	-	-
Pharmaceuticals	Atenolol	29122-68-7	-	-	-	-
Pharmaceuticals	10,11-Dihydro-10-	29331-92-8	-	-	-	-
	hydroxycarbamazepine					
Pharmaceuticals	Carbamazepine	298-46-4	-	-	-	-
Pharmaceuticals	Mexiletine	31828-71-4	-	-	-	-
Pharmaceuticals	Climbazol	38083-17-9	-	-	-	-
Pharmaceuticals	Sotalol	3930-20-9	-	-	-	-
Pharmaceuticals	bezafibrate	41859-67-0	-	-	-	-
Pharmaceuticals	Genistein	446-72-0	-	-	-	-
Pharmaceuticals	Tiapride	51012-32-9	-	-	-	-
Pharmaceuticals	Metoprolol	51384-51-1	-	-	-	-
Pharmaceuticals	Propranolol	525-66-6	-	-	-	-
Pharmaceuticals	Flufenamic acid	530-78-9	-	-	-	-
Pharmaceuticals	Flecainide	54143-55-4	-	-	-	-
Pharmaceuticals	Furosemide	54-31-9	-	-	-	-
Pharmaceuticals	Amitriptyline	549-18-8	-	-	-	-
Pharmaceuticals	Metoprolol acid	56392-14-4	-	-	-	-
Pharmaceuticals	Phenytoin	57-41-0	-	-	-	-
Pharmaceuticals	Progesterone	57-83-0	-	-	-	-
Pharmaceuticals	Testosterone	58-22-0	-	-	-	-
Pharmaceuticals	Theophylline	58-55-9	-	-	-	-

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP classification <sup>13</sup>
Pharmaceuticals	Citalopram	59729-33-8	-	-	-	-
Pharmaceuticals	Oxazepam	604-75-1	-	-	-	-
Pharmaceuticals	Mirtazapine	61337-67-5	-	-	-	-
Pharmaceuticals	Gabapentin-Lactam	64744-50-9	-	-	-	-
Pharmaceuticals	Metformin	657-24-9	-	-	-	-
Pharmaceuticals	Ranitidine	66357-35-5	-	-	-	-
Pharmaceuticals	Bisoprolol	66722-44-9	-	-	-	-
Pharmaceuticals	Norfloxacin	70458-96-7	-	-	-	-
Pharmaceuticals	Amisulpride	71675-85-9	-	-	-	-
Pharmaceuticals	Sulfamethoxazole	723-46-6	-	-	-	-
Pharmaceuticals	trimethroprim	738-70-5	-	-	-	-
Pharmaceuticals	Amantadine	768-94-5	-	-	-	-
Pharmaceuticals	Clarithromycin	81103-11-9	-	-	-	-
Pharmaceuticals	4-Aminoantipyrine	83-07-8	-	-	-	-
Pharmaceuticals	N-Acetyl-4-aminoantipyrine	83-15-8	-	-	-	-
Pharmaceuticals	Cetirizine	83881-51-0	-	-	-	-
Pharmaceuticals	Azithromycin	83905-01-5	-	-	-	-
Pharmaceuticals	Lamotrigine	84057-84-1	-	-	-	-
Pharmaceuticals	Ciprofloxacin	85721-33-1	-	-	-	-
Pharmaceuticals	Fluconazole	86386-73-4	-	-	-	-
Pharmaceuticals	Bicalutamide	90357-06-5	-	-	-	-
Pharmaceuticals	O-Desmethylvenlafaxine	93413-62-8	-	-	-	-
Pharmaceuticals	Venlafaxine	93413-69-5	-	-	-	-
PFAS	Perfluorooctanesulfonic acid (PFOS)	1763-23-1	-	-	Yes	Carc. 1B
PFAS	Perfluoropentanoic acid (PFPeA)	2706-90-3	-	-	-	-

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP classification <sup>13</sup>
PFAS	6:2 fluorotelomer sulfonic acid	27619-97-2	-	-	-	-
PFAS	Perfluorohexanoic acid	307-24-4	-	-	-	-
PFAS	Pentadecafluorooctanoic acid (PFOA)	335-67-1	SVHC	Restriction proposal under evaluation	Yes	Carc. 1B Muta. 1B Asp. Tox. 1
PFAS	Pentafluorobutanoic acid (PFBA)	375-22-4	-	Restriction proposal under evaluation	-	-
PFAS	Perfluoro-n-heptanoic acid (PFHpA)	375-85-9	SVHC	Restriction proposal under evaluation	Yes	Carc. 1B Muta. 1B Asp. Tox. 1
PFAS	Perfluoro-n-nonanoic acid (PFNA)	375-95-1	SVHC	Listed	Yes	Carc. 1B Muta. 1B Asp. Tox. 1
PFAS	Perfluoropropionic acid	422-64-0	-	Restriction proposal under evaluation	-	-
PFAS	Perfluorobutane sulfonate (PFBS)	45187-15-3	-	Restriction proposal under evaluation	-	-
PFAS	Perfluorosulfonamide	754-91-6	-	Restriction proposal under evaluation	-	-
Pesticides	Tebuconazol	107534-96-3	-	-	-	Acute Tox. 4 * Aquatic Acute 1 Aquatic Chronic 1
Pesticides	Thiacloprid	111988-49-9	-	-	-	%
Pesticides	Fipronil	120068-37-3	-	-	-	Asp. Tox. 1
Pesticides	Acetamiprid	135410-20-7	-	-	-	-
Pesticides	Imidacloprid	138261-41-3	-	-	-	-
Pesticides	Atraton	1610-17-9	-	-	-	-
Pesticides	Atrazine (ATZ)	1912-24-9	-	-	-	-
Pesticides	Metribuzin	21087-64-9	-	-	-	Aquatic Chronic 1

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP
						classification <sup>13</sup>
Pesticides	Chlorpyriphos (CPR)	2921-88-2	-	-	-	Aquatic Chronic 4
Pesticides	Diuron	330-54-1	-	-	-	Skin Sens. 1
						Aquatic Chronic 2
Pesticides	Isoproturon	34123-59-6	-	-	-	Skin Irrit. 2
						Eye Dam. 1
						Skin Sens. 1
Destisides		470.00.0				Aquatic Chronic 2
Pesticides		470-90-6	-	-	-	Eye Dam. 1
Pesticides	Metolachior	51218-45-2	-	-	-	-
Pesticides	Propanil	709-98-8	-	-	-	-
Pesticides	Fenoxycarb	72490-01-8	-	-	-	Aquatic Chronic 4
Pesticides	Ametryn	834-12-8	-	-	-	-
Pesticides	Terbutryn	886-50-0	-	-	-	-
Pesticides	Dinoseb (Subitex)	88-85-7	SVHC	-	Yes	Carc. 1B
Personal Care Products	Mepiquat	15302-91-7	-	-	-	-
Personal Care Products	Oxybenzone	131-57-7	-	-	-	-
Personal Care Products	Diethyltoluamide (DEET)	134-62-3	-	-	-	-
Personal Care Products	Methylparaben	99-76-3	-	-	-	-
Industrial chemicals	Tri-isobutylphosphate	126-71-6	-	-	-	-
Industrial chemicals	Tris(1-chloro-2-	13674-84-5	-	-	-	-
	propyl)phosphate					
Industrial chemicals	Phenylbenzimidazole sulfonic	27503-81-7	-	-	-	-
	acid					
Industrial chemicals	Hexa(methoxymethyl)melami	3089-11-0	-	-	-	-
	ne					
Industrial chemicals	Benzophenone-4	4065-45-6	-	-	-	-
Industrial chemicals	4,4-Diaminodiphenylmethane	101-77-9	SVHC	-	-	-
Industrial chemicals	1,3-Diphenylguanidine	102-06-7	-	-	-	-

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP classification <sup>13</sup>
Industrial chemicals	Tripropylamine	102-69-2	-	-	-	-
Industrial chemicals	p-Toluenesulfonic acid	104-15-4	-	-	Yes	Carc. 2 Repr. 1B Lact. Acute Tox. 4 Acute Tox. 4 STOT RE 1 Eye Dam. 1
Industrial chemicals	Caprolactam	105-60-2	-	-	-	-
Industrial chemicals	Dibutylphosphate	107-66-4	-	-	-	-
Industrial chemicals	Bis(fluorosulfonyl)imide	1079129-48-8	-	-	-	-
Industrial chemicals	Melamine	108-78-1	SVHC	-	-	-
Industrial chemicals	Cyanuric acid	108-80-5	-	-	-	-
Industrial chemicals	Cyclohexylamine	108-91-8	-	-	-	-
Industrial chemicals	2-[2-(3- Aminopropoxy)ethoxy]ethano	112-33-4	-	-	-	-
Industrial chemicals	Tris(trifluoromethanesulfonyl) methanide	114395-69-6	-	-	-	-
Industrial chemicals	Tris(2-chloroethyl)phosphate	115-96-8	SVHC	-	-	Eye Dam. 1 Skin Sens. 1 Aquatic Chronic 3
Industrial chemicals	o-Dianisidine	119-90-4	-	-	-	-
Industrial chemicals	Sulfanilic acid	121-47-1	-	-	-	-
Industrial chemicals	Galaxolid	1222-05-5	-	-	-	Acute Tox. 4 * Eye Irrit. 2 Aquatic Chronic 3
Industrial chemicals	4'-Aminoacetanilide	122-80-5	-	-	-	-
Industrial chemicals	Hexafluorophosphate	1257647-66-7	-	-	-	-

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP classification <sup>13</sup>
Industrial chemicals	Tri-n-butyl phosphate (TnBP)	126-73-8	-	-	-	Aquatic Chronic 4
Industrial chemicals	2,4,7,9-Tetramethyldec-5-in- 4,7-diol (TMDD)	126-86-3	-	-	-	-
Industrial chemicals	3-Nitrobenzenesulfonate	127-68-4	-	-	Yes	Carc. 1B
Industrial chemicals	Tri-(2- chloroisopropyl)phosphate	13674-84-5	-	-	-	-
Industrial chemicals	5-Methyl-1H-benzotriazole	136-85-6	-	-	-	-
Industrial chemicals	Decamethyltetrasiloxane(L4)	141-62-8	The substance is/was part of an assessment as follows: vPvB (Article 57e) Status: Intention	-	-	-
Industrial chemicals	Tetraphenylborate	143-66-8	-	-	-	-
Industrial chemicals	Trifluoromethane sulfonic acid (PFMS)	1493-13-6	-	-	-	-
Industrial chemicals	2-Methyl-2-propene-1- sulfonic acid	1561-92-8	-	-	-	-
Industrial chemicals	Bis(trifluoromethanesulfonyl)i mide	161401-25-8	-	-	-	-
Industrial chemicals	Tetrabutylammonium	1643-19-2	-	-	-	-
Industrial chemicals	Tributylmethylphosphonium	1702-42-7	-	-	-	-
Industrial chemicals	2-(2- (Dimethylamino)ethoxy)ethan ol	1704-62-7	-	-	-	-
Industrial chemicals	3,5-Di-tert-butylsalicylic acid	19715-19-6	-	-	-	-
Industrial chemicals	Trimethylsulfonium	2181-42-2	-	-	-	-
Industrial chemicals	Dicyclohexyl sulfosuccinate	23386-52-9	-	-	-	-
Industrial chemicals	beta-Methylcholine	2382-43-6	-	-	-	-

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP classification <sup>13</sup>
Industrial chemicals	Dimethylbenzenesulfonic acid (mix of isomers)	25241-16-1, 1300-72-7	-	-	-	-
Industrial chemicals	Xylenesulfonate	25321-41-9	-	-	-	-
Industrial chemicals	Trihexyl(tetradecyl)phosphoni um	258864-54-9	-	-	-	-
Industrial chemicals	4,4'-bis(2-sulfostyryl)biphenyl	27344-41-8	-	-	-	-
Industrial chemicals	1,4-Diazabicyclo[2.2.2]octane	280-57-9	-	-	-	-
Industrial chemicals	Isophorone diamine	2855-13-2	-	-	-	-
Industrial chemicals	1,2,4-Triazole	288-88-0	-	-	-	-
Industrial chemicals	Bis(2- dimethylaminoethyl)methyla mine	3030-47-5	-	-	-	-
Industrial chemicals	Vinylsulfonic acid	3039-83-6	-	-	-	-
Industrial chemicals	Tributylmethylammonium	3085-79-8	-	-	-	-
Industrial chemicals	3-Sulfonatopropyl acrylate	31098-20-1	-	-	-	-
Industrial chemicals	1-Ethyl-4-methylpyridinium	32353-49-4	-	-	-	-
Industrial chemicals	Ethyl sulfate	342573-75-5	-	-	-	-
Industrial chemicals	Tricyanomethanide	36603-80-2	-	-	-	-
Industrial chemicals	N,N-dimethyl-1- adamantanamine	3717-40-6	-	-	-	-
Industrial chemicals	Tris(pentafluorethyl)trifluorph osphate	377739-43-0	-	-	-	-
Industrial chemicals	Dimethyl-5-sulfoisophthalate	3965-55-7	-	-	-	-
Industrial chemicals	Cyanoguanidine	461-58-5	-	-	-	-
Industrial chemicals	Denatonium	47324-98-1	-	-	-	-
Industrial chemicals	Benzo(a)pyrene	50-32-8	SVHC	Listed	-	Flam. Liq. 2 Acute Tox. 3 * Acute Tox. 3 *



Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP classification <sup>13</sup>
						Acute Tox. 3 *
						Aquatic Chronic 2
Industrial chemicals	Methacrylamido propyl trimethyl ammonium	51410-72-1	-	-	-	-
Industrial chemicals	2-Acrylamido-2- methylpropanesulfonic acid	5165-97-9	-	-	-	-
Industrial chemicals	N,N,N- Trimethylethanammonium	51-93-4	-	-	-	-
Industrial chemicals	N-(3-(dimethylamino)- propyl)methacrylamide	5205-93-6	-	-	-	-
Industrial chemicals	3-Allyloxy-2-hydroxy-1- propanesulfonate	52556-42-0	-	-	-	-
Industrial chemicals	4-Hydroxy-1-(2-hydroxyethyl)- 2,2,6,6-tetramethylpiperidine	52722-86-8	-	-	-	-
Industrial chemicals	Sulfaminsäure	5329-14-6	-	-	Yes	Carc. 2 Aquatic Acute 1 Aquatic Chronic 1
Industrial chemicals	1-(3,3-Dimethyl-2-oxo-butyl)- pyridinium	5397-45-5	-	-	-	-
Industrial chemicals	Decamethylcyclopentasiloxan e(D5)	541-02-6	SVHC	Listed	-	-
Industrial chemicals	6-Methyl-1,3,5-triazine- diamine	542-02-9	-	-	-	-
Industrial chemicals	Octamethylcyclotetrasiloxane (D4)	556-67-2	SVHC	Listed	-	Self-react. D **** Skin Sens. 1 Aquatic Acute 1 Aquatic Chronic 1
Industrial chemicals	Benzyltrimethylammonium	56-93-9	-	-	-	-
Industrial chemicals	Hexadecyltrimethylammoniu m	57-09-0	-	-	-	-
Industrial chemicals	1-Cetylpyridinium	6004-24-6	-	-	-	-

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP classification <sup>13</sup>
Industrial chemicals	2-(Methylthio)benzothiazole	615-22-5	-	-	-	-
Industrial chemicals	2-Pyrrolidone	616-45-5	-	-	-	-
Industrial chemicals	2-Morpholinoethanol	622-40-2	-	-	-	-
Industrial chemicals	Benzalkonium	63449-41-2	-	-	-	-
Industrial chemicals	3-Methylsulfanilate	63450-43-1	-	-	-	-
Industrial chemicals	2,2'-Dimorpholinyldiethyl ether	6425-39-4	-	-	-	-
Industrial chemicals	1-Methyl-3-octylimidazolium	64697-40-1	-	-	-	-
Industrial chemicals	1-Butyl-4-methylpyridinium	65350-59-6	-	-	-	-
Industrial chemicals	p-Toluenesulfonamide	70-55-3	-	-	-	-
Industrial chemicals	4-(2-Hydroxyethyl)piperazine- 1-ethanesulfonic acid	7365-45-9	-	-	-	-
Industrial chemicals	Triethylcitrate	77-93-0	-	-	-	-
Industrial chemicals	Triethylphosphate	78-40-0	-	-	-	Aquatic Chronic 4
Industrial chemicals	Tributoxyethyl phosphate (TBEP)	78-51-3	-	-	-	-
Industrial chemicals	Triphenylphosphine oxide	791-28-6	-	-	-	-
Industrial chemicals	6-PPD (N-(1,3- Dimethylbutyl)-N'-phenyl-p- phenylendiamin) und das Transformationsprodukt 6-PPDC (N-(1,3- Dimethylbutyl)-N'-phenyl- pphenylendiamin chinon)	793-24-8	-	-	-	-
Industrial chemicals	Bisphenol S (BPS)	80-09-1	SVHC	-	-	Acute Tox. 4 * STOT RE 2 * Aquatic Chronic 3
Industrial chemicals	1,5-Naphthalenedisulfonic acid	81-04-9	-	-	-	-

Substance group	Substance name	CAS	SVHC	Restriction (REACH)	CMR	Harmonized CLP classification <sup>13</sup>
Industrial chemicals	Vincubine	826-36-8	-	-	-	-
Industrial chemicals	Tris(2-hydroxyethyl) isocyanurate	839-90-7	-	-	-	-
Industrial chemicals	Naphthalenesulfonic acid	85-47-2	-	-	-	-
Industrial chemicals	1-Butylpyridinium	874-80-6	-	-	-	-
Industrial chemicals	Tetrafluoroborate	886059-84-3	-	-	-	-
Industrial chemicals	m-Xylene-4-sulfonic acid	88-61-9	-	-	-	-
Industrial chemicals	N,N-diethylaniline	91-66-7	-	-	-	-
Industrial chemicals	Benzoguanamine	91-76-9	-	-	-	-
Industrial chemicals	Methyloctylpyrrolidinium	927021-43-0	-	-	-	-
Industrial chemicals	2-Hydroxybenzothiazole	934-34-9	-	-	-	-
Industrial chemicals	2-Benzothiazolesulfonic acid	941-57-1	-	-	-	-
Industrial chemicals	1H-Benzotriazole	95-14-7	-	-	-	-
Industrial chemicals	Benzothiazole	95-16-9	-	-	-	-
Industrial chemicals	1,3-Di-o-tolylguanidine	97-39-2	-	-	-	-
Industrial chemicals	Benzenesulfonic acid	98-11-3	-	-	-	-
Industrial chemicals	1-Butyl-2,3- dimethylimidazolium	98892-75-2	-	-	-	-
Food ingredients	Cyclamate	100-88-9	-	-	-	-
Food ingredients	Acesulfame	55589-62-3	-	-	-	-
Food ingredients	Sucralose	56038-13-2	-	-	-	-
Food ingredients	Caffeine	58-08-2	-	-	-	-
Food ingredients	Saccharin	81-07-2	-	-	-	-

#### **APPENDIX 2 - MONITORING DATABASES FOR WATER**

In addition to the national programmes and scientific literature, there are various environmental databases available for surface waters (and partly wastewater). Some of these are presented below.

The NORMAN network has developed a chemical occurrence database called <u>EMPODAT</u>. It is a database of geo-referenced monitoring and biomonitoring data on emerging substances in the following matrices: water (including wastewater), sediments, biota, SPM, soil, sewage sludge and air. The database is free accessible and does contain 4,567 substances and 96,107,746 data points (as of January 2025). Data on wastewater represents approximately 26% of the total data but is rather old (currently no data collected after 2020 is included). The database does include data from various use categories including biocides, flame retardants, food additives, food contact chemicals, industrial chemicals, metals and their compounds, per- and polyfluoroalkyl substances (PFAS), personal care products (PCP), pharmaceuticals, plant protection products (PPP), plastic additives.

Water Research Australia in partnership with Griffith University have developed a chemical information database called <u>ECHIDNA</u> (Emerging CHemIcals Database for National Awareness) to support science-based decision making and management of Contaminants of Emerging Concern (CEC). ECHIDNA prioritises close to 1,800 potential CEC covering common compound classes including DBPs, herbicides, pharmaceuticals, per- and polyfluoroalkyl compounds and transformation products. CEC are first prioritised based on in silico assessment of their persistent, bioaccumulative and toxic (PBT) properties, then based on toxicity, occurrence and removal data collected for prioritised chemicals. Risk Quotients (RQ) for both human health and ecosystem health are estimated to assist with management decision-making in the absence of regulatory guidance. Ramboll does not have access to this database, but according to a research article on the development of the database occurrence data was collected from scientific literature and the NORMAN database (Neale et al., 2023). It was stated that occurrence data can be limited due to little active monitoring for CEC and values are extrapolated using available removal data when necessary.

The <u>RIWA</u> (River Water Association) database contains information on detected substances in several rivers in the Netherlands, particularly the Meuse river. The RIWA organization focus on monitoring and improving the quality of river water. Substances are including pharmaceuticals, industrial compounds, and pesticides. This database is not free accessible.

#### **APPENDIX 3 - DOCUMENT REVIEW LIST INCL. GUIDING QUESTIONS**

Reference	Title	Which micropollutants are considered?	Is there an indication of quantity ratios (total share of micropollutants, subgroups of micropollutants, specific substances)?	Is there an indication on the toxicity/hazard of the micropollutants?	What is the source of the data (e.g. measurements, other studies)?	Uncertainties / validity of data
(Finckh et al., 2024)	A risk-based assessment approach for chemical mixtures from wastewater treatment plant effluents	Wide-scope chemical target screening of 499 emerging chemicals including - pharmaceuticals - pesticides - other parent compounds (surfactants, food, plastic and rubber additives, PFAS, UV filters, corrosion inhibitors)	No information on the total share of the measured water sample, but 32 chemicals were established as consensus mixture risk contributors of high concern, including a high percentage (66%) of pesticides and biocides. Median concentrations determined (µg/L) for substances reported for 499 micropollutants Top 5: Sucralose (Sweetener): 15,346 µg/L 1H-Benzotriazole (Corrosion inhibitor): 3,590 µg/L Hydrochlorothiazide (Pharmaceutical): 2,340 µg/L 5-Methyl-1H-benzotriazole (Corrosion inhibitor): 1,781 µg/L	The detected chemicals were categorized with respect to critical information relevant for risk assessment and management prioritization including: (1) frequency of occurrence, (2) measured concentrations, (3) use groups, (4) persistence & bioaccumulation, and (5) modes of action.	56 effluent samples from 52 European wastewater treatment plants (WWTPs) were investigated for the occurrence of 499 emerging chemicals (ECs) and their associated potential risks to the environment.	NA
(Ayoub et al., 2022)	A Short Cost-Effective Methodology for Tracing the Temporal and Spatial Anthropogenic Inputs of Micropollutants into Ecosystems: Verified Mass-Balance Approach Applied to River Confluence and WWTP Release	1 plastic additive (Bisphenol A) 17 pharmaceuticals 1 PCP (triclosan) 2 PFAS (PFOA and PFOS)	No information on the total share in the measured water samples. However, there is information on the concentrations, for example: - Clarithromycin: 639 ng/L (October): 140 ng/L (January) - Bisphenol A: 236 ng/L (September); 80-90 ng/L (January, October) - PFOS: detected in all sites with levels as high as 34 ng/L (well above the above the EU Environmental Quality Standards (EQS) of 0.65 ng/L) - PFOA: less consistently detected with a maximum concentration of 15.7 ng/L Concentrations of other micropollutants are provided in the study. The estimation of possible mass flux of micropollutants from the WWTP (average value): PFOS: 10 g/day Bisphenol A: 93 g/day Clarithromycin: 218 g/day	Νο	Concentrations of micropollutants were measured at several river locations in France, with the highest concentrations observed in the Meurthe river, downstream of the WWTP and upstream of the confluence. Additionally, the study estimated the potential mass flux of micropollutants from the WWTP. Along with clarithromycin, bisphenol A also exhibited a high mass flux, averaging 93 g/day. Further analysis revealed that bisphenol A is also poorly removed by the WWTP located in Nancy, France.	ΝΑ
(Rapp-Wright et al., 2023)	A year-long study of the occurrence and risk of over 140 contaminants of emerging concern in	Investigation of 140 contaminants of emerging concern (CECs), including	No indication on the total share of micropollutants. In total, 58 CECs were detected. Along with	The environmental CEC risks were estimated using RQs calculated in wastewater effluent and receiving river	Influent, effluent and receiving surface waters at both urban and a rural location (72 samples in total) in Ireland	NA

Reference	Title	Which micropollutants are considered?	Is there an indication of quantity ratios (total share of micropollutants, subgroups of micropollutants, specific substances)?	Is there an indication on the toxicity/hazard of the micropollutants?	What is the source of the data (e.g. measurements, other studies)?	Uncertainties / validity of data
	wastewater influent, effluent and receiving waters in the Republic of Ireland	pharmaceuticals, pesticides, and PCPs	pharmaceuticals and PCPs, pesticides were also detected - 11 pesticides in influent, 6 in effluent, and 1 in surface waters. Propamocarb was found in all matrices. In conclusion it appears that all pesticides appeared to be removed before discharge from these WWTPs to the natural environment apart from propamocarb.	water by dividing the measured environmental concentration in each matrix at each site by the lowest PNEC obtained from NORMAN Ecotoxicology database. Performed ERA revealed that in surface waters, total RQ fo all CECs was an order of magnitude lower than in effluents. The majority of CECs in surface waters posed a lower risk except E2 and EE2 which presented a medium risk (RQs of 3.5 and 1.1, respectively) in the rural area.	over a 12-month period in 2018-2019.	
(Torres-Padrón et al., 2020)	An update of the occurrence of organic contaminants of emerging concern in the Canary Islands (Spain)	6 UV stabilisers 8 cytostatic compounds 15 steroid compounds	No information on the total share in the measured water samples. There is information on the concentrations of micropollutants measured as part of the study: - UV stabilizers were detected at all locations, with concentrations ranging from 13.12 to 1933 ng/L. Influent concentrations were higher than effluent concentrations, likely due to compound adsorption onto suspended solids during treatment. UV-329 was the most frequently detected compound, found in 33% of influent samples (106–1933 ng/L) and 10% of effluent samples (49.54–570.9 ng/L), indicating incomplete removal.	No	Influent and effluent wastewater samples collected from 5 WWTPs of the island of Gran Canaria. Detailed on the sampled WWTPs are included in the study.	NA
(Manetti & Tomei, 2024)	Anaerobic removal of contaminants of emerging concern in municipal wastewater: Eco-toxicological risk evaluation and strategic selection of optimal treatment	21 analysed CECs: pharmaceuticals, personal care products, plasticizer, stimulants	No information on the total share in the measured water samples. Average frequency of CECs found in WWTPs effluent from other literature studies. Most commonly found: TMP, CBZ, BPA, CAF, HHCB, AHTN, AZT, CIP, DCF, GEM, TCS	Risk Quotient (RQ), defined as predicted environmental concentration (PEC)/ predicted no-effect concentration (PNEC)	Literature review and risk assessment	NA
(Ofrydopoulou et al., 2022)	Assessment of a wide array of organic micropollutants of emerging concern in wastewater treatment plants in Greece: Occurrence, removals, mass loading and potential risks	A total of 172 Emerging Contaminants including - 135 PPCPs (Pharmaceuticals and Personal Care Products- 17 IDs (illicit drugs)- 11 PFCs (poly- and perfluoroalkyl substances)- 9 OPFRs (organophosphate flame retardants) and	No information on the total share in the measured water samples. 80 compounds (46% of the method's total scope) were detected at least in one sample. Average effluent concentrations ranged from below the method quantification limits ( <mql) to<br="">remarkably high values (µg L-1 scale), such as for caffeine, acetaminophen, diclofenac, irbesartan and valsartan, among others.</mql)>	Ecotoxicological risk assessment including risk quotient (RQ), risk quotient considering frequency (RQf) and toxic units (TU)	influent and effluent of two wastewater treatment plants (WWTPs) in Greece	It was mentioned that there is a need to record more ecotoxicological data on chronic exposure for certain omnipresent groups (i.e., antihypertensives) is mandatory to modulate future hazard investigation.

Reference	Title	Which micropollutants are considered?	Is there an indication of quantity ratios (total share of micropollutants, subgroups of micropollutants, specific substances)?	Is there an indication on the toxicity/hazard of the micropollutants?	What is the source of the data (e.g. measurements, other studies)?	Uncertainties / validity of data
(Svahn & Borg, 2024)	Assessment of full-scale 4th treatment step for micro pollutant removal in Sweden: Sand and GAC filter combo	22 Pharmaceuticals 1 industrial chemical (corrosion inhibitor) 1 pesticide	No information on the total share in the measured water samples. Concentrations of measured micropollutants are given. Concentration of non- pharmaceuticals were as follows: - benzotriazole: 386 ng/L - imidacloprid: 6 ng/L	Νο	Samples taken prior to the 4th treatment step of the WWTP in Sweden.	NA
(Kilpinen et al., 2023)	Catchment area, fate, and environmental risks investigation of micropollutants in Danish wastewater	291 target micropollutants (full list available in SI), including pharmaceuticals, PCPs, pesticides, industrial chemicals, etc.	No information on the total share in the measured water samples. Out of the 291 micropollutants analyzed, 79 were identified and quantified in either influent or effluent wastewater from at least one WWTP. The distribution of these micropollutants is as follows: - Pharmaceuticals: 12 were quantified in influent samples, and 16 in effluent samples. - Antibiotics: 8 were detected in both influent and effluent wastewater. - Food Additives: 4 were found in both influent and effluent wastewater. - Industrial Chemicals: 8 were present in both influent and effluent wastewater, 8 were unique to effluent wastewater, and 9 were unique to influent wastewater. - Pesticides: 18 were quantified in effluent wastewater, while 6 were found only in influent wastewater. - Other Micropollutants: 8 of mixed origin were identified in effluent wastewater, and 13 were found in influent wastewater.	To estimate the environmental risk of the quantified micropollutants, RQs have been calculated according to the following equation: RQ=MEC/PNEC.	Influent (n=20) and effluent (n=26) wastewater samples collected from 8 WWTPs with activated sludge treatment. Samples were collected between June and July in 2020 and all of them are located in Denmark. Six of them are located in larger cities, and 2 of them in smaller villages.	As reported in the study: the detection frequencies are biased due to the different numbers of influent (n=20) and effluent (n=26) wastewater samples analysed. Influent samples collected from 5 WWTPs and effluent samples from 8 WWTPs.
(Lopez- Herguedas et al., 2022)	Characterization of the contamination fingerprint of wastewatertreatment plant effluents in the Henares River Basin (central Spain)based on target and suspect screening analysis	Combined approach of suspect and screening and targeted approach. The list of 162 target compounds that are considered as contaminants of emerging concern (CECs) includes:- 103 Pharmaceuticals- 2 Personal care products- 51 Pesticides- 6 Industrial chemicals	Suspect screening annotated 297 chemicals from a suspect list over40,000 compounds. Target analysis revealed 82 out of 162 emerging pollutants. Share of the 82 CECs that were quantified:- 76% of the compounds quantified corresponded to pharmaceuticals,- 21% to pesticides and- 3% to industrial chemicals.	Finally, a risk prioritization approach was applied based on risk quotients (RQs) for algae, invertebrates, and fish. Azithromycin, diuron, chlortoluron, clarithromycin, sertraline and sulfamethoxazole were identified as having the largest risks to algae. As for invertebrates, the compounds having the largest RQs were carbendazim, fenoxycarb and eprosartan, and for fish acetaminophen, DEET, carbendazim, caffeine, fluconazole, and azithromycin.	Effluents of five WWTPs in the Henares River basin (central Spain) during two sampling campaigns (summer and autumn).	NA

Reference	Title	Which micropollutants are considered?	Is there an indication of quantity ratios (total share of micropollutants, subgroups of micropollutants, specific substances)?	Is there an indication on the toxicity/hazard of the micropollutants?	What is the source of the data (e.g. measurements, other studies)?	Uncertainties / validity of data
(Jucyte-Cicine et al., 2024)	Coastal wastewater treatment plants as a source of endocrine disrupting micropollutants: a case study of Lithuania in the Baltic Sea	Plasticizer, Oestrogens, Phthalic acid esters, Steroidal hormones	No information on the total share in the measured water samples, but concentration of substances.	NA	144 samples from WWTPs situated at two seaside resorts in Lithuania > assessment of wastewater and effluent quality	NA
(Ferreiro et al., 2020)	Contaminants of emerging concern removal in an effluent of wastewater treatment plant under biological and continuous mode ultrafiltration treatment	39 contaminants of emerging concern (CEC) were monitored, including pharmaceuticals (n= 25), industrial additives (n= 5), food additives (n= 4), herbicides (n=4), and PCPs (n=1)	No information on the total share in the measured water samples. Concentrations provided in the study. 3 food additives were among the top 10 CECs with highest concentrations in influent samples.	In order to assess the toxicity levels of UF influent and effluent samples Microtox <sup>®</sup> toxicity bioassays were performed.	Influent of the biological WWTP in Spain.	NA
(Weitere et al., 2021)	Disentangling multiple chemical and non- chemical stressors in a lotic ecosystem using a longitudinal approach	Measuring of 149 organic compounds including pharmaceuticals and personal care products (PCPs), pesticides, biocides and industrial compounds	No information on the total share in the measured water samples, but concentration of substances.	WWTPs were the predominant source of toxic stress, resulting in a rapid increase of the toxicity for invertebrates and algae with only one order of magnitude below the acute toxic levels. This toxicity correlates negatively with the contribution of invertebrate species being sensitive towards pesticides (SPEARpesticides index), probably contributing to the loss of biodiversity recorded in response to WWTP effluent	Germany, upstream and downstream of major point sources (WWTPs, stormwater drainage) and tributaries	NA
(Spina et al., 2020)	Ecofriendly laccases treatment to challenge micropollutants issue in municipal wastewaters	15 compounds were investigated: pesticide (1), personal care products (2), varnish (1), plasticizer (3), herbicide (2), surfactant (1), and drug (3)	No information on the total share of the measured water sample. Concentration of individual compounds was discussed. The most abundant were e bis(2- ethylhexyl) phthalate, diethyl phthalate and ketoprofen (most dominant)	Two in vitro tests (E-screen test and MELN assay) were used to evaluate the estrogenic activity. The aim of this study was to investigate the actual potential of the enzymatic treatment of some micropollutants as EDCs, pharmaceuticals, PCPs, etc. in real municipal wastewaters.	municipal WTP in Italy (Torino)	NA
(Ansorge et al., 2024)	Emerging contaminants in wastewater – results of Joint Danube Survey 4 evaluated via the grey water footprint	419 CECs including pharmaceuticals, agricultural chemicals, antibiotics, antipsychotic drugs, drugs of abuse and tobacco ingredients, food additive, industrial chemicals, others.	Partly, the largest proportion of detected CECs were pharmaceuticals. With a total of 165 substances, they represent 39.4 % of all detected CECs in wastewater. A total of 419 CECs found in wastewater during JDS4 were included in the analysis. Of these, 311 CECs were detected in treated wastewater discharged from WWTPs, and 306 CECs were detected in wastewater entering WWTPs.	YesData presented also with PNECs	Waters of the Danube River basin, including wastewater from selected wastewater treatment plants (not specified in the paper)	Authors stated that comparing the results of this study with other studies highlights the main issues that such studies currently have to face. The first issue is the selection of PNEC values. For particular CECs, very different PNEC values can be found in the literature, which can differ by

RAMBOLL					ENVIRONMENT & HEALTH		
Reference	Title	Which micropollutants are considered?	Is there an indication of quantity ratios (total share of micropollutants, subgroups of micropollutants, specific substances)?	Is there an indication on the toxicity/hazard of the micropollutants?	What is the source of the data (e.g. measurements, other studies)?	Uncertainties / validity of data	
			Only 198 substances were found both in the influents and effluents to/from WWTPs.			several orders of magnitude. The second issue is the selectivity of most studies, which usually include only a selection of a few CECs. From this point of view, JDS4 provided a unique dataset, even though it only covered 11 selected WWTPs in the Danube river basin. However, the available data did not allow an assessment of absolute significance, for which it is necessary to know the total amount of particular CECs in the wastewater monitored, not just the maximum and minimum concentrations. However, the variability of CECs in wastewater is subject to seasonal and daily dynamics. Daily dynamics can be suppressed by taking 24-hour composite samples. Seasonal dynamics cannot be captured by the screening measurements within JDS4. it can be assumed that these data also reflect short-term variability caused by a range of other factors.	
(Pistocchi et al., 2022)	European scale assessment of the potential of ozonation and activated carbon treatment to reduce micropollutant emissions with wastewater	Compiled list of 1337 chemicals commonly found in wastewater effluents based on several different datasets. Allocation of substances to specific groups is not provided. The study states that "the list includes several pharmaceuticals and personal care products, substances used in households, metabolites and transformation products, and inorganic substances including metals."	The study assumed for each substance a representative, uniform concentration in the raw sewage entering the WWTP in order to make a comparison of wastewater treatment scenarios independent of the specific composition of wastewater at each plant. Attribution of concentrations was based on available databases. Allocation of substances to specific groups is not provided. The study states that "the list includes several pharmaceuticals and personal care products, substances used in households, metabolites and transformation products, and inorganic substances including metals."	The study assessed mixture toxicity using multiple thresholds (including EC50 for fish, crustaceans, D. magna, and algae), HC50, and PNEC.	The study relies on other databases including: - a measurement campaign in the context of the 4th Joint Danube Survey (JDS4, http://www.danubesurvey.org /jd54/about), - the abovementioned Dutch WATSON database, - the measurements of the campaign by Finckh et al., 2022, - concentrations derived from emission estimates available in the European Environmental	Some of the uncertainties and limitations mentioned in the study: assumption-based relative toxicity estimation, limited pollutant scope - some substances may have been overlooked, uniform concentrations assumptions, and lack of systematic monitoring	

Reference	Title	Which micropollutants are considered?	Is there an indication of quantity ratios (total share of micropollutants, subgroups of micropollutants, specific substances)?	Is there an indication on the toxicity/hazard of the micropollutants?	What is the source of the data (e.g. measurements, other studies)?	Uncertainties / validity of data
			estimated. For this the equations of the SimpleTreat model v. 4.0 were used. Further details are included in the study.		Footprint 3.0 exercise (Saouter et al., 2020).	
(Lopez- Herguedas et al., 2024)	Evaluating membrane bioreactor treatment for the elimination of emerging contaminants using different analytical methods	The combination of a suspect screening approach using liquid chromatography tandem high-resolution mass spectrometry (LC-HRMS) and multitarget analysis by gas chromatography-mass spectrometry (GC-MS) allowed the detection of approximately 200 compounds in the WWTP effluents.	No information on total share in the measured water sample. A total of 96 compounds including PPCPs, pesticides, industrial agents, phthalates and hormones were quantified in all the analysed effluents. Supplementary material presents data for individual micropollutants (without information about the source group).	Yes, calculation of risk RQ; The environmental risk posed by the non-eliminated compounds after both treatments remained similar, being anthracene, clarithromycin, bis(2- ethylhexyl) phthalate (DEHP) and dilantin the most concerning pollutants (RQ > 1).	21 samples from WWTP in the Basque Country, Spain	ΝΑ
(Nas et al., 2022)	Evaluation of occurrence, fate and removal of priority phthalate esters (PAEs) in wastewater and sewage sludge by advanced biological treatment, waste stabilization pond and constructed wetland	Phthalate esters (PAEs): - Di(2-ethylhexyl)phthalate (DEHP) - Di-n-octyl phthalate (DNOP) - Benzyl butyl phthalate (BBP)	No information on the total share in the measured water samples, but concentration on PAEs.	No	Wastewater and sludge lines of three different WWTPs in Konya, Turkey	NA
(Nas et al., 2023)	Fate and removal of pesticides in solid and liquid phases of metropolitan, urban and rural-scale wastewater treatment plants	Pesticides, Atrazine (ATZ), Chlorpyriphos (CPR) and Chlorfenvinphos (CFV)	No information on the total share in the measured water samples, but concentration of substances.	No	Samples from three different WWTPs	NA
(Muschket et al., 2024)	Fate of persistent and mobile chemicals in the water cycle: From municipal wastewater discharges to river bank filtrate	127 PM (persistent and mobile) chemicals:- 105 REACH-registered industrial chemicals- 4 pharmaceuticals- 7 transformation products- 1 pesticide- 2 sweeteners	No information on the total share in the measured water samples.Among the 20 most abundant ones found in surface water were many industrial chemicals (REACH), pharmaceuticals, sweeteners and transformation products.	According to the study authors it appears that all these chemicals fulfil the regulatory criterion for classification as "mobile" or "very mobile".Health-related Indicator Values (HRIV) for selected substances.	Effluent and surface water was investigated. Effluent of six German WWTPs (from 52,000 to 1 350 000 population equivalents), all with mechanical and biological treatment stages, was collected 3 to 14 times (n = 38) between January and October 2021.	NA
(Guillossou et al., 2021)	Fluorescence excitation/emission matrices as a tool to monitor the removal of organic micropollutants from wastewater effluents by adsorption onto activated carbon	20 pharmaceuticals 5 pesticides 2 hormones 1 perfluorinated acid	No information on the total share in the measured water samples, but information on concentration for individual compounds.	No	Sampling wastewater effluent from the Seine Centre WWTP	NA
(Müller et al., 2020)	Influence of Emission Sources and Tributaries on the Spatial and	97 organic micropollutants (target compounds) - pesticides	No information on the total share in the measured water samples.	2 bioassays were performed covering oxidative stress response (AREc32) and	Measurements of 2 different sampling points	NA

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	Temporal Patterns of Micropollutant Mixtures and Associated Effects in a Small River	- pharmaceuticals - industrial and household chemicals	Two sampling points alongside a river (Ammer, Germany) after a storm event Sample point 1: 11 pesticides, 9 pharmaceuticals, 7 industrial and household chemicals Sample point 2: 10 pesticides, 17 pharmaceuticals, 6 industrial and household chemicals (note: Supplementary material presents measured concentrations of all target compounds)	induction of hydrocarbon receptor-chemical-activated luciferase gene expression (AhR-CALUX). The mixture effects of all chemicals were assessed.		
(Diogo et al., 2023)	Insights into environmental caffeine contamination in ecotoxicological biomarkers and potential health effects of Danio rerio	Caffeine	caffeine concentrations in different waterbodies and geographies are cited	Study results indicated that environmentally relevant concentrations of caffeine affected metabolic pathways in D.rerio, i.e. caffeine induces: i) significant disruptions in antioxidant defence pathways (SOD, GRed, and GSH); ii) cellular energy allocation mechanisms somewhat affected as LDH activity and lipids content; iii) the highest concentrations of caffeine were responsible for neuro- oxidative disturbances in D. rerio	Review of studies on scientific studies of caffeine	ΝΑ
(Kizgin et al., 2024)	Integrating Biological Early Warning Systems with High-Resolution Online Chemical Monitoring in Wastewater Treatment Plants	Mixed targeted and non- targeted approach. Pharmaceuticals (targeted screening) and insecticides (2,4-Dichlorophenol, Carbofuran) (non target screening) and industrial chemical (Tributyl phosphate) (non target screening).	No information on the total share in the measured water samples, but concentration are provided.2,4-Dichlorophenol (1,000 ug/L) Carbofuran (1.4 ug/L) Tributyl phosphate (15.3 ug/L)lidocaine (1.2 ug/L)xylazine (1.8 ug/L)aminoantipyrine (4.2 ug/L)	Νο	Measurement of samples at a full-scale WWTP (Canton St. Gallen, Switzerland) that receives municipal wastewater from about 39 000 population equivalents (3.6 million m3/a).	Authors indicate that results should be considered with caution due to matrix effects.
(Salgado et al., 2022)	Microalgal Cultures for the Bioremediation of Urban Wastewaters in the Presence of Siloxanes	7 Siloxanes were investigated: D3-D6 and L3-L5	Concentrations of siloxanes in primary effluent (raw and filtered) and secondary effluent (raw and filtered)	No	Samples effluents (primary and secondary) from a Portuguese WWTP with over 10,000 PE.	NA
(Proctor et al., 2021)	Micropollutant fluxes in urban environment – A catchment perspective	The study examined 142 CECs in a river catchment impacted by 5 urban areas.	Study revealed that a wide range of contaminants were detected, with 112 out of 138 CECs identified in the aqueous phase (influentAQ) and 74 out of 96 found in the solid particulate matter (influentSPM). Of these, 39 chemicals were consistently present in all samples across both phases. These included antidepressants, analgesics, stimulants like cocaine, and industrial chemicals such as bisphenol A (BPA) and	No	Samples were collected from 5 WWTP in the UK over 7 consecutive days between June and October 2015. The WWTPs varied in treatment technologies and served populations of different sizes. Sampling methods included: - volume-proportional sampling for influent	NA

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			benzophenone-1. The chemical composition differed notably between the two phases. The aqueous phase primarily contained lifestyle chemicals like caffeine and nicotine, nonsteroidal anti- inflammatory drugs (NSAIDs), and antidiabetics, with over 96% of these compounds residing in this phase. In contrast, the solid phase was dominated by BPA, which accounted for 69.6% of the load, followed by antidepressants at 12.9% and antifungal agents at 4.1%.		wastewater. - time-proportional sampling for effluent. - grab sampling for river water upstream and downstream of discharge points, and for digested sludge at two WWTWs. This approach allowed for comprehensive data collection on wastewater and environmental conditions.	
(lanes et al., 2024)	Monitoring (micro- )pollutants in wastewater treatment plants: Comparing discharges in wet- and dry-weather	78 target compounds - 7 conventional pollutants - 19 metals - 52 micropollutants (23 pesticides, 25 PFAS, MEBICAR, 2-Methyl 5-Methylthio 1,3,4- Thiadiazole (MMTD), Dimetridazole (DMZ), and Tris(2-chloroethyl) phosphate (TCEP))	No information on the total share in the measured water samples, but information on concentration for individual compounds. Out of the 78 compounds analyzed, 3/19 metals, 12/23 pesticides, and 18/25 PFAS were below the LOQ in all samples.	Ecotoxicity was analyzed through immobilization on Daphnia magna. Results suggests that samples with highest concentrations of nutrients, namely those at the beginning of the event (storm) or collected during small rain events, have a higher toxicity, while at the end of the events when concentrations of pesticides are higher, but the concentrations of conventional pollutants and metals are lower, the toxicity is also lower.	A WWTP in the outskirt of Milan was sampled during dry and wet weather conditions	ΝΑ
(Langeveld et al., 2023)	Monitoring organic micropollutants in stormwater runoff with the method of fingerprinting	Concentration in stormwater runoff of 403 organic micropollutants was estimated by fingerprint method: - 254 pesticides - 28 organochlorine pesticides - 63 pharmaceuticals - 15 PAHs - 7 PCBs - 33 other substances	No information on the total share in the measured water samples, but the concentration was estimated. Detected micropollutants in stormwater portion in WWTPs - 24 out of 254 pesticides - 6 out of 28 organochlorine pesticides - 45 out of 63 pesticides - 15 out of 15 PAHs - 2 out of 7 PCBs - 20 out of 33 other substances	No	Samples collected at the influent of 5 different WWTPs in The Netherlands; portion of stormwater runoff in WWTP was calculated and concentrations of micropollutants were detected based on a new method, called fingerprinting	ΝΑ
(Aggerbeck et al., 2024)	Non-target Analysis of Wastewater Treatment Plant Effluents: Chemical Fingerprinting as a Monitoring Tool.	A non-target screening without analytes of particular interest prior to conducting the research. Analysis revealed substances belonging to several different groups:Natural substances:- Amino acids- Endogenous MetabolitesSynthetic	4094 unique substances were detected in the water samples with 1482 filtered out as background noise. A tiered identification system was used to categorize substances, from confirmed compounds with experimental data to those identified only by mass spectrometry data. Using this system, 785 compounds were confirmed, with 451 having assigned compound classes. 38	NA	Effluent samples from 3 WWTP in Denmark, ranging in PE from 12,000 to 400,000 and different proximity to city, hospitals, industry and rural areas.	Some limitations mentioned in the study:- bias from pre- assembled libraries (the reliance on pre-existing libraries for compound identification may introduce bias, particularly toward known substances, which is evident in the higher

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		substances:- industrial chemicals- PCP- pesticides- reagents and standards- therapeutics and drugs	compounds were confirmed with in house libraries.Additionally, Compound Discoverer identified 16 compounds that varied significantly in their presence between sites. These included 10 compounds from the therapeutics and drugs category (such as the antibiotic clarithromycin and anticonvulsant oxcarbazepine), 4 pesticides (e.g., propiconazole and prosulfocarb), 1 flame retardant (tributyl phosphate), and 1 personal care product (the sunscreen component 2-ethylhexyl salicylate).			proportion of therapeutics and drugs identified. This bias may decrease over time as more compounds are added to libraries)- limited sample size (the study only examined a small number of samples from three WWTPs, making it difficult to draw broad statements)- cytotoxicity concerns (the impact of identified compounds, especially metabolites from different sources on microbial communities requries further research)- quantification challenges (the study detected compounds at very low concentrations, but the mere presence of a compound doesn't necessarily imply that it poses a significant risk)- computational challenges (the analysis of large datasets containing thousands of compounds presents computational difficulties)	
(Chiriac et al., 2020)	Occurrence and Fate of Bisphenol A and its Congeners in Two Wastewater Treatment Plants and Receiving Surface Waters in Romania	Bisphenol A and its Congeners	Bisphenol A: 69.9-75.2 ng/L 4-hydroxyacetophenone: 17.8-20.8 ng/L	Concentrations determined pose no risk to human health if they were used as drinking water sources. Moreover, the BPA and BPS values determined in effluents show no more than a low risk for aquatic organisms.	Samples originating from municipal WWTPs corresponding to cities of Braila and Targu-Jiu. Braila city (A) is located in the Eastern part of Romania, whereas Targu-Jiu city (B) is situated in the South-West part of Romania	NA	
(Golovko et al., 2021)	Occurrence and removal of chemicals of emerging concern in wastewater treatment plants and their impact on receiving water systems	Targeted analysis of 164 contaminants of emerging concern (CECs): - 96 Pharmaceuticals - 4 Personal care products - 9 Industrial chemicals - 10 Per- and polyfluoroalkyl substances (PFASs) - 34 Pesticides - 3 Parabens - 3 Stimulants - 2 Vitamins - 1 Drug	No information on the total share in the measured water samples. 119 of 154 target CECs were detected in most samples, including pharmaceuticals, personal care products, industrial chemicals, PFASs, pesticides, parabens, stimulants and vitamins. The dominant groups were NSAIDs (nonsteroidal anti-inflammatory drug), stimulants, antidiabetic drugs, and industrial chemicals. Highest concentrations and high frequency of detection (> 50%) were found for three industrial chemicals, 15 pharmaceuticals and the stimulants caffeine	No	Influent and effluent wastewater samples from 15 WWTPs in Sweden	NA	



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		- 1 Fatty acid - 1 Isoflavone	and nicotine. For individual CECs, the highest concentrations were found for metformin (up to 54,000 ng/L), caffeine (64,000 ng/L) and nicotine (9600 ng/L) in wastewater influent and effluent.	·		
(Đurišić- Mladenović et al., 2024)	Occurrence of contaminants of emerging concern in different water samples from the lower part of the Danube River Middle Basin – A review	70 contaminants of emerging concern (CECs) in wastewater - Pharmaceuticals - Industrial chemicals - PFAS - Pesticides - Personal care products	No information on the total share in the measured water samples. Widest concentration of CECs in wastewater was found for pharmaceutically active compounds, followed by pesticides and industrial chemicals. Highest value in wastewater samples was more than 2000 µg/L for linear alkyl benzene sulfonate (grouped in industrial chemicals). Highest value of pharmaceuticals (39.15 µg/L of carboxy-cyclophosphamide) was found in a sample from Slovenia, representing hospital effluents. The ranges of pharmaceuticals within the lower part of the Middle Danube Basin were similar, with maximum values around 20 µg/L. PFAS levels in wastewater span over a similar range of concentrations	No	Review of 38 scientific papers that reported the occurrence of CECs in different water types from the countries belonging to the lower part of the Middle Danube Basin	NA
(Beltrán De Heredia et al., 2024) (Montes et al., 2023)	Occurrence of emerging contaminants in three river basins impacted by wastewater treatment plant effluents: Spatio- seasonal patterns and environmental risk assessment Occurrence of persistent and mobile chemicals and other contaminants of	Targeted analysis of 270 compounds - pharmaceuticals - other consumer products - pesticides - industrial chemicals Investigated CECs:PPCPs and their metabolites (n=22), pesticides (n=8), food	No information on the total share in the measured water samples. 68 analytes out of the 270 compounds were not detected at all. 187 compounds were detected in at least one WWTP: - 115 pharmaceuticals - 7 other consumer products - 32 pesticides - 33 industrial chemicals No information on the total share in the measured water samples., concentrations provided in the study including both raw and	No RQ were calculated for each substances.	Samples taken in three river basins located in the Basque Country (northern Spain). These river basins were selected, since they are impacted by the treated effluents from WWTPs. Raw and treated wastewater from WWTP located in Spain and Portugal.	NA
	emerging concern in Spanish and Portuguese wastewater treatment plants, transnational river basins and coastal water	additives (n=2), industrial chemicals (n=18), and cleaning agents (2).	treated wastewater.		-	
(Nas et al., 2020)	Occurrence, loadings and removal of EU-priority polycyclic aromatic hydrocarbons (PAHs) in wastewater and sludge by advanced biological treatment, stabilization pond and constructed wetland	8 polycyclic aromatic hydrocarbon (PAH) compounds which have been accepted as priority micropollutants by European Union (EU) were analyzed both in wastewater Benzo[a]pyrene (B[a]P)	No information on the total share in the measured water samples. Selected CECs average concentrations: See selected substances tab	No	Turkey - three different WWTPs located in different points in the same city between September of 2017 and August of 2018 over 1 year Large scale WWTP (Konya) in which industrial activities exist Medium scale WWTP (Eregli)	ΝΑ

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		Benzo[b]fluoranthene (B[b]F) Benzo[g,h,i]perylene (B[g,h,i]P) Benzo[k]fluoranthene (B[k]F) Fluoranthene (FLU) Naphthalene (NAP) Anthracene (ANT) Indeno(1,2,3-cd)pyrene (I[1,2,3-cd]P)			in which industrial activities limited, Small scale WWTP (Zincirlikuyu) in which there is no industrial activities.	
(Kaiser et al., 2021)	Ozone as oxidizing agent for the total oxidizable precursor (TOP) assay and as a preceding step for activated carbon treatments concerning per- and polyfluoroalkyl substance removal	13 PFAS, 1 corrosion inhibitor (Benzotriazole (BTA)), 2 pharmaceuticals (Carbamazepine (CBZ) and Trimethoprim (TMP))	PFAS concentrations in effluent (ng/L): PFBA (11.01) PFPeA (3.91) PFHxA (6.83) PFHpA (1.54) PFOA (1.54) PFOA (0.70) PFDA (0.70) PFDA (0.57) PFUnDA ( <lod) PFBS (2.16) PFHxS (1.14) PFOS (2.77) DONA (2.62) GenX (4.45) Other substances: BTA (1311.3) CBZ (114.5) TMP (38.2)</lod) 	Νο	Effluents from WWTP in Austria. No further details in the study.	ΝΑ
(Neef et al., 2022)	Performance of Micropollutant Removal during Wet-Weather Conditions in Advanced Treatment Stages on a Full-Scale WWTP	A total of 26 organic micropollutants were measured in the samples collected from WWTP: pharmaceuticals (n=12) food (n=1) corrosion inhibitor (n=2) industrial chemical (n=4) flame retardant (n=3) insect repellent (n=2) herbicide (n=2)	No information on the total share in the measured water samples, but concentrations in the effluent of the secondary clarifier are provided. The highest concentrations during both dry and wet weather were observed for the corrosion inhibitors 1H-benzotriazole and tolytriazole. In dry weather their concentrations reached 15.8 µg/L and 16.8 µg/L, respectively, which is double the levels detected in wet-weather samples. Notably, these concentrations are up to 100 times higher than those measured for ibuprofen or herbicide tertbutyl. Further, concentrations are provided in effluent after PAC treatment and effluents after GAC filter. Investigation showed that different removal performances are observed for both processes related to impacts such as HRT, feed concentrations, pH, temperature, and different properties of the two activated	ΝΟ	A case study conducted at the WWTP in Mannheim, Germany. The WWTP has a size of 725,000 PE and an inflow of around 78,000 m3 per day. Approximately 50% of the wastewater volume comes from industries such as chemical industry, metal processing industry and food industry. WWTP has a full scale additional treatment stage with PAC in partial flow operation and a GAC filter for further investigation on micropollutant removal. Both treatment stages were sampled once during dry- weather and twice during wet- weather conditions.	some of uncertainties identified in the study: 1. uncontrollable external influences such as rain events 2. limited sampling and temporal scope 3. resource constraints 4. Lack of broader validation 5. The results cannot be generalized beyond the specific conditions studied (e.g., wet weather conditions in Mannheim)



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			carbon products (concentrations provided only in the figure).			
(Scheurer et al., 2022)	Persistent and mobile organic chemicals in water resources: Occurrence and removal options for water utilities	26 Persistent and mobile (PM) substances	For the Rhine river, substance concentrations and for the Rhine and Alb river, figures showing the quantitative distribution of the substances at different sampling spots are displayed.	NA	> 120 surface water samples from various sampling spots at the Alb and Rhine river	NA
(Ullberg et al., 2021)	Pilot-scale removal of organic micropollutants and natural organic matter from drinking water using ozonation followed by granular activated carbon	99 target compounds: - PFAS - pharmaceuticals - other organic micropollutants	No information on the total share in the measured water samples, but concentration of substances. 29 compounds were detected (22 pharmaceuticals, 2 PFAS, 6 other OMPs) at a WWTP in Görväln, Sweden and substance concentrations of ingoing wastewater are shown. The highest concentrations were detected for caffeine (22+-3.8 ng/L) and Tolyltriazole (13+-6.9 ng/L).	NA	Measurements (Sample points at various stages of a WWTP)	NA
(Tasselli et al., 2021)	Polycyclic musk fragrance (PMF) removal, adsorption and biodegradation in a conventional activated sludge wastewater treatment plant in Northern Italy. The wastewater treatment plant (WWTP) pipeline includes initial treatment stages such as coarse screening and primary settling, followed by a conventional activated sludge (CAS) system comprising an anoxic tank and an aerobic tank. The final stage involves tertiary treatment, which consists of filtration and ultraviolet (UV) disinfection.	5 polycyclic musk fragrances (PMF)	Concentration of PMF were discussed. Galaxolide (HHCB) has been the compound with the highest concentrations and, together with HHCB-lactone, has been in the µg L-1 range.	Other studies are cited stating the following hazards: - acute toxicity to aquatic organisms ranges from hundreds of µg L-1 to amounts of <20 mg/L - no data are currently available regarding chronic toxicity whilst only few studies focussing on subchronic effects were published - oxidative stress	Measurements (Samples of water and sludge at a WWTP in Northern Italy)	ΝΑ
(García-Vara et al., 2023)	Prioritization of organic contaminants in a reclaimed water irrigation system using wide-scope LC-HRMS screening	Suspect screening of sample without pre-defined selection of analytes	158 contaminants of emerging concern (CECs) including pharmaceuticals, industrial chemicals, and pesticides, among others were identified. More than 50% of the CECs tentatively identified were pharmaceuticals, which was assumed to be in agreement with the domestic origin of the wastewater. Pharmaceuticals, pesticides, and industrial chemicals were the CEC classes most	Yes, PNEC values and RQ derived:Regarding their ecotoxicological risk, 14 out of 119 tentatively identified CECs showed an individual RQ over 1 and, therefore, presented a concentration potentially toxic for the aquatic environment. From these, O-desmethyl-	Monitoring of water regeneration plant (WRP) influent (A) and effluent (B) of urban and industrial origin in Spain. Reclaimed water discharged into the channels (C) and water abstracted for irrigation downstream (mix of	As stated by the authors this approach presents some analytical limitations, e.g., highly polar and apolar compounds may not be covered, and missing compounds in the suspect lists used (e.g. transformation products).

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			frequently detected in the investigated waters.Semi-quantified concentrations of the CECs found in the water used for irrigation in winter and summer.	venlafaxine would pose the highest risk with an RQ value of 175; then, venlafaxine and galaxolidone (a metabolite of the personal care product galaxolide) would present high risk (RQ > 10) and the rest of compounds moderate risk (1 < RQ < 10). This last category included industrial chemicals (2-ethylhexyl diphenyl phosphate, N-phenyl-1- naphthylamine, and caprolactam), pharmaceuticals (carbamazepine, sulfamethoxazole, and temazepam), tire wear compounds (N,N'- diphenylguanidine), and caffeine and its metabolite theophylline.	reclaimed and surface water) (D).	
(García-Galán et al., 2021)	Removal and environmental risk assessment of contaminants of emerging concern from irrigation waters in a semi-closed microalgae photobioreactor	<ul> <li>13 Contaminants of emerging concern (CECs) were investigated:</li> <li>- 6 pharmaceuticals,</li> <li>- 4 personal care products,</li> <li>- 2 flame retardant and</li> <li>- 1 surfactant</li> </ul>	No information on the total share in the measured water samples. Concentration are provided. Average concentrations of selected CECs : - Diclofenac (DCF): 1106 ± 111 ng/g - Carbamazepine (CBZ) : 717 ± 59 ng/g - N,N-diethyl-m-toluamide (DEET): 699 ± 90 ng/g - Tris(2-chloroethyl) phosphate (TCEP): 284 ± 29 ng/g - Surfinol 104 (TMDD): 256 ± 42 ng/g	Yes, ecotoxicity endpoints and hazard quotients estimated.	Reclaimed wastewater from an urban WWTP and agricultural run-off from agricultural land (irrigation water) from Spain	NA
(Bogunović et al., 2021)	Removal of selected emerging micropollutants from wastewater treatment plant effluent by advanced non- oxidative treatment - A lab-scale case study from Serbia	48 micropollutants were analyzed including active pharmaceutical ingredients, bisphenols, parabens and UV filters.Examples for substances include:2,4- dihydroxybenzophenone (DH- BP)bisphenol F (BPF)bisphenol S (BPS)ketoprofen (KP)diclofenac (DF)carbamazepine (CBZ)	No information on the total share in the measured water samples. Information on concentration are included.Only 16 substances were above the LOQ in at least one sample.	No	Wastewater samples were collected three times during Septemberand October 2017, at the "Vodokanal" Sombor municipal WWTP inSerbia.	NA
(Delli Compagni et al., 2020)	Risk assessment of contaminants of emerging concern in the context of wastewater reuse for irrigation: An	13 Contaminants of emerging concern (CECs):- clarithromycin (CLA)- sulfamethoxazole (SMX)- diclofenac (DCF)- ibuprofen (IBU)- paracetamol (PAR)-	No information on the total share in the measured water samples but predicted concentration.	Environmental and human health risks were evaluated	Predicted CEC concentrations from the river model in Denmark; Model applied to a case study in Italy	NA

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	integrated modelling approach	carbamazepine (CBZ)- furosemide (FUR)- 17-a ethinylestradiol (EE2)- 17-b oestradiol (E2)- estrone (E1) - perfluorooctanoic acid (PFOA) - perfluorooctane sulfonate (PFOS)- triclosan (TCS)				
(Narain-Ford, van Wezel, et al., 2022)	Soil self-cleaning capacity: Removal of organic compounds during sub-surface irrigation with sewage effluent	89 Contaminants of emerging concern (CoECs) - herbicides, industrial chemicals, pharmaceuticals,personal care products, and their transformation products.	No information on the total share in the measured water samples, but measured concentrations of measured substances. Top 5: 1H-benzotriazole (industrial chemicals)Metoprolol (pharmaceutical)Sotalol (pharmaceutical)Triethyl phosphate (industrial chemicals)Furosemide (pharmaceutical)	The CoECs are assigned to four persistency-mobility classes, i.e. highpersistency and high mobility (PM), high persistency and low mobility(Pm), low persistency and high mobility (pM), and low persistency andlow mobility (pm)	STP effluent from 1 STP in Netherlands. Five sampling episodes from September 2017 to April 2019 were carried out.	NA
(Seelig et al., 2024)	Sources of persistent and mobile chemicals in municipal wastewater: a sewer perspective in Leipzig, Germany	67 PM (persistency-mobility) chemicals	No information on the total share of the measured water sample, but concentration of selected analytes. CSA (4-isopropylbenzenesulfonic acid) showed the highest concentration in a single sample (11 mg L-1). It was detected in almost every sample, but with highly variable concentrations ranging over two orders of magnitude. This is also demonstrated by the chemicals vast range of applications. CSA is used widely in industry, in manufacturing, and in household products like bleach and air freshener or is applied for the production of surfactants. In this study, highest concentrations of CSA were found in the discharge of nursing homes and samples belonging to the traffic-related and cleaning industry.	NA	19 wastewater samples were collected in the sewer system of Leipzig, Germany, from different catchment areas categorized in clinical, domestic, and industrial wastewater.	NA
(Hinnenkamp et al., 2022)	Target, suspect and non- target screening analysis from wastewatertreatment plant effluents to drinking water using collision crosssection values as additional identification criterion	A total of 51 substances were found in the treated water discharged from WWTPs in different concentration ranges. Out of these, 19 substances were also detected in the drinking water sample.	Substances detected in WWTP effluents (n=2) in the concentration range >1000 ng/L with the quantitative screening:corrosion inhibitor (1H-benzotriazole)pharmaceuticals (4- Aminoantipyrine, Candesartan, Carbamazepine, diclofenac, Gabapentin, Metoprolol, Telmisartan, Valsartan, Valsartan acid).	The study stated there are currently no regulatory limit values for the detected compounds in drinking water. There are however, health related guideline values available for 10 of these compounds:0.3 µg/L: for substances such as 10,11- dihydroxy-10,11- dihydrocarbamazepine, candesartan, carbamazepine, and valsartan acid.1 µg/L: for gabapentin, gabapentin- lactam, and iopamidol.3 µg/L:	The study analyzed several environmental compartments including drinking water, surface water, raw water, process water and two WWTP effluents.	The study states that non- target screening which involves analyzing unknown compounds in water, faces challenges such as data complexity and the need for advanced processing techniques. Prioritization methods help identify the most relevant features, and data sources like ChemSpider or PubChem assist in matching detected compounds to known substances. However, some substances are so novel

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				for 1H-benzotriazole, chlorothalonil M-12, and methyl-desphenyl- chloridazon.The study concluded there no human health risk is currently associated with the levels of these substances in the analyzed drinking water samples.		that they cannot be identified using these methods alone.
(Kilpinen et al., 2024)	Temporal trends and sources of organic micropollutants in wastewater	Both targeted and suspect screening approaches were employed, allowing for the full quantification of 64 micropollutants and the identification of 90 additional compounds through suspect screening.Biocides: 12Pharmaceuticals: 35Sweeteners: 2Personal Care Products and Additives: 5Persistent Organic Pollutants (POPs): 7Natural Compounds and Metabolites: 3	No information on the total share in the measured water samples, 64 micropollutants were quantified. Concentrations provided in the study.	No	168 effluent samples in Denmark over three months from the same WWTP	NA
(Freeling et al., 2020)	Under the radar – Exceptionally high environmental concentrations of the high production volume chemical	Sulfamic acid only	Sulfamate concentrations in the influent and effluent of the studied WWTPs ranged from 520 mg/L to 1900 mg/L and from 490 mg/L to 1600 mg/L, respectively. This means that typical sulfamate concentrations in WWTP effluent in Germany are more than 1000 times higher than the effluent concentrations of the commonly used pharmaceuticals CBZ and diclofenac, which are generally detected in the mid ng/L-range	Yes, hazards are discussed.	measurement of influent and effluent from five conventional (i.e. conventional activated sludge system) WWTPs in Germany	NA
(Ng et al., 2023)	Wide-scope target screening characterization of legacy and emerging contaminants in the Danube River Basin by liquid and gas chromatography coupled with high-resolution mass spectrometry	Targeted screening of 212 contaminants of emerging concern (CECs) - PPCPs, industrial chemicals and PPPs	No information on the total share in the measured water samples, concentrations of individual CECs are provided.	Mentions with the CECs is on the Watch List established by the Commission Implementing Decision (EU 2018/840)	11 effluent wastewater treatment plants along the Danube river in 10 EU countries	NA
(Gago-Ferrero et al., 2020)	Wide-scope target screening of>2000 emerging contaminants	Target screening of>2000 emerging contaminants in wastewater samples and	No information on the total share in the measured water samples.	No	Influent and effluent wastewater samples were collected from the WWTP of	NA

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	in wastewater samples with UPLC-Q-ToF- HRMS/MS and smart evaluation of its performance through the validation of 195 selected representative analytes	smart evaluation of its performance through the validation of 195 selected representative analytes: - 66 pesticides - 215 drugs - 4 sweeteners - 10 perfluorinated compounds - 8 amino acids - 31 industrial chemicals	Information on concentrations are available. LAS surfactants, metformin and its metabolite guanylurea, and N-desmethylvenlafaxine were present at the highest concentrations		Athens (Greece) on the 15th of March 2014		