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Urban Input Pathways and Spatial-Temporal Distribution of Tire-Derived Compounds in the Danube River and Its Tributaries in Vienna

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Abstract

Tire wear particles (TWP) are among the largest sources of microplastics and act as a significant pathway for tire-derived compounds (TDC) into the environment, where they may pose risks to ecosystems and human health. The Danube River receives continuous inputs of TWP and TDC through multiple pathways such as road runoff, wastewater treatment plants (WWTP) effluents, or atmospheric deposition, with urban areas representing key hotspots. In this study, the occurrence and spatial-temporal distribution of selected TDC were investigated along the Danube in Vienna and its tributaries. Samples were collected during four sampling campaigns at 15 locations, including the Danube, the Danube Channel, and two tributaries. Water samples were filtered to separate the dissolved phase and suspended particulate matter (SPM), and sediments were collected at selected locations. All samples were quantified using Triple quadrupole liquid chromatography-mass spectrometry (LC-MS/MS). TDC were detected across all samples, confirming their continuous presence in urban surface waters. The highest concentrations were observed in urban tributaries and WWTP effluents, identifying these as the major entry pathways. TDC concentrations in water and sediment increased from upstream Vienna to downstream Vienna, while compound profiles remained largely consistent, suggesting that urban inputs mainly increase TDC loads without changing the compound composition. No uniform temporal pattern for TDC was revealed for any of the dissolved, particulate, and sediment phases. The highest concentrations were detected in sampling campaign 4, where the most dominant compounds Hexa(methoxymethyl)melamine (HMMM) and 5-methyl-1h-benzotriazole (5-Me BTR) reached up to 23832.47 ng/L and 38927.86 ng/L, respectively, in individual locations. This study provides an overview of the main pathways and the occurrence of TDC in surface waters of Vienna, as well as the phase distribution of these contaminants.

Kurzfassung

Reifenabriebpartikel (TWP) gehören zu den größten Quellen für Mikroplastik und stellen einen bedeutenden Eintragspfad für aus Reifen freigesetzte Zusatzstoffe (TDC) in die Umwelt dar, wo sie Risiken für Ökosysteme und die menschliche Gesundheit bergen können. Die Donau nimmt kontinuierlich TWP und TDC über Wege wie Straßenabfluss, Abwässer aus Kläranlagen (WWTP) oder atmosphärischen Stoffeintrag auf, wobei städtische Gebiete wichtige Hotspots darstellen. In dieser Studie wurden das Vorkommen und die räumlich-zeitliche Verteilung ausgewählter TDC entlang der Donau in Wien und ihrer Nebenflüsse untersucht. Die Probenahmen erfolgten im Rahmen von vier Probenahmekampagnen an 15 Standorten in der Donau, dem Donaukanal und zwei Nebenflüsse. Die Wasserproben wurden gefiltert, um die gelöste Phase und die Schwebstoffe (SPM) voneinander zu trennen, an ausgewählten Standorten wurden Sedimentproben entnommen. Alle Proben wurden mittels Triple-Quadrupol-Flüssigchromatographie-Massenspektrometrie (LC-MS/MS) quantifiziert. TDC wurden in allen Proben nachgewiesen, was ihr kontinuierliches Vorkommen in städtischen Oberflächengewässern bestätigt. Die höchsten Konzentrationen wurden in städtischen Nebenflüssen und Kläranlagenabläufen beobachtet, was diese als die wichtigsten Eintragspfade identifiziert. Die Konzentrationen in Wasser und Sediment stiegen von stromaufwärts bis stromabwärts von Wien an, während die Stoffprofile weitgehend konsistent blieben. Das deutet darauf hin, dass städtische Einträge hauptsächlich die TDC-Belastung erhöhen, ohne die Stoffzusammensetzung zu verändern. Es zeigte sich kein einheitliches zeitliches Muster für TDC in den gelösten, partikulären und sedimentären Phasen. Die höchsten Konzentrationen wurden in der Probenahmekampagne 4 festgestellt, wo die dominierenden Verbindungen Hexa(methoxymethyl)melamine (HMMM) und 5-Methyl-1h-Benzotriazole (5-Me BTR) an einzelnen Standorten Werte von bis zu 23832.47 ng/L bzw. 38927.86 ng/L erreichten. Diese Studie bietet einen Überblick über die Haupteintragspfade und das Vorkommen von TDC in den Oberflächengewässern in Wien, sowie über die Phasenverteilung dieser Schadstoffe.

Keywords

tire-derived compounds, emerging pollutants, phase distribution, urban runoff pathways, Danube River

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List of Abbreviations

2-amino BTH	2-aminobenzothiazole
2-Me BTH	2-methylbenzothiazole
2-OH BTH	2-hydroxybenzothiazole
2-S BTH	2-mercaptobenzothiazole
5-Me BTR	5-methyl-1h-benzotriazole
6PPD	N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylenediamine
6PPDq	2-anilino-5-[(4-methylpentan-2-yl)amino]-cyclohexa-2,5-diene-1,4-dione
ACN	Acetonitrile
AO2246	2,2-Methylenebis(6-tert-butyl-4-methylphenol)
BHA	Butylated hydroxyanisole
BHT	Butylated hydroxytoluene
BTH	Benzothiazole
CAS	Chemical Abstract Service
CBS	N-Cyclohexyl-2-benzothiazolesulfenamide
CPPD	N-Cyclohexyl-N'-phenyl-p-phenylenediamine
CPPDq	2-(Cyclohexylamino)-5-(phenylamino)-2,5-cyclohexadiene-1,4-dione
DCM	Dichloromethane
DPG	1,3-Diphenylguanidine
DPPD	N,N'-Diphenyl-p-phenylenediamine
DPPDq	2,5-bis(phenylamino)cyclohexa-2,5-diene-1,4-dione
DPTU	N,N'-Diphenylthiourea
DTG	1,3-Di-o-tolylguanidine
HMMM	Hexa(methoxymethyl)melamine
IPPD	N-Isopropyl-N'-phenyl-p-phenylendiamin
IPPDq	2-[(1-Methylethyl)amino]-5-(phenylamino)-2,5-cyclohexadiene-1,4-dione
LC-MS/MS	Triple quadrupole liquid chromatography-mass spectrometry
LOD	Limit of detection
$\log K_{ow}$	n-octanol-water partition coefficient
LOQ	Limit of quantification
MeOH	Methanol
MQ	MilliQ, ultrapure water
Neozone	N-Phenyl-2-naphthylamine
NR	Natural rubber

PBD	Polybutadiene
PPD	p-Phenylenediamine
PPDs	p-Phenylenediamines
SBR	Styrene butadiene rubber
SPE	Solid-phase extraction
SPM	Suspended particulate matter
TDC	Tire-derived compounds
TSS	Total suspended solids
TWP	Tire wear particles
WWTP	Wastewater treatment plant

1 Introduction

Extensive anthropogenic pressures on the Earth system represent one of the most urgent global challenges. These pressures are conceptualized within the planetary boundaries framework, which defines a safe operating space for humanity. Crossing these boundaries increases the risk of irreversible and abrupt environmental changes, leading to an unstable, civilization-unfriendly environment. As of 2025, seven out of the nine boundaries have already been crossed, including the boundary for novel entities. Novel entities are new or modified substances and materials anthropogenically introduced into the environment. These substances include plastics, heavy metals, pharmaceuticals, and plastic additives, which can have adverse effects on ecosystems and human health. [1]

Regulations for these environmentally concerning substances often lag behind their production and application, due to the large amounts of newly registered substances every year, resulting in largely unregulated release into the environment. [1] Globally, more than 275 million substances are registered in the Chemical Abstract Service (CAS) Registry, with approximately 15 000 new substances added every day. [2] This vast and continuously growing number of chemicals makes comprehensive hazard assessment and safety testing of individual substances extremely challenging. [1]

As a subset of novel entities, microplastics and plastic additives are a great concern. Tire wear particles (TWP) are considered one of the largest sources of microplastic pollution, which are generated through abrasion between tires and road surfaces. [3] During tire application, tire-derived compounds (TDC) can be released together with TWP during abrasion or leach from the particles after entering the environment. This leaching occurs when TWP interact with environmental media such as water and soil, introducing TDC into surrounding ecosystems. This widespread contamination and the associated release of hazardous substances pose a significant and growing global concern. [4]

TDC are detected worldwide in road runoff, wastewater treatment plants (WWTPs), sediment, soil and surface waters. [5], [6], [7], [8], [9] Among them, compounds such as 6PPDq and HMMM have attracted considerable attention due to their environmental relevance. 6PPDq has been shown to cause adverse effects to some fish like coho salmon and zebrafish. [10], [11] HMMM, which is used as a crosslinking agent in tire rubber, is frequently detected in urban surface waters and has been discussed as a precursor of melamine, a substance identified as being of very high concern due to its persistence, mobility, and toxicological properties. [12], [13]

Surface waters are particularly vulnerable to TDC contamination, as they receive input from multiple pathways simultaneously, such as surface road runoff, stormwater drainage systems, effluents from WWTPs, and atmospheric deposition. Consequently, rivers are important transport pathways for traffic related contaminants, and it is crucial to understand the occurrence, distribution and transport of TDC. [14]

As the second largest river in Europe, with a river basin of 801 463 km^2 and 83 million people living in that area, the Danube River is particularly relevant for investigating the occurrence and transport of emerging contaminants such as TDC. The Danube is an important resource for drinking water supply, agriculture, industry, transportation, and recreation. [15]

Throughout its course, various types of pollution enter the river. These include point source pollution, such as municipal, industrial, and agricultural wastewater, and diffuse source pollution, such as direct surface runoff and atmospheric deposition. Throughout these pathways, traffic-related emissions, including TWP and TDC, may be transported into urban river systems. Due to these pathways, urban rivers often function as hotspots for emerging pollutants and play a key role in transporting these downstream. [15]

With over 2 million inhabitants (2025) Vienna is the largest city located along the Danube [16], making it highly relevant for investigating the fate and transport of anthropogenic contaminants. Although Vienna has the lowest car ownership rate among all Austrian federal states, with 363 cars per 1000 inhabitants at the end of 2024 compared to the national average of 569 cars per 1000 inhabitants, the city is characterized by high traffic density and high mobility demands. [17] Major traffic corridors, including the A23 Südosttangente, one of Austria's busiest motorways, pass through the city and crosses the Danube and Danube Channel. [18] Furthermore, Vienna has a complex urban water infrastructure, including both combined and separate sewer systems and a centralized wastewater treatment system for the whole city. [19]

These characteristics make the Danube River in Vienna a suitable natural system to investigate urban input pathways, spatial concentration gradients, and hydrologically driven temporal variability of TDC in a large urban river system.

2 State of Knowledge

2.1 Tire-Derived Compounds

TDC are substances released from tires and TWP into the environment. TWP are formed during vehicle operation, such as braking or accelerating, through mechanical friction between tires and road surfaces. The particles accumulate on road surfaces and enter the environment via different pathways, such as surface rainfall runoff, WWTPs [20] or atmospheric deposition. [21] TWP contribute to microplastic emissions with amounts of 5-6 Mt/y worldwide, making it one of the largest sources of microplastic pollution. [22]

Tire rubber typically consists of a complex mixture of natural rubber (NR), styrene butadiene rubber (SBR), and polybutadiene (PBD). Additives such as antiozonants, antioxidants, crosslinking agents, vulcanization agents, curing agents, fillers, and reinforcement agents are added to improve the performance and longevity of tire rubber. These additives account for 5-10% of the total tire composition. [23], [24] While the exact composition of tires is generally not publicly disclosed, many additives are known to be added to tires. [25]

Antiozonants and anti-aging agents such as p-phenylenediamine (PPD) and its derivatives prolong the lifespan of tires by protecting them from ozone attack, oxidation, and mechanical fatigue. Common compounds, some of which are also investigated in this study, include N-Isopropyl-N'-phenyl-p-phenylendiamin (IPPD), N-cyclohexyl-N' phenyl-p-phenylenediamine (CPPD), N,N'-diphenyl-p-phenylenediamine (DPPD), N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylenediamine (6PPD). [26] Following their release into the environment, these compounds can undergo rapid oxidative transformation, leading to the formation of quinone derivatives like 2-[(1-methylethyl)amino]-5 (phenylamino)-2,5-cyclohexadiene-1,4-dione (IPPDq), 2-(cyclohexylamino)-5-(phenylamino)-2,5-cyclohexadiene-1,4-dione (CPPDq), 2,5 bis(phenylamino)cyclohexa-2,5-diene-1,4-dione (DPPDq), and 2-anilino-5-[(4-methylpentan-2 yl)amino]-cyclohexa-2,5-diene-1,4-dione (6PPDq). [26]

Antioxidants such as butylated hydroxytoluene (BHT), butylated hydroxyanisole (BHA), N-phenyl-2-naphthylamine (Neozone), and 2,2-,methylenebis(6-tert-butyl-4 methylphenol) (AO2246) are also added to inhibit oxidative reactions and delay aging of the rubber in tires. [27]

Vulcanization accelerators including benzothiazole (BTH), 2-mercaptobenzothiazole (2-S BTH), 5-methyl-1h-benzotriazole (5-Me BTR), and N-cyclohexyl-2-benzothiazolesulfenamide (CBS) are added to tires as vulcanization accelerators.[20], [28] Related compounds like 1,3-diphenylguanidine (DPG), 1,3-di-o tolylguanidine (DTG) and N,N'-diphenylthiourea (DPTU) serve

as co-accelerators or activators. [7], [27], [28] Transformation products such as 2-aminobenzothiazole (2-amino BTH), 2-methylbenzothiazole (2-Me BTH) and 2-hydroxybenzothiazole (2-OH BTH) are frequently detected in environmental samples associated with tire wear. [20], [29]

Hexamethoxymethylmelamine (HMMM) is used in rubber formulations as a crosslinking and curing agent to improve the mechanical properties and durability of rubber materials. [7], [27] Aniline is an important industrial intermediate used in the synthesis of various rubber additives, including aromatic amine antioxidants and vulcanization accelerators. [30]

Some of these additives are not exclusive to tire rubber but are also applied in other plastics and coatings, as is the case for HMMM, BTH and BHA. [7] AO2246 is used in lubricants and mineral oil as part of hydraulic oil. [31] PPDs are widely applied in industrial rubber products and conveyor belts. [32] 6PPD and 6PPDq have been detected in samples of crumb rubber and sneaker soles. [33]

Many of these tire-derived compounds are biologically toxic to aquatic organisms, causing a range of adverse effects, including neurobehavioral alterations and reproductive dysfunction. [20], [26] One of the most prominent cases is the acute toxicity of 6PPDq, which has been shown to cause rapid mortality in coho salmon [10], the same effect has been shown for rainbow trout. [11] It has also been shown to cause developmental toxicity in embryonic zebrafish.[34] Additionally, exposure to DPGs, BTRs, and BTHs has been associated with inflammatory responses and contact dermatitis.[9]

2.2 Pathways of TDC into Aquatic Systems

TDC can reach aquatic environments through multiple pathways, such as surface road runoff, stormwater drainage systems, effluents from WWTPs, and atmospheric deposition. [14] Urban areas are hotspots for TDC emissions due to higher traffic and road infrastructure density, which increases the generation and accumulation of TWP and associated additives. [35]

One of the important pathways by which TDC enter surface waters is stormwater and surface runoff. TWP and associated TDC accumulate on road surfaces and are mobilized during precipitation events, after which they are transported directly into nearby surface waters or urban sewer systems. [14]

In Europe, approximately 75% of all sewer systems are combined sewer systems [36], in which domestic and industrial wastewater, as well as stormwater, are collected in the same pipelines. This is also the case in Vienna. [19], [37] Under “normal” conditions, the collected water is

transported to WWTPs and discharged into surface waters after treatment. During heavy storm events, the capacity of combined sewer systems can be exceeded, resulting in combined sewer overflows (CSOs). This results in the direct discharge of untreated wastewater, including stormwater-derived TDC, into surface waters and can lead to elevated concentrations during and after rain events in the surrounding surface waters. It therefore represents an important pathway for TDC input into urban aquatic systems. [38], [39] 6PPDq, HMMM, DPG, 2-Me BTH have been reported in CSO discharges. [40] 6PPDq has been detected in CSO with concentrations around 242 ng/L. [41] In the context of the present study, CSO events may contribute to temporal peaks in TDC concentrations, since combined sewer systems dominate the drainage structure in Vienna.

WWTPs are points on pathways for TDC to enter the environment, discharging treated effluent into receiving surface waters. Vienna is served by a single municipal WWTP located in Simmering in the south of the city, which discharges the treated effluent into the Danube Channel. The WWTP has a treatment capacity equivalent to 4 million inhabitants (EW_{60}). [42] Another WWTPs in this study includes WWTP Klosterneuburg, which has a treatment capacity equivalent to 55000 inhabitants (EW_{60}) and discharges into the Danube [43] and WWTP Breitenfurt-Laab has a treatment capacity equivalent to 12000 inhabitants (EW_{60}) and discharges into Liesingbach. [44] All three WWTPs are two-stage municipal mechanical-biological WWTPs, which includes mechanical pre-treatment, followed by two-stage biological treatment. [42], [43]

Depending on physicochemical properties of the TDC and the treatment technologies of WWTP, removal efficiencies and transformation processes in WWTP may vary. Consequently, WWTPs can act as sources or sinks of TDC, as some compounds can be efficiently removed, while others persist or are formed from precursor substances. [9]

A study conducted in China investigated the removal efficiency of PPDs and their quinones (PPDqs) at two WWTPs, both are secondary WWTPs, using sequencing batch reactor (Plant A) and anaerobic/anoxic/oxic tanks (Plant B). 6PPD was removed at a rate of around 95%, DPPD of around 80% IPPDq of around 55% in both plants. 6PPDq showed rates of approximately 70% in plant A and 85% in plant B and IPPD had removal efficiency of approximately 70% in Plant A and 100% in Plant B, indicating, that the removal strongly depends on the type of treatment used in the WWTPs. [32]

Removal efficiencies of selected organic compounds, including TDC, in wastewater treatment plants were also assessed during the Joint Danube Survey 4. Comparing influent and effluent concentrations, the removal rates of 2-OH BTH exceeded 80 %. In contrast, the removal of 5-Me BTR was negative, meaning that effluent concentrations exceeded influent concentrations. This

observation may indicate formation of the compound in the WWTP or transformation of precursor substances. [45]

A study from the United States further demonstrated large variability in WWTP removal efficiencies for tire- and plastic-related additives by measuring removal rates in one WWTP comparing those to efficiencies measured in other studies. The WWTP has a treatment capacity equivalent to 75000 inhabitants and uses activated-sludge treatment, including aeration tanks and biological processes. Average removal efficiencies of 54.1% for 6PPD and 57.8% for 6PPDq were calculated. An increase of the removal efficiencies of 6PPD and 6PPDq after the secondary treatment was observed and attributed to transformation processes occurring during activated sludge treatment, although the specific transformation pathways were not further resolved. DPG and DTG showed removal efficiencies of 0.4 and 3.0% after primary treatment, which decreased to -30 and -10% respectively, after the secondary treatment. [9]

To indicate the contribution of WWTP pathways to the total TDC concentrations, and to assess whether effluent was captured directly by the grab samples or still contributes to downstream samples, electrical conductivity can be used as a general indicator, or a suitable chemical marker can be applied.

Chemical tracers can be used as indicators of wastewater influence. Carbamazepine is particularly suitable for this purpose, as it is continuously emitted from WWTPs and is highly persistent in aquatic environments. In contrast to TDC, whose concentrations are additionally affected by traffic-related emissions and runoff processes, carbamazepine concentrations are expected to remain comparatively stable over time. Consequently, investigating carbamazepine concentrations can help distinguish wastewater-related inputs from other urban sources and will therefore be used in this study. [46]

The atmospheric deposition of TWP represents an additional pathway for TDC to reach soil and water and thereby contaminating the environment. [14], [47] About 10% of freshly generated TWP become airborne and are transported through air before settling in water or soil. [47] Although atmospheric deposition is not the primary pathway for TDC to reach the environment, it contributes to the background concentrations of TDC, especially in urban areas with high road and traffic density. [47]

2.3 Environmental Behavior and Fate of TDC in Aquatic Systems

The environmental behavior and fate of TDC in aquatic systems depend on a combination of physicochemical properties and environmental conditions. One of the key factors influencing the environmental behavior of TDC is their partitioning between dissolved, particulate, and sediment

phases, which is influenced by hydrophobicity, often expressed as the n-octanol-water partition coefficient ($logK_{ow}$). [48], [49] The selected compounds represent a diverse group, regarding the physicochemical properties. Based on the $logK_{ow}$ in Tab. 1, these compounds can be broadly divided into three groups regarding their environmental behavior in a river system. More hydrophobic compounds with higher $logK_{ow}$ ($logK_{ow} > 3$) tend to sorb to sediment and organic matter. This includes the compounds IPPD, 6PPD, CPPD, and DPPD and their respective transformation products (IPPDq, 6PPDq, CPPDq, and DPPDq), as well as compounds such as Neozone, AO2246, HMMM, CBS, and DTG. [48], [49] Compounds with $logK_{ow} \approx 2–3$ are moderate hydrophilic and may be distributed between both dissolved and particulate phases depending on environmental conditions. This includes the compounds BTH, 2-amino BTH, 2-Me BTH, 2-S BTH, 2-OH BTH, DPG, and DPTU. [50] Compounds with lower $logK_{ow}$ ($logK_{ow} < 2$) are hydrophilic and tend to stay in the dissolved phase. This includes the compounds 5-Me BTR, PPD, Aniline, and HMMM. [51], [52] This compound-specific behavior highlights the importance of investigating both dissolved and particulate phases when assessing the occurrence and fate of TDC in aquatic systems.

To evaluate the distribution behavior of the analyzed TDC in water and SPM, the water-SPM distribution coefficient K_D (L/kg) can be calculated with the following equation [49]:

$$K_D = \frac{C_{SPM}}{C_W}$$

where C_W is the concentration of the TDC in water and C_{SPM} is the concentration of the TDC in SPM.

Lower $log(K_D)$ values suggest that compounds are predominantly present in the dissolved phase and are therefore more mobile within the river system. In contrast, higher $log(K_D)$ values indicate a stronger association with suspended particulate matter and a higher potential for sedimentation and particle-bound transport. [49] The K_D is therefore an important factor for understanding the environmental fate and transport of TDC. However, environmental conditions such as organic carbon content, flow conditions, and particle composition can further influence the distribution behavior. Additionally, a combination of compound-specific properties, such as the K_{ow}, biodegradation rate, and molecular weight have an influence. [49]

In addition to partitioning, the fate of pollutants is influenced by transport processes that govern mixing and dispersion within the river system. These processes depend on factors such as junction angle, momentum flux ratio and channel geometry. [53] As well as by variations in environmental conditions such as pH, temperature, total suspended solids (TSS) and microbial community composition. [5], [8] In urban environments, transport processes such as stormwater runoff or CSO can lead to short-term increases in SPM and associated contaminants. [38], [54]

SPM is a highly dynamic phase in aquatic systems and influences the transport and fate of organic pollutants in rivers such as the Danube. Processes like deposition and resuspension influence the exchange of particle bound contaminants between water and sediments. Contaminants can accumulate in in sediments through deposition and therefore act as a sink. Hydrodynamic conditions mobilize sediments and SPM in rivers and remobilize these compounds, potentially releasing these compounds back into the water column. Hydrological events like heavy rainfall can further mobilize particle bound contaminants leading to higher contamination loads in the river. [55], [56]

In addition to partitioning, transformation processes play an important role in determining the environmental fate of TDC. They undergo these processes in the production process, in contact with the road surface or after they are released into WWTP or surface waters. [8], [20] PPDs are released into the environment, like surface waters and undergo rapid oxidative transformation, leading to the formation of quinone derivatives (PPDqs). A well-known example is the antioxidant 6PPD, which reacts with ozone or other oxidants to form the highly toxic 6PPDq. [26] Microbial transformation of TDC is especially relevant in WWTP but can result in higher concentrations of even more toxic transformation products. [32], [57]

2.4 Spatial and Temporal Distribution of TDC in River Systems

Previous studies have investigated the concentrations of TDC in surface waters, sediments, SPM and WWTP. Stormwater runoff has been identified as a major pathway for TDC entering surface waters. A study conducted in Australia demonstrated that concentrations of TDC in urban tributaries increased by up to a factor of 40 during stormwater events compared to baseflow conditions. Peak concentrations reached up to 248 ng/L HMMM, 1079 ng/L DPG, 88 ng/L 6PPDq, 449 ng/L 2-OH BTH, 274 ng/L 2-S BTH and 462 ng/L 5-Me BTR. [7]

Similarly, a comprehensive study from China investigated TDC in road runoff and surface waters of the Pearl River Delta. Significantly higher concentrations were observed in road runoff, reaching up to 9292 ng/L for 2-OH BTH, 15430 ng/L for BTH, 58780 ng/L for DPG. In contrast, PPDs like DPPD (0.11 ng/L), IPPD (0.8 ng/L), CPPD (1.10 ng/L) and 6PPD (3.06 ng/L) showed comparatively low concentrations. In surface waters, TDC were detected in a range from <LOD to 1993 ng/L, while 2-OH BTH (1993 ng/L) and DPG (1894 ng/L) showed the highest concentrations and BTH (502 ng/L) and 2-S BTH (422 ng/L) were present at lower levels with PPD concentrations occurring at the lowest (0.03–1.29 ng/L). [20]

The Joint Danube Survey 4 analyzed microplastic content in Danube River Basin and identified tire-related polymers such as SBR, highlighting the impact of urban runoff and traffic emissions

on river systems. Despite their widespread occurrence, no consistent longitudinal trends were observed, suggesting that the distribution of traffic-related pollutants is primarily controlled by local inputs rather than large-scale river processes. Additionally, several TDC have been investigated in surface waters and eleven different WWTP, including analyses of influent and effluent concentrations as well as removal efficiencies. 2-OH BTH has been efficiently removed (removal rate ≥80 %), with concentration ranges of 11-267 ng/L in influent and 7.7-21 ng/L in effluent samples. While 5-Me BTR has been poorly removed, with concentration ranges of 34-4930 ng/L in influent and 18-3123 ng/L in effluent samples. 5-Me BTR has also been detected in surface water samples with average concentrations of 145 ng/L, and 2-amino BTH with average concentrations of 3.7 ng/L. [6]

These findings highlight the importance of both spatial and temporal variability, as well as localized emission sources, in controlling the occurrence and distribution of TDC in river systems such as the Danube. Nevertheless, the combined assessment of spatial patterns, phase distribution, and urban input pathways remains limited, demonstrating the need for integrated studies to better understand the environmental behavior of TDC in complex urban river systems.

2.5 Sampling Strategies and Mass Load

Grab sampling is one of the most common methods for chemical monitoring, primarily used for targeted sampling and the collection of point data. [58] A significant advantage of this method is that it allows the collection of both the dissolved and particle-associated fractions, which is specifically important for the compounds of interest in this study. The mass load can be directly calculated by coupling the concentration with the discharge, and the method is cost-effective, with minimal field installation. The primary disadvantage is that compound concentrations can vary strongly in time and space, since surface waters like rivers are variable. Grab samples might not represent the true chemical quality of the water body as compounds are not always equally distributed and grab samples might capture peaks and lows. [58], [59]

In contrast, passive samplers collect water samples and environmental data over a defined period, providing time-weighted average concentrations. This method smooths short-term fluctuations but primarily only monitors the dissolved fraction.[58] Additionally, no single membrane or sorbent is capable of retaining all relevant TDC investigated in this study, which may limit the detection of certain compounds [60] and SPM can potentially create a barrier and host biodegradation of the additives.[61]

For this study, grab sampling was selected as the sampling strategy, as it allows targeted collection of precipitation events and seasonal changes and was compatible with the available

sampling equipment. To ensure the collection of representative, well-mixed grab samples, sampling should be conducted in the main channel flow of the river, where the highest mass transport is expected. Dead zones, backwaters and eddies should be avoided. The grab sample should be obtained in the upper third of the river, typically at a depth of 10-20 cm, with the bottle opening against the flow. [59]

3 Aims and Hypotheses

Large-scale studies such as the Joint Danube Surveys [62] and SUNDANSE [63] investigate water, suspended particulate matter (SPM), and sediments for emerging pollutants, including TDC and microplastics, in the Danube. These studies provide a broad overview across the whole river basin but do not investigate urban-scale input pathways or temporal variability within major metropolitan areas such as Vienna. More detailed studies of TDC have been conducted in other regions like the Pearl River Delta in China, which investigated the occurrence of TDC in surface waters in 2015, with a focus on surface runoff and WWTP inputs. While this study highlights the importance of urban sources, due to their large spatial scale, it does not investigate short-term temporal variability. [20] In contrast, a study in Australia studied the influence of stormwater events on TWP and TDC in Cubberla Creek near Brisbane in 2020. Although limited to a single sampling location, this study demonstrated elevated TWP and TDC concentrations associated with stormwater inputs, highlighting the relevance of rainfall-driven transport processes. [7]

To date, data on the occurrence and distribution of TDC in European urban river systems is lacking, especially considering different urban input pathways such as direct road runoff, wastewater effluents, and tributary inflows, together with short-term temporal variability. To address this knowledge gap, we conducted a sampling campaign in the Vienna section of the Danube and two of its tributaries, the Wienfluss and Liesingbach. By quantifying the concentrations of selected TDC in water, SPM, and sediments, this study aims to assess the spatial and temporal distribution and pathways of these compounds in an urban river system. Sampling sites were selected to represent different types of urban influence, including upstream and downstream sites, as well as locations influenced by road runoff and WWTP effluents. Repeated sampling across different hydrological conditions allows the investigation of short-term temporal variability, since one of the important pathways by which TDC enter surface waters is stormwater and surface runoff. [7] These insights improve the understanding of TDC inputs into urban surface waters and provide an essential foundation for future monitoring efforts and the development of effective mitigation strategies.

It is hypothesized that the tributaries Wienfluss and Liesingbach as well as WWTP effluents contribute significantly to TDC concentrations and loads in the Danube, due to direct road runoff and limited dilution [7], [39], [53], [64]. Consequently, TDC concentrations are expected to be higher downstream than upstream of Vienna, reflecting cumulative urban inputs. Furthermore, rainfall events are hypothesized to enhance the transport of road-derived contaminants, leading to increased TDC loads compared to dry-weather conditions. [7], [65] Finally, hydrophobic TDC are expected to exhibit a stronger association with suspended particulate matter than more hydrophilic TDC.

4 Materials and Methods

4.1 Chemicals, Standards and Preparations

Compound mixtures were prepared by weighing in pure compounds and dissolving them in Acetonitrile (ACN) (Fisher Scientific, LC-MS grade), which were subsequently combined to prepare a mixed compound stock solution. The list of all 25 compounds used can be found in Tab. 1. These stocks were then adjusted to a final concentration of 10 µg/mL in ACN and stored in the fridge at 4°C in a brown glass vial with Teflon septa.

An internal standard (INST) for the TDC quantification of 6PPDq-d5 and BTH-d4 was mixed with ACN, to achieve a 50 µg/mL concentration. The INST was stored in the fridge at 4°C.

A list of all CAS numbers and vendors of all used compounds and INST can be found in Appendix 1.

The glassware was cleaned in a dishwasher without detergent, rinsed three times with ultrapure water (MQ) (Purelab® Chorus 1, ELGA LAB Water, Veolia Water Technologies, Celle, Germany), and baked out in a muffle furnace at 550°C for 5 hours (Nabertherm N11/R with Programme Controller C19). All caps were soaked in water to remove organic residues, then rinsed three times with tap water and three times with MQ. PTFE septa caps were rinsed with acetone (Honeywell, Riedel-de-Haën™, Schwerte, Germany) and isopropanol (Merck, Darmstadt, Germany). The components of the solid-phase extraction (SPE) setup were soaked in isopropanol for 30 minutes and dried before use.

Tab. 1: List of compounds with abbreviations, full names, their molecular formula and logK_{ow} values

	Abbreviation	Compound Name	Molecular Formula	logK_{ow}
1	BTH	Benzothiazole	C_7H_5NS	2.17 [66]
2	2-amino BTH	2-aminobenzothiazole	$C_7H_6N_2S$	2.00 [66]
3	2-Me BTH	2-methylbenzothiazole	C_8H_7NS	2.72 [66]
4	2-S BTH	2-mercaptobenzothiazole	$C_7H_5NS_2$	1.83 [66]
5	2-OH BTH	2-hydroxybenzothiazole	C_7H_5NOS	2.35 [66]
6	5-Me BTR	5-methyl-1h-benzotriazole	$C_7H_7N_3$	1.13 [67]
7	PPD	p-Phenylenediamine	$C_6H_8N_2$	-0.3 [68]
8	IPPD	N-Isopropyl-N'-phenyl-p-phenylendiamin	$C_{15}H_{18}N_2$	3.28 [69]
9	IPPDq	2-[(1-Methylethyl)amino]-5-(phenylamino)-2,5-cyclohexadiene-1,4-dione	$C_{15}H_{16}N_2O_2$	2.58 [69]
10	6PPD	N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylenediamine	$C_{18}H_{24}N_2$	4.47 [69]
11	6PPDq	2-anilino-5-[(4-methylpentan-2-yl)amino]-cyclohexa-2,5-diene-1,4-dione	$C_{18}H_{22}N_2O_2$	3.98 [69]
12	CPPD	N-Cyclohexyl-N'-phenyl-p-phenylenediamine	$C_{18}H_{22}N_2$	4.64 [69]
13	CPPDq	2-(Cyclohexylamino)-5-(phenylamino)-2,5-cyclohexadiene-1,4-dione	$C_{18}H_{20}N_2O_2$	3.94 [69]
14	DPPD	N,N'-Diphenyl-p-phenylenediamine	$C_{18}H_{16}N_2$	4.93 [69]
15	DPPDq	2,5-bis(phenylamino)cyclohexa-2,5-diene-1,4-dione	$C_{18}H_{14}N_2O_2$	3.46 [69]
16	Aniline	Aniline	C_6H_7N	0.9 [68]
17	CBS	N-Cyclohexyl-2-benzothiazolesulfenamide	$C_{13}H_{16}N_2S_2$	3.47 [70]
18	DPG	1,3-Diphenylguanidine	$C_{13}H_{13}N_3$	2.89 [49]
19	DPTU	N,N'-Diphenylthiourea	$C_{13}H_{12}N_2S$	2.2 [68]
20	DTG	1,3-Di-o-tolylguanidine	$C_{15}H_{17}N_3$	3.1 [68]
21	HMMM	Hexa(methoxymethyl)melamine	$C_{15}H_{30}N_6O_6$	1.61[49]
22	Neozone	N-Phenyl-2-naphthylamine	$C_{16}H_{13}N$	5.1[68]
23	AO2246	2,2-Methylenebis(6-tert-butyl-4-methylphenol)	$C_{23}H_{32}O_2$	7.2 [68]
24	BHT	Butylated hydroxytoluene	$C_{15}H_{24}O$	5.3 [68]
25	BHA	Butylated hydroxyanisole	$C_{11}H_{16}O$	3.2 [68]

For the SPE the Waters 20-Position Cartridge Extraction Manifold was connected to a vacuum pump. The cartridges (Oasis HLB 6cc (200 mg) extraction cartridges (plastic) and Oasis HLB Glass 5cc (200 mg) extraction cartridge (glass)) were loaded by attaching a TFE Tubing with an inner diameter of 3.76 mm (Waters) on one side to the cartridges with a connection part and on the other side into the 1L bottle with the respective sample, as shown in Fig. 1. The solvents used for

the SPE were methanol (MeOH) (Fisher Scientific, LC-MS grade), ACN (Fisher Scientific, LC-MS grade), and Dichloromethane (DCM) (Fisher Scientific).

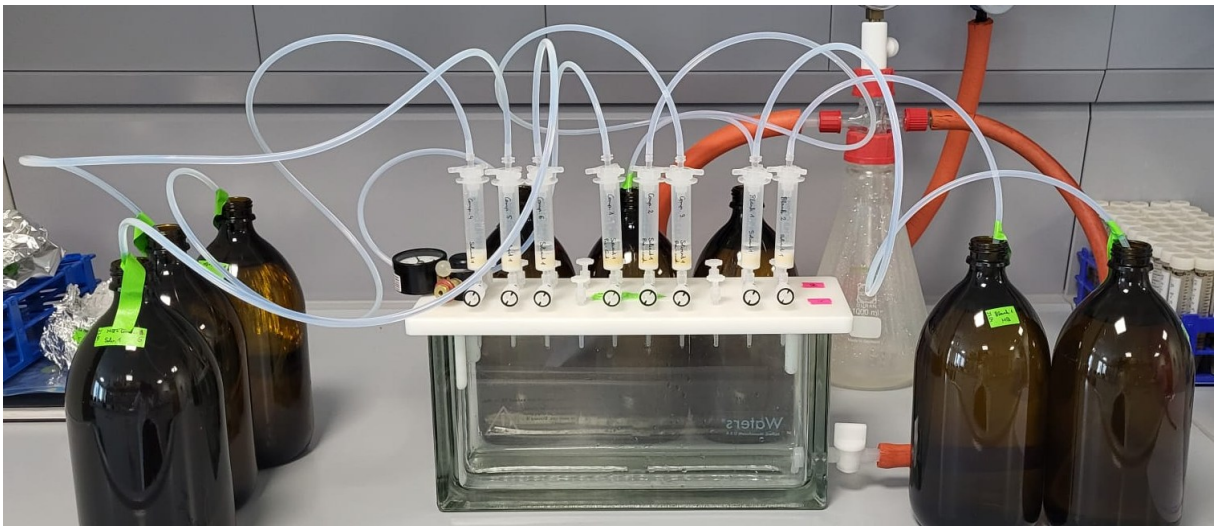

Fig. 1: SPE setup with tubing and plastic cartridges.

4.2 Recovery Experiment

The recovery test aimed to evaluate the efficiency of different solvents for eluting the target compounds from the SPE cartridges and to identify the optimal elution conditions for subsequent sample processing. This step was essential to ensure that the extraction method allows for reliable quantification of TDC in environmental water samples.

The basic setup already exists from the Individual Research Project where we developed a reliable method to analyze the presence of TDC and phthalates in Antarctic seawater samples. This method was adapted to make the laboratory process more efficient by adding plastic tubing to the system. Since no contamination was detected from the SPE cartridges or tubing, their use to enhance extraction efficiency was validated with a recovery test using both glass and plastic cartridges. With this setup, 16 samples could be processed simultaneously. This ensured that the field samples could be processed as quickly as possible, minimizing the potential degradation of the target compounds.

For the recovery tests, 1000 g of MQ water was weighed into amber glass bottles (1 L) and 100 µL of the mixed compound stock solution (C=10 µg/mL) was spiked into the MQ to achieve a concentration of 1000 ng/L. Triplicate blanks (MQ without compounds) were added to account for background contamination.

For the first round of recovery tests 13 samples with compounds and three blanks were prepared as listed in Tab. 2. The pre-conditioning of the cartridges was done with 5 mL of MeOH and 5 mL of MQ at a flow rate of approximately one drop per second. The target compounds were extracted

using 3 x 5 mL of MeOH, ACN or DCM at a flow rate of approximately one drop per second. For the second round of recovery tests, three samples containing compounds and three blanks were prepared (Tab. 2). The pre-conditioning of the cartridges was done as in recovery test 1. For the extraction of the compounds, 5 mL MeOH and 5 mL ACN were used at a flow rate of approximately one drop per second. The eluate was collected in 20 mL screw-cap vials for further processing. After the extraction, 20 µL of the INST (C=50 µg/mL) was spiked into the sample. A Barkey nitrogen evaporator was used to further concentrate the samples. This process concentrated the solvent with compounds to approximately 1 mL for subsequent analysis.

To ensure no particles enter the LC-MS/MS, 1 mL of each sample was filtered using 0.2 µm nylon syringe filters (Altmann Analytik, Munich, Germany) attached to 5 mL Luer lock plastic syringes (Fisher Scientific, Pittsburgh, USA). The first drop was discarded, to avoid contamination from the filters, and the remaining filtrate was transferred into 2 mL LC-MS/MS vials with PTFE septum. The vials were then stored in a fridge at 4°C until analysis.

Tab. 2: Summary of the recovery tests using different solvents and cartridges.

Samples	Pre-conditioning (yes/no)	Solvent	Cartridge material
Recovery Test 1			
3 blanks	no	ACN	plastic
3 spiked	yes	ACN	plastic
3 spiked	no	ACN	plastic
3 spiked	no	MeOH	Plastic
3 spiked	no	DCM	plastic
1 spiked	no	ACN	glass
Recovery Test 2			
3 blanks	yes	ACN + MeOH	plastic
3 spiked	yes	ACN + MeOH	plastic

4.3 Sampling and Locations

The sampling strategy was developed to ensure representative coverage of potential sources and transport pathways of TDC in the Danube River system in and around Vienna. Sampling focused on surface water to assess the occurrence and distribution of TDC in the dissolved and suspended phases. At each location, duplicate grab samples were collected, and field blanks were included to identify possible contamination during collection and sample processing.

4.3.1 Locations

To capture a gradient of potential TDC pathways, sampling sites were selected to represent both urban and rural influences, as well as direct inputs from WWTP effluents and stormwater discharges. In total, 15 sampling locations were chosen across the Danube River and its tributaries around Vienna. This approach allowed the assessment of spatial variations in TDC concentrations and provided insights into how different environmental and anthropogenic factors influence their distribution within the river system.

The locations of all samples are shown in Fig. 2 along with the sample numbers and full names in Tab. 3. At each location two samples were collected as duplicates, indicated by numbers 1 and 2.

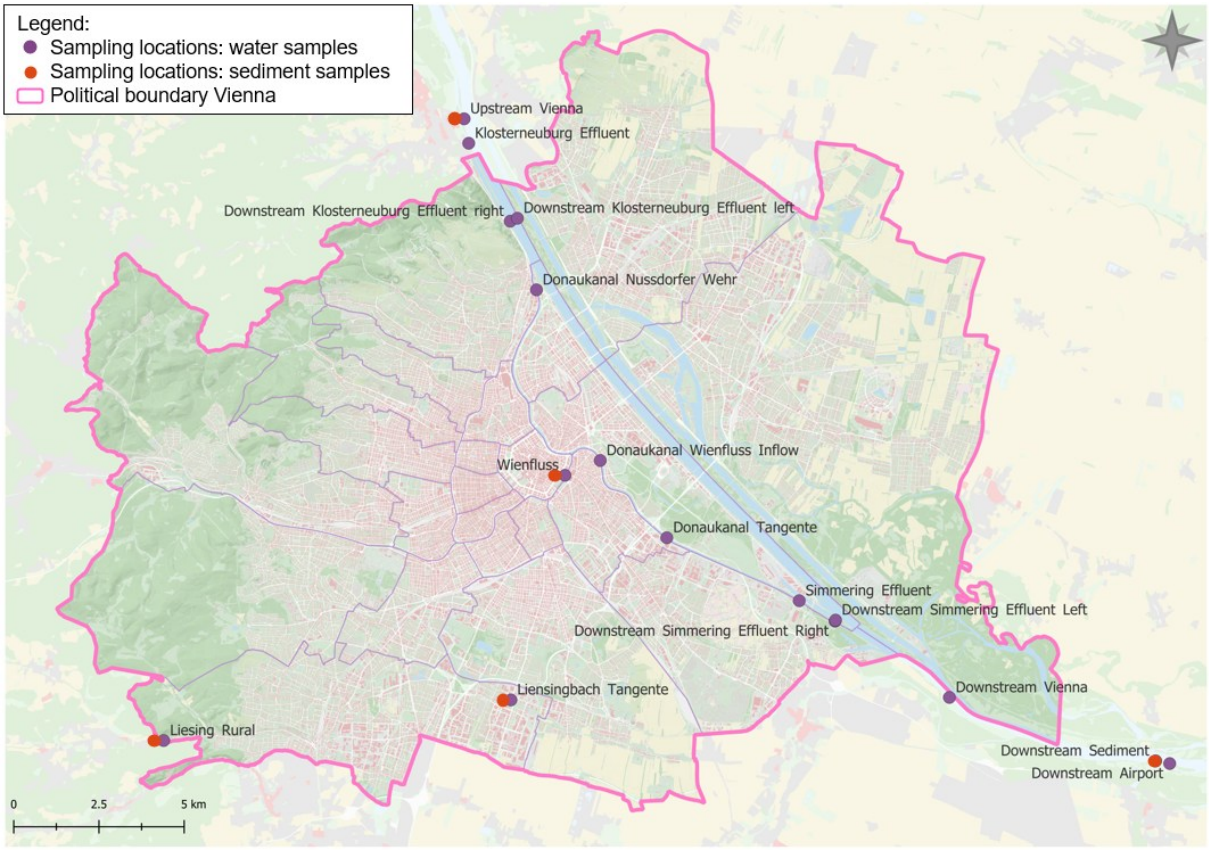

Fig. 2: Map of the sampling locations for water (purple) and sediment (red) samples in the Danube River, Danube Channel, Liesingbach, and Wienfluss. The political boundary of Vienna is marked in pink.

Tab. 3: Samples numbers and full location names. The numbers 1 and 2 indicate the duplicates.

No.	Sample Name	No.	Sample Name
1	Wienfluss 1	17	WWTP Simmering Downstream other 1
2	Wienfluss 2	18	WWTP Simmering Downstream other 2
3	Liesingbach Rural 1	19	Danube Upstream 1
4	Liesingbach Rural 2	20	Danube Upstream 2
5	Liesingbach Tangente 1	21	WWTP Klosterneuburg Effluent 1
6	Liesingbach Tangente 2	22	WWTP Klosterneuburg Effluent 2
7	Danube Channel Nussdorfer Wehr 1	23	WWTP Klosterneuburg Downstream 1
8	Danube Channel Nussdorfer Wehr 2	24	WWTP Klosterneuburg Downstream 2
9	Danube Channel Wienfluss Inflow 1	25	WWTP Klosterneuburg Downstream Other 1
10	Danube Channel Wienfluss Inflow 2	26	WWTP Klosterneuburg Downstream Other 2
11	Danube Channel Tangente 1	27	Danube Downstream 1
12	Danube Channel Tangente 2	28	Danube Downstream 2
13	WWTP Simmering Effluent 1	29	Danube Airport 1
14	WWTP Simmering Effluent 2	30	Danube Airport 2
15	WWTP Simmering Downstream 1	31	Field Blank (Danube upstream)
16	WWTP Simmering Downstream 2	32	Field Blank (Danube downstream)

One site was selected along the Wienfluss (Samples 1–2) near Stadtpark, just before it flows into the Danube Channel. Road runoff from streets near the river throughout the city is going into the Wienfluss [71], especially during rainfall. It is therefore expected to contribute elevated TDC loads to the Danube system.

The Liesingbach (Samples 3–6), a small stream about 30 km long originating in Lower Austria, flows through Vienna's 23rd and 10th districts before discharging into the River Schwechat, which ultimately enters the Danube. [72] Upstream samples (Samples 3-4) were collected near the border with Upper Austria to represent a background area with minimal urban impact. Downstream samples (Samples 5–6) were taken approximately one kilometer downstream of the "Südosttangente Wien A23" highway, one of Vienna's most heavily trafficked roads. [73]

In the Danube Channel several sampling sites (Samples 7-12) were selected. The first spot (Samples 7-8) at the Nußdorfer Wehr represents the upstream entry of the Danube Channel. There, the Danube River flows into the Danube Channel and can therefore be used as a reference point before the water passes through the whole city. To determine the input of TDC from the whole Wienfluss into the Danube, samples were taken to catch the inflow of the Wienfluss into the Channel (Samples 9-10). Another set of samples (Samples 11-12) was collected approx. 500m downstream of the "Südosttangente Wien A23" highway, which also crosses the Danube Channel. Throughout the entire Danube Channel, discharge points from Vienna's sewer and

drainage system release road runoff directly into the water. To determine the sampling points, we assessed the sewer network of Vienna via KANIS. [74]

Samples from the WWTP Simmering were taken directly at the effluent (Samples 13-14) and 1 km downstream of the effluent (Samples 15-16), as well as on the same height as the downstream sample but on the other side of the river (Samples 17-18). To determine the mixing of the effluent into the river water and its influence on downstream concentrations, samples were taken both on the side of the WWTP discharge and on the opposite side to assess whether complete mixing had occurred.

The upstream Danube River samples (Samples 19-20) were collected right before the Vienna border, since the Danube River already splits up into the Neue Danube right after the border. These samples therefore be used as a reference point before the water passes through the whole city. Samples from WWTP Klosterneuburg include the effluent (Samples 21-22) and downstream on both river sides (Samples 23-26) to assess the influence of a smaller WWTP discharging into the Danube River.

Downstream of Vienna, one location was selected (Samples 27-28) to determine the total influence of the city and the tributaries. The Danube Airport sites (Samples 29-30) were sampled to determine the potential input of the runoff from runways and paved surfaces of Vienna International Airport “Flughafen Wien-Schwechat" into the Danube River. According to the airport’s drainage concept, some of the rainwater collected on the runways are discharged directly into the river. [75]

The distance of the sampling sites downstream of the WWTPs (Simmering and Klosterneuburg) and the inflow of the Wienfluss was determined based on the Consolidated Federal Law on the Quality Objectives Ordinance Chemistry Surface Waters (QZV Chemie OG). According to §4, subsection 4, “In the case of wastewater discharges, the environmental quality standards must be complied with within the mixing zone at a certain distance downstream of the discharge. This distance should generally be ten times the width of the waterbody at the point of discharge, but in any case should be at least one kilometer” (translated from German).[76] Based on this regulation, samples 9 and 10 were collected one kilometer downstream of the Wienfluss inflow, as the channel width at this point is approximately 60m, ten times this width would correspond to 0.6km, which is below the minimum distance required. The same reasoning applies to samples 15 and 16, taken downstream of the WWTP Simmering effluent. Here, the channel width is approximately 47 m, corresponding to 0.47 km, and thus the distance was set to 1 km downstream in compliance with the regulation. Samples 23 and 24 were collected at 2.8 km downstream of the WWTP Klosterneuburg effluent. The width of the Danube River measures

approx. 280 m, ten times this width corresponds to 2.8 km. The widths of the rivers at the respective locations were determined with the “Distance Measurement Tool” of Google Maps. [77]

Two field blanks (Samples 31–32) were collected, one upstream and one downstream of Vienna, to account for potential contamination during sampling and handling.

4.3.2 Time period

Sampling campaigns were planned to include both dry-weather conditions and periods following rainfall, allowing the assessment of stormwater-related TDC inputs. The time periods of the sampling campaigns were determined based on both hydrological and logistical factors. According to precipitation data in Vienna from the years 2019 to 2025, the months with the highest mean monthly precipitation (in mm) (excluding November to May due to logistics), are June August, and September, and the months with the most days with rainfall are June, July, and Oktober. [78] This is consistent with the climatological monthly means for the period 1991–2020 from GeoSphere Austria [79] where the months with the highest precipitation values (in mm) are June, July, and August. Based on these datasets, we decided to sample in June, July, and September/October 2025. To have approximately six to eight weeks in between the sampling campaigns. One additional sampling in December 2026 was later added, to assess the seasonal variability.

All data about the sample coordinates, sampling date and time can be found in Appendix 2.

4.4 Sampling and River Data

The first set of samples was collected from June 3rd to 5th, 2025. Samples 1–6 were taken on the first day, 19–30 on the second day, and 7–18 on the third day. The second set of samples was collected on July 16th and 17th, 2025. During this campaign, samples 7–30 were taken on the first day, and samples 1–6 on the second day. The third set of samples was collected on September 30th and October 1st, 2025. As in the previous campaign, samples 7–30 were taken on the first day, and samples 1–6 on the second day. The fourth sampling set was collected on December 2nd (samples 9–28) and samples 1–6 on December 3rd. For this last sampling campaign, the sampling points 7 and 8 and 29 and 30 were excluded, to keep the route as short as possible in cold weather conditions. The exclusion of these sampling points was based on previously collected data, indicating that TDC concentrations at these locations did not differ significantly from nearby sampling sites.

Only one upstream field blank (sample 31) was collected during the first sampling campaign. For all other sampling campaigns, field blanks were collected upstream (sample 31) and downstream (sample 32) of the Danube.

After visiting the potential sampling location in person, it was clear that not all sites were accessible by foot, particularly those situated in the middle of the Danube River, where samples from the well-mixed main flow were desired.

For sampling in the Danube River and Danube Channel, kayaks were used to access the designated locations. As soon as we reached one location, we stopped paddling, rinsed a 1 L glass bottle once with river water, then filled it up completely at approx. 20 cm below the surface with the bottle opening against the flow and closed it securely. The duplicate sample was collected immediately afterward in the same manner. During sampling, the kayak drifted freely with the river flow. This means that the duplicate was taken a few meters downstream from the first sample. Sampling the effluent of the WWTP Klosterneuburg (samples 21 and 22) was not always possible. The effluent pipe is located below the water surface and is only visible when the water level is low, such as during sampling campaign 2 (h_2 = 245 cm), sampling campaign 3 (h_3 = 220 cm), and sampling campign4 (h_4 = 228 cm). During sampling campaign 1, when the water level was higher (h_1 = 347 cm), the outlet was not visible. [80]

For sampling at the Liesingbach and Wienfluss, the rivers were accessible by foot with wading suits. At each site, we stepped into the middle of the stream. A 1 L glass bottle was rinsed once with river water before being filled completely, securely closed and labeled. For the field blanks, clean bottles were filled with 1L of MQ at the respective locations.

The sediment samples have been collected in five locations, namely Wienfluss, Liesingbach Tangente, Liesingbach rural, Danube upstream and Sediment downstream. The samples were collected with a TeleScoop Water Sampler and transferred into 100 mL amber glass bottles.

To measure flow velocity in the Liesingbach and Wienfluss, the OTT C31 Universal Current Meter for discharge measurements was used. For the Danube River and the Danube Channel, however, measurements with this device were not feasible, as we wanted to determine the flow velocity directly at the sampling points. Since the samples from these sites were collected from kayaks that moved with the river current, the current meter, which requires a stationary position during measurement, could not be operated under these conditions. For this reason, the volume flow rate of the Danube River was determined with the “RiverApp” application. [81] It provides data from the Hydrographic Service of Lower Austria (Hydrographischer Dienst Niederösterreich) at different locations of the Danube River. The data we used is from Korneuburg, the nearest gauging station upstream of the Danube Upstream sampling sites. For the Danube Channel no data about

the flow velocity or volume flow rate was found. The water level of the Danube Channel at the Schwedenbrücke and of the Danube River at Korneuburg is provided by the Danube River Information Service (DORIS). [80] Data about water level, flow velocity and volume flow rate can be found in Appendix 5.

The precipitation data in Vienna were obtained from GeoSphere Austria [82], whose Data Hub is freely accessible by the public. For this study, the 24h sum precipitation data (mm) from four gauging stations (Schwedenplatz, Stammersdorf, Brunn am Gebirge, and Schwechat Flughafen) were analyzed. The selection of these stations was based on their proximity to the sampling locations and their spatial distribution to ensure representative coverage of the Vienna area. The focus was on precipitation occurring on the sampling dates and during the 30 days preceding each sampling event. Precipitation data can be found in Appendix 6.

4.5 Sample Processing

In the laboratory the pH and electric conductivity of all samples were measured (Appendix 3 and Appendix 4), and all samples were spiked with 200 µL of Sodium Azide (C = 250 mg/mL) to prevent bacterial growth. All samples were stored in the fridge at 4°C until processing.

All samples were filtered before the SPE. A vacuum filtration setup was used using a 0.2 µm Nylon membrane filter (Whatman, Buckinghamshire, UK) to remove particulate matter and allow to determine the concentration of compounds sorbed to particulate matter. The weight of the water was determined by weighing the empty sample bottles and then weighing them with the filtered water, which was poured back in. The empty bottles were rinsed three times with MQ before being filled again to ensure that all particulate matter was gone. The water samples were then processed using the same method as for recovery test 2 and measured on the LC-MS/MS. For all samples from the first sampling campaign a total of 20 µL of INST was spiked after the SPE like in the recovery tests. For the second and third sampling campaign, based on a recovery test from a previous campaign, a total of 60 µL was spiked before the SPE to correct for potential extraction losses and matrix effects during sample preparation.

After filtering the filters were transferred into 20 mL vials, which were weighed with the empty filters, then dried in the drying oven overnight at 60°C and then weighed with the full used dried filters to quantify the weight of the particulate matter. The weights of the water and SPM samples are provided in Appendix 7, together with the calculated TSS.

For each sample, the filters were spiked with 20 µL of INST. The filters were extracted once with 3 mL MeOH (LC-MS grade) in the ultrasonication bath for 15 min. Each filter extract was filtered through a 0.45 µm filter (Altmann Analytik, München, Germany) using a 5 mL plastic syringe into

a new 20 mL vial. The filters were extracted one more time with 3 mL ACN (LC-MS grade) in the ultra-sonication bath for 15 min and filtered to the respective vials already containing the MeOH. A new plastic syringe and pre-filter were used for each filter extract to avoid contamination. The filtered extracts were concentrated in the Nitrogen Barkey to 1 mL and transferred to 2 mL LC-MS/MS vials with PTFE septum. The concentrates were measured on the LC-MS/MS.

The sediment samples have been processed within another project and will therefore not be discussed in the method section.

4.6 Quantification and Data Evaluation

To determine the concentrations of the TDC, triple quadrupole LC-MS/MS was used. This system consists of an ultra-high performance liquid chromatograph (UHPLC) (Agilent Infinity 1290 II, Agilent Technologies, Santa Clara, USA) coupled with a 6470 LC/TQ triple quadrupole mass spectrometer (Agilent Technologies, Santa Clara, USA) operating in multiple reaction monitoring (MRM) mode. Separation was achieved using a C18 column (Acquity UPLC HSS T3, 1.8 µm, 100 mm, Waters). The liquid chromatography operated at a flow rate of 0.6 mL/min with the column maintained at a temperature of 40 °C. The mobile phase consisted of MQ (Phase A) and ACN (Phase B), both containing 0.1 % formic acid. The eluent gradient was set to the following: 0 min, 95 % of phase A and 5 % phase B, which switched to 5 % of phase A and 95% of phase B at 10 min, where it was held for 3 min until it went back to 95 % of phase A and 5 % of phase B at minute 13. The injection volume was set to 5 µL, and the autosampler operated with standard needle-wash conditions. To improve peak shape, needle mixing was enabled in the injector program. First, 4 µL of the sample is drawn, followed by a needle wash. The autosampler then adds 6 µL of MQ and performs another needle wash. The mixture is homogenized through five air-mixing cycles, after which 1 µL is discarded to remove any air. Finally, 5 µL of the homogenized solution are injected. The draw and eject speeds were both set to 50 µL/min, and vial bottom sensing was activated to ensure precise sampling. For quantification, a calibration curve with 8 standards (0.1 ng/mL – 1000 ng/mL in ACN) for each compound of interest with 20 µL of both INSTs (50 µg/mL) was used to calculate the different amounts of TDC in each sample. We evaluate the data using MassHunter Quantitative Analysis software (Agilent Technologies, Santa Clara, USA). Peak integration was performed automatically and manually inspected where necessary.

The limit of detection (LOD) and limit of quantification (LOQ) of the method were determined using the residual standard deviation of the calibration curve for the samples (Tab. 4). Concentrations below the LOD were treated as non-detects and excluded from further evaluation.

It should be noted that the analytical uncertainty differs between compounds due to variations in recovery rates and method sensitivity. Compounds with low recoveries may be underestimated, whereas compounds with high LODs and LOQs, such as PPD, IPPDq, and DPPDq may remain undetected even when present at environmentally relevant concentrations. Not detecting these compound does not necessarily mean that the compound is not present in the environment. These limitations should be considered when interpreting the results.

Tab. 4: LOD and LOQ in ng/L for all measured TDC.

Compound	**LOD (ng/L)**	**LOQ (ng/L)**
BTH	286.92	869.46
2-amino BTH	0.37	1.12
2-Me BTH	4.38	13.26
2-S BTH	19.43	58.87
2-OH BTH	35.64	108.00
5-Me BTR	0.06	0.19
PPD	3997.40	12113.35
IPPD	0.86	2.61
IPPDq	895.72	2714.30
6PPD	4.71	14.28
6PPDq	45.13	136.75
CPPD	1.02	3.10
CPPDq	47.09	142.71
DPPD	13.24	40.12
DPPDq	462.37	1401.11
Aniline	16.92	51.28
CBS	0.34	1.04
DPG	0.17	0.51
DPTU	1.11	3.35
DTG	0.11	0.32
HMMM	1.02	3.08
Neozone	15.13	45.83
AO2246	1.00	3.03
BHT	not detected	not detected
BHA	not detected	not detected

5 Results and Discussion

5.1 Recovery Experiments

In the first set of experiments, extraction with ACN resulted in recoveries above 70% for 14 compounds when pre-conditioned cartridges were used, and for 11 compounds without pre-conditioning. (Appendix 8) Extraction with MeOH resulted in 13 compounds exceeding 70% recovery, while DCM achieved this threshold for 12 compounds. These results indicate that extraction efficiency is compound-specific and strongly dependent on the solvent used. The observed differences in extraction efficiency can be attributed to the varying polarity of the solvents and the physicochemical properties of the target compounds. MeOH, being a polar solvent, showed higher recoveries for more hydrophilic compounds such as DPG, DTG, and PPD, while the less polar solvent DCM was more effective for hydrophobic compounds such as IPPDq and DPPDq. ACN exhibited intermediate behavior, resulting in relatively balanced recoveries across a wide range of compounds. [68]

Pre-conditioning of the cartridges with MQ water improved the recovery of certain compounds, particularly 5-Me BTR (+11.08%), IPPD (+7.97%), CPPD (+7.97%), 6PPD (+7.47%), and IPPDq (+19.82%). Other compounds, such as AO2246, Neozone, 6PPDq, and CPPDq, showed improved recoveries of a few percent (<2%). Overall, the effect of pre-conditioning was compound-specific but generally beneficial as it activates the sorbent material and ideally lowers background contamination. (Appendix 8)

A comparison between glass and plastic SPE cartridges showed similar performance. Using ACN as the extraction solvent, 11 compounds achieved recoveries above 70% for both cartridge types. Slight differences were observed for individual compounds, such as higher recovery of AO2246 and lower recovery of IPPD in glass cartridges. Due to the more complex handling of glass cartridges (e.g., incompatibility with plastic tubing), plastic cartridges were selected for all subsequent experiments. The results of the recovery rates of the first recovery test can be found in Appendix 8.

Based on these findings, a second recovery experiment was conducted using a combined extraction with MeOH followed by ACN. The results are summarized in Tab. 5. This method improved overall performance, with 18 compounds showing recoveries above 70%, ranging from 70% to 138%. The improved recoveries suggest that the combined use of solvents with different polarities enhances the extraction of compounds with diverse physicochemical properties.

Recoveries exceeding 100% were observed for some compounds, which may indicate matrix effects or analytical variability leading to signal enhancement. For this study, recovery rates between 70-120% were considered acceptable, as this threshold is commonly applied in environmental analysis to ensure reliable quantification. [83]

A few compounds consistently showed lower recoveries, including CPPD (59.36%), 6PPD (65.41%), and Aniline (44.11%), even with the optimized method. DPTU with 0.00% and 2-S BTH with 9.37% could not be reliably recovered in any of the experiments. Possible explanations could be strong sorption to the cartridges or insufficient elution during extraction. It should be noted that DPTU was nevertheless detected in a few water and sediment samples. This may indicate that the concentration used in the recovery experiments was too low to allow reliable quantification. Therefore, the reported concentrations of DPTU should be interpreted with caution.

The calibration for BHT and BHA was unsuccessful, preventing their quantification under the applied conditions.

2-amino BTH and DPG exhibited recoveries significantly above 100%, with recovery rates of 460.73% and 202.99%, respectively. Such elevated recoveries indicate potential matrix effects or background contamination [84] and suggest that quantification for these compounds should be interpreted with caution.

Overall, the combined MeOH and ACN extraction with pre-conditioned plastic cartridges was selected as the best method for field sample analysis, as it provided the best compromise between recovery efficiency and practical handling.

Based on these findings, 23 out of the 25 target compounds were considered for further analysis, while BHA and BHT were excluded due to unsuccessful calibration.

Tab. 5: Measured recovery rates (%) and standard deviation (%) of all compounds of the second recovery test.

Compound	Recovery (%)	Standard Deviation (%)
BTH	133.56	7.37
2-amino BTH	460.73	18.14
2-Me BTH	114.42	3.81
2-S BTH	9.37	1.86
2-OH BTH	103.33	5.82
5-Me BTH	100.53	4.31
PPD	95.72	1.63
IPPD	111.28	3.34
IPPDq	76.47	2.42
6PPD	65.41	3.35
6PPDq	83.38	1.24
CPPD	59.36	3.91
CPPDq	81.95	0.36
DPPD	81.41	2.18
DPPDq	70.15	1.9
Aniline	44.11	1.72
CBS	98.18	5.27
DPG	202.99	9.26
DPTU	0.00	0.00
DTG	138.52	5.73
HMMM	118.92	5.33
Neozone	80.88	1.77
AO2246	83.66	4.33
BHA	0.00	0.00
BHT	0.00	0.00

5.2 Widespread Occurrence of TDC throughout the Vienna River System

Overall, TDC have been detected in all samples at all sites in all sampling campaigns. This indicates continuous TDC input throughout the Vienna river system.

5.2.1 Water Samples are Dominated by a Small Number of Frequently Detected TDC

The sum concentrations of all analyzed compounds in the water samples varied across locations and sampling campaigns. The total concentrations of all measured TDC in individual locations range from 15.03 ng/L to 64572.99 ng/L. (Appendix 10)

Out of the 23 compounds, 16 were detected in at least one sample. The most frequently detected compounds are 5-Me BTR, DPG, 2-amino BTH, HMMM, AO2246, and 2-OH BTH, which were found in all four sampling campaigns. All these compounds were also detected in 100% of the samples in at least one campaign, except for 2-OH BTH, with detection frequencies of <15% in all four sampling campaigns. Aniline and DTG were detected in three out of four sampling campaigns with detection frequencies between 13.33% and 73.33%. The compounds BTH and 6PPD have only been detected in singular locations, but always in both duplicates. DPTU, IPPD, 2-Me BTH, 2-S BTH, CPPD, and CBS were only detected in singular grab samples in singular locations. The low recovery of 2-S BTH (9.37%) may have contributed to its low detection frequency and could result in an underestimation of its environmental occurrence. The compounds PPD, IPPDq, DPPDq, CPPDq, 6PPDq, DPPD, and Neozone have not been detected in any samples. It should be noted that the high LOD of PPD, IPPDq, and DPPDq could be a reason for not detecting any concentrations in the sample, which does not necessarily mean that they are not present in any of the samples.

During sampling campaign 1, total concentrations of all compounds ranged from 71.14 ng/L in "Danube Channel Nussdorfer Wehr" up to 2445.98 ng/L at "Wienfluss". In sampling campaign 2, concentrations ranged from 15.03 ng/L at "WWTP Klosterneuburg Downstream Other" up to 343.91 ng/L at "WWTP Simmering Effluent". In sampling campaign 3, the total detected concentrations ranged from 96.64 ng/L at "Danube Downstream" up to 1396.31 ng/L at "WWTP Klosterneuburg effluent". For sampling campaign 4, concentrations ranged from 48.24 ng/L at "Danube Airport" up to 64572.99 ng/L at "Danube Downstream".

Detection frequencies (%), concentration ranges (ng/L), and mean concentrations (ng/L) for all compounds across all samples (n = 30) are summarized in Tab. 6.

Tab. 6: Detection frequencies (%), concentration ranges (ng/L), and mean concentrations (ng/L) of all analyzed compounds in water samples (n = 30) across all sampling locations and campaigns. "–" indicates concentrations below the LOD. Compounds are grouped by detection frequency (dark green = detected in all four sampling campaigns, medium green = detected in three campaigns, light green = detected in only a few samples) and are additionally ranked from highest to lowest overall detection frequency (sum across all four sampling campaigns).

Water	Frequency (%)				Range (ng/L)				Mean (ng/L)			
Compounds	**1**	**2**	**3**	**4**	**1**	**2**	**3**	**4**	**1**	**2**	**3**	**4**
5-Me BTR	100.00	100.00	96.67	95.83	6.70-309.20	3.48-178.71	21.18-885.42	3.20-55067.22	55.88	25.83	164.77	9343.97
DPG	100.00	100.00	96.67	79.17	19.31-436.22	2.16-134.40	11.69-170.4	11.57-2487.85	111.89	13.25	37.48	648.44
2-amino BTH	100.00	40.00	96.67	54.17	1.89-56.71	0.42-4.06	0.58-27.44	22.8-819.56	10.72	1.84	3.14	261.95
HMMM	100.00	6.67	96.67	87.50	17.88-554.47	1.16-1.77	7.95-110.59	6.28-35585.50	140.60	1.46	35.70	5721.17
AO2246	20.00	100.00	66.67	4.17	10.43-60.98	1.18-15.08	1.36-25.64	-	27.36	5.18	12.64	71.57
2-OH BTH	6.67	3.33	13.33	4.17	113.11-139.98	-	45.11-521.13	-	126.54	39.69	175.63	4168.08
DTG	0.00	20.00	73.33	29.17	-	0.16-0.28	3.34-2.13	3.35-104.00	-	0.20	0.58	43.40
Aniline	33.33	30.00	13.33	0.00	99.67-930.39	17.47-83.15	34.46-56.70	-	342.89	45.01	46.23	-
BTH	20.00	0.00	0.00	0.00	340.55-791.47	-	-	-	591.32	-	-	-
DPTU	0.00	0.00	16.67	0.00	-	-	5.73-8.25	-	-	-	6.57	-
IPPD	0.00	10.00	0.00	0.00	-	7.75-9.08	-	-	-	8.26	-	-
2-Me BTH	0.00	3.33	3.33	0.00	-	-	-	-	-	4.42	32.71	-
6PPD	0.00	6.67	0.00	0.00	-	25.78-25.82	-	-	-	25.80	-	-
2-S BTH	0.00	0.00	3.33	0.00	-	-	-	-	-	-	280.53	-
CPPD	0.00	3.33	0.00	0.00	-	-	-	-	-	17.66	-	-
CBS	3.33	0.00	0.00	0.00	-	-	-	-	0.60	-	-	-

5.2.2 TDC Occurrence in SPM is Highly Variable

The sum concentrations of all analyzed TDC in SPM showed spatial and temporal variability across the sampling campaigns. Concentrations at individual sampling sites ranged from 1093.43 µg/kg to 607987.17 µg/kg. (Appendix 11)

Out of the 23 compounds, 16 were detected in at least one sample. The most frequently detected compounds were DPG, 5-Me BTR, AO2246, and 2-amino BTH, with detection frequencies consistently above 10% across all sampling campaigns and reaching up to 96.67%. No compounds were detected in all SPM samples. DTG, 2-Me BTH, Aniline, and 6PPD were detected in three out of four sampling campaigns, with detection frequencies ranging from 3.33% to 76.67%. The compounds PPD, 2-OH BTH, 6PPDq, IPPDq, HMMM, IPPD, 2-S BTH, and BTH were only detected in singular grab samples. The compounds CPPD, DPTU, DPPDq, CPPDq, DPPD, Neozone, and CBS were not detected in any samples.

Across the four sampling campaigns, substantial differences in total concentration were observed. In sampling campaign 1, total concentrations ranged from 1.09 µg/kg at "Danube Airport" up to 19277.36 µg/kg at "Liesingbach rural". During sampling campaign 2, concentrations ranged from 72.44 mg/kg at "Danube Channel Tangente" up to 1973222.50 µg/kg at "WWTP Simmering Effluent". In sampling campaign 3, the total detected concentrations ranged from 133.92 µg/kg at "Danube Channel Tangente" up to 947724.32 µg/kg at "WWTP Klosterneuburg Effluent". For sampling campaign 4, concentrations ranged from 1093.43 µg/kg at "Danube Downstream" up to 40104.74 µg/kg at "Danube Channel Tangente".

Detection frequencies (%), concentration ranges (µg/kg), and mean concentrations (µg/kg) for all compounds across all samples (n = 30) are summarized in Tab. 7.

Tab. 7: Detection frequencies (%), concentration ranges (µg/kg), and mean concentrations (µg/kg) of all analyzed compounds in SPM samples (n = 30) across all sampling locations and campaigns. "–" indicates concentrations below the LOD. Compounds are grouped by detection frequency (dark green = detected in all four sampling campaigns, medium green = detected in three campaigns, light green = detected in only a few samples) and are additionally ranked from highest to lowest overall detection frequency (sum across all four sampling campaigns).

SPM	Frequency (%)				Range (µg/kg)				Mean (µg/kg)			
Compound	**1**	**2**	**3**	**4**	**1**	**2**	**3**	**4**	**1**	**2**	**3**	**4**
DPG	36.67	93.33	73.33	95.83	1.85-148.08	0.16-17640.84	26.84-4478.62	7.92-4342.64	46.46	820.30	1042.05	997.72
5-Me BTR	10.00	10.00	96.67	95.83	2.68-33.69	0.21-11379.95	55.98-16365.47	17.46-13959.97	22.17	3797.78	1541.99	1105.20
AO2246	50.00	43.33	13.33	95.83	101.52-30577.46	3100.15-3849746.70	72139.62-1872372.61	138.36-42540.12	9005.70	309498.07	780660.21	11140.32
2-amino BTH	13.33	10.00	33.33	41.67	1.36-167.21	2.96-5362.86	5.94-750.91	6.37-52854.98	44.57	1956.92	162.39	8979.87
6PPD	10.00	6.67	73.33	0.00	1.05-192.26	5876.52-6779.70	26.84-4478.62	-	66.33	6328.11	1042.05	-
DTG	0.00	6.67	70.00	8.33	-	172.91-2154.40	1.52-3574.40	387.70-2061.83	-	1163.66	448.71	1224.76
2-Me BTH	76.67	3.33	3.33	0.00	0.92-30.53	-	-	-	8.92	191.09	1753.12	-
Aniline	26.67	36.67	10.34	0.00	44.78-1255.01	70.00-52781.77	2567.20-11294.17	-	433.32	8685.86	6045.51	-
PPD	0.00	30.00	0.00	0.00	-	251.57-4811.54	-	-	-	1979.57	-	-
2-OH BTH	0.00	20.00	6.67	0.00	-	535.39-17126.70	4828.36-6381.98	-	-	5987.07	5605.17	-
6PPDq	6.67	0.00	13.33	0.00	4.55-13.98	-	389.28-1484.48	-	9.27	-	712.73	-
IPPDq	10.00	0.00	0.00	0.00	1.05-192.26	-	-	-	66.33	-	-	-
HMMM	0.00	0.00	0.00	8.33	-	-	-	1122.20-1519.47	-	-	-	1320.83
IPPD	0.00	6.67	0.00	0.00	-	322.27-15811.65	-	-	-	8066.96	-	-
2-S BTH	0.00	0.00	0.00	4.17	-	-	-	-	-	-	-	54680.15
BTH	0.00	3.33	0.00	0.00	-	-	-	-	-	1942.67	-	-

It is important to note that the quantification of the investigated TDC in SPM is associated with considerable uncertainty due to the low mass of collected particles. The mass of SPM collected from approximately 1 L of water was generally low across all sampling campaigns. While water

masses were close to 1 kg per sample, particle masses typically ranged from approximately 20–230 mg in sampling campaign 1, 1–35 mg in sampling campaign 2, 1–14 mg in sampling campaign 3, and 1-150 mg in sampling campaign 4. This corresponds to TSS concentrations on the order of a few mg/L, indicating relatively low particle loads in the 1L samples analyzed. The low particle mass may contribute to increased variability and uncertainty in the calculated concentrations.

A detailed list of water and particle masses, as well as calculated TSS values, is provided in Appendix 7.

5.2.3 Sediments Act as a Sink for Hydrophobic TDC

Spatial and temporal variability was also observed in sediment samples across the five locations and sampling campaigns. The sum concentrations of all measured TDC at individual sites ranged from 0.62 µg/kg to 12405.96 µg/kg. (Appendix 12)

Out of the 23 compounds, 18 were detected in at least one sample. The most frequently detected compounds are 5-Me BTR and 6PPD, which were detected in all four sampling campaigns. 5-Me BTR showed detection frequencies reaching up to 100% in sampling campaigns 1, 3, and 4 and 6PPD was detected in 100% of the samples in sampling campaign 2. Several compounds, including AO2246, 2-amino BTH, DPG, 2-OH BTH, HMMM, 6PPDq, and Neozone were detected in three out of four sampling campaigns, with detection frequencies between 20% and 100%. Other compounds, such as DTG and DPPD, were detected in two sampling campaigns. IPPD, DPPDq, CPPD, DPTU, and 2-S BTH were detected in one sampling campaign, with detection frequencies also between 20% and 100%. The compounds PPD, BTH, 2-Me BTH, IPPDq, Aniline, CPPDq, and CBS were not detected in any samples.

The compounds DPPD, DPPDq, and Neozone were only detected in sediment samples. This is consistent with their high hydrophobicity ($\log K_{ow}$ values of 4.93, 3.46, and 5.1) (see Tab. 1), which promotes sorption to particulate matter and accumulation in sediments. CPPD and 6PPD were only detected in one singular water sample in sampling campaigns 1 and 2, respectively, also showing higher $\log K_{ow}$ values of 4.64 and 4.47. (see Tab. 1), further supporting their preferential association with solid phases. The results indicate that sediments act as an important sink for hydrophobic TDC, reflecting accumulation processes and particle-associated transport. Compared to the water phase, the broader detection of compounds in sediments suggests reduced mobility but increased persistence in this environmental compartment.

Detection frequencies (%), concentration ranges (µg/kg), and mean concentrations (µg/kg) for all compounds across all samples (n = 5) are summarized in Tab. 8.

Tab. 8: Detection frequencies (%), concentration ranges (µg/kg), and mean concentrations (µg/kg) of all analyzed compounds in sediment samples (n = 5) across all sampling locations and campaigns. "–" indicates concentrations below the LOD. Compounds are grouped by detection frequency (dark green = detected in all four sampling campaigns, medium green = detected in three campaigns, light green = detected in only a few samples) and are additionally ranked from highest to lowest overall detection frequency (sum across all four sampling campaigns).

Sediment	Frequency (%)				Range (µg/kg)				Mean (µg/kg)			
Compound	**1**	**2**	**3**	**4**	**1**	**2**	**3**	**4**	**1**	**2**	**3**	**4**
5-Me BTR	100.00	40.00	100.00	100.00	3.95-5.72	0.17-1.50	2.14-57.15	2.54-9.38	4.96	0.84	15.45	5.66
6PPD	33.33	100.00	60.00	80.00	-	0.27-15.52	0.40-7.57	2.16-14.04	0.49	4.49	3.38	5.87
AO2246	66.67	0.00	100.00	80.00	434.36-1254.07	-	303.42-12063.52	3.62-4.53	844.22	-	2792.44	4.00
2-amino BTH	66.67	60.00	100.00	0.00	0.39-1.73	0.03-0.34	8.72-213.06	-	1.06	0.24	52.92	-
DPG	0.00	20.00	100.00	80.00	-	-	1.42-45.94	1050.97-2115.56	-	6.44	19.07	1557.68
2-OH BTH	100.00	20.00	0.00	20.00	6.65-35.20	-	-	-	16.31	7.85	-	40.91
HMMM	33.33	40.00	0.00	40.00	-	2.06-2.67	-	3.10-3.69	1.33	2.36	-	3.39
6PPDq	33.33	60.00	0.00	20.00	-	0.85-12.21	-	-	3.26	5.48	-	0.92
Neozone	33.33	20.00	0.00	60.00	-	-	-	0.07-0.69	0.94	0.08	-	0.43
DTG	0.00	0.00	100.00	80.00	-	-	4.11-26.29	1.20-6.20	-	-	8.72	3.50
DPPD	33.33	80.00	0.00	0.00	-	0.36-5.29	-	-	6.10	1.79	-	-
IPPD	0.00	80.00	0.00	0.00	-	0.57-0.92	-	-	-	0.71	-	-
DPPDq	66.67	0.00	0.00	0.00	0.70-1-23	-	-	-	0.96	-	-	-
CPPD	0.00	40.00	0.00	0.00	-	0.59-0.60	-	-	-	0.59	-	-
DPTU	0.00	0.00	0.00	40.00	-	-	-	0.40-1.44	-	-	-	0.92
2-S BTH	0.00	0.00	0.00	20.00	-	-	-	-	-	-	-	183.28

Overall, 5-Me BTR is the most detected compound in all three phases, followed by AO2246, DPG, and 2-amino BTH. CPPDq is the only compound that has not been detected in any sample.

5.2.4 Dynamic Distribution of TDC between Dissolved and Particulate Phases

The log(K_D) values were calculated for all compounds for which concentrations in both the dissolved and particulate phases were available and can be found in Appendix 9.

The resulting log(K_D) values ranged from 0.73 to 8.56, indicating a broad variability in partitioning behavior among the investigated TDC. Considerable variability in log(K_D) values was observed both between sampling locations and campaigns for individual compounds. For example, logK_D values ranged from 2.07 to 6.25 for 2-amino BTH, 1.41-6.01 for DPG, 0.73-5.58 for 5-Me BTR, and 3.22-8.56 for AO2246. This wide range demonstrates that the phase distribution of these compounds is not constant but influenced by changing environmental conditions. [5] It should be noted that the observed range in log(K_D) values is relatively large. However, these values represent

all four sampling campaigns combined. When individual sampling campaigns are considered separately, the variability is substantially smaller. For example, log(K_D) values for DPG ranged from 1.41 to 2.65 during sampling campaign 1 and from 3.10 to 6.01 during sampling campaign 2. This suggests that temporal changes in environmental conditions contribute considerably to the overall variability. Similar observations have been reported previously, where lower log(K_D) values for DPG, 2-OH BTH, DPPD, and 6PPDq during the wet season compared to the dry season, linking these shifts to changes in sources, environmental behavior, and hydrodynamic conditions. [49]

Overall, the observed variability in log(K_D) values indicates that partitioning of TDC in the investigated system is dynamic and governed by both compound-specific properties and environmental factors such as suspended solids concentration and hydrological conditions. This finding is consistent with the results from the water, SPM, and sediment analyses, which indicate that the distribution of TDC between dissolved and particulate phases varies considerably across compounds, sampling locations, and campaigns.

5.3 Spatial Distribution of TDC Reflects Urban Inputs

5.3.1 Tributaries and WWTP Effluents are TDC Hotspots in Water Samples

The highest sum concentrations were observed in WWTP effluents and urban tributaries. In sampling campaigns 1–3, concentrations in the WWTP effluents reached 13150.34 ng/L in Simmering and 1396.31 ng/L in Klosterneuburg. Urban tributaries also showed elevated concentrations up to 2445.98 ng/L in “Wienfluss”, 562.26 ng/L “Liesingsbach rural”, and 1566.53 ng/L “Liesingbach Tangente”. Elevated concentrations in urban tributaries can be attributed to their limited dilution capacity, while high concentrations detected in WWTP effluents indicate incomplete removal of TDC during wastewater treatment processes. [9], [32], [39] Furthermore, during dry weather conditions and minor rainfall conditions of conditions, a substantial fraction of urban runoff is collected via the combined sewer system and routed to WWTPs, resulting in a centralized discharge of TDC into receiving waters through effluent release. [19], [38]

The sum concentrations of all analyzed TDC in the water samples across all locations and sampling campaigns are shown in Fig. 3 and all measured mean concentrations are listed in Appendix 10.

It must be noted that during sampling campaign 1, no effluent was captured at the sampling locations “WWTP Klosterneuburg Effluent” (Sample 21 and 22) due to high water levels (h_1 = 347 cm), which obscured the outlet. This is supported by measured water parameters (pH_{21} = 8.25 and pH_{22} = 8.17 and EC_{21} = 358.00 µS/cm and EC_{22} = 341.00 µS/cm), which differ significantly from typical WWTP effluent values (pH ~ 7 [85] and EC ranges from 600-1200 µS/cm). [85], [86] The EC

and pH in the other WWTP Klosterneuburg effluent samples (sampling campaigns 2-4) ranged from 635-1504 µS/cm and 7.51-7.81, and in Simmering (sampling campaigns 1-4) from 833-1048 µS/cm and 6.93-7.34, respectively. All measured water parameters can be found in Appendix 3. The carbamazepine concentrations in sampling campaign 1 also reflected the absence of effluent in these samples. While the concentrations of WWTP Simmering reached 566.95 ng/L, the concentration at WWTP Klosterneuburg was 6.72 ng/L. This value falls into the range of the other river samples (0.00-108.01 ng/L).

Comparing the downstream samples at both WWTP sites, the differences between the two river sides (WWTP Klosterneuburg downstream and WWTP Klosterneuburg downstream other, WWTP Simmering downstream and WWTP Simmering downstream other) were generally more pronounced at the WWTP Simmering than at WWTP Klosterneuburg. At WWTP Simmering, sum TDC concentrations at the "downstream other" site were consistently lower, with decreases of approximately 80.5%, 68.9%, 46.3%, and 77.0% across sampling campaigns 1 to 4, respectively. The carbamazepine samples also reflected this pattern in sampling campaigns 1 to 3. At WWTP Simmering, concentrations at the "downstream other" site were consistently lower, with decreases of approximately 96.5%, 74.6%, and 72.0%, respectively.

In contrast, differences downstream of WWTP Klosterneuburg were substantially smaller in most sampling campaigns, with reductions of TDC concentrations of 49.6%, 21.0%, and 0.1% observed in sampling campaigns 1 to 3. Differences downstream of WWTP Klosterneuburg were smaller in most sampling campaigns, with reductions of 68.4%, 16.2%, and 1.6% observed in sampling campaigns 1 to 3 in carbamazepine concentrations. This indicates a much more homogeneous distribution between the two river sides at the location of Klosterneuburg. These observations suggest less efficient mixing and dilution processes in the Danube Channel relative to the main Danube River. Hydrodynamic factors such as flow velocity and turbulence likely influence these patterns. [53] An exception was observed during sampling campaign 4, downstream of WWTP Klosterneuburg, where carbamazepine concentrations at the "downstream other" site exceeded those at the "downstream" site by approximately 265%, indicating a reversal of the pattern and highlighting strong temporal variability at this location. The detected TDC in both samples are also constantly higher in the "downstream other" site, suggesting a potential influence of changing hydrological conditions.

The lowest TDC concentrations were consistently detected in the Danube Channel (Nußdorf, Wienfluss, Tangente) and the main Danube (upstream, downstream, and Airport) in sampling campaigns 1-3 with sum concentrations below approx. 250 ng/L. This reflects the efficient dilution and effective mixing processes in larger water bodies. [53] An increase in sum concentrations

from “Danube upstream” to “Danube downstream” was observed in three out of four sampling campaigns: from 146.88 to 250.96 ng/L (sampling campaign 1), 18.28 to 28.37 ng/L (sampling campaign 2), and 23304.27 to 64572.99 ng/L (sampling campaign 4), corresponding to increases of approximately 71%, 55%, and 177%, respectively. In sampling campaign 3, concentrations slightly decreased from 129.61 to 96.64 ng/L. This suggests that the loads in the Danube are increased by Urban Vienna.

Comparing the upstream (“Liesingbach rural”) and downstream (“Liesingbach Tangente”) sites of the Liesingbach, no consistent spatial trend in sum TDC concentrations was observed across sampling campaigns. The concentrations increased from upstream to downstream during sampling campaigns 1 and 2 (from 562.20 to 1566.53 ng/L and from 87.95 to 172.63 ng/L, respectively), while a decrease was observed in sampling campaigns 3 and 4 (from 208.51 to 104.92 ng/L and from 358.84 to 82.56 ng/L, respectively). The absence of a consistent spatial trend at Liesingbach suggests that local factors, such as variable runoff inputs and site-specific emission sources have a strong influence on the concentrations in smaller rivers.

In contrast, carbamazepine concentrations showed a consistent decrease from “Liesingbach rural” to “Liesingbach Tangente” across all four sampling campaigns. Notably, concentrations at the upstream site were in some cases even higher than those observed at locations within the Danube Channel and the Danube. This pattern prompted further investigation into potential upstream sources. One plausible explanation is the discharge from the wastewater treatment plant Breitenfurt-Laab, which is located approximately 1 km upstream of the rural sampling site, just outside the Vienna city boundary. [44] Such an input could explain both the elevated carbamazepine concentrations and the inconsistent spatial patterns observed for TDC.

In contrast to carbamazepine, no consistent spatial trend was observed for TDC in Liesingbach. This difference indicates that TDC concentrations are controlled by additional local sources and not by wastewater inputs alone. While carbamazepine is emitted continuously and predominantly by WWTP effluents into surface waters, TDC concentrations are additionally controlled by traffic-related emissions, runoff events, and site-specific inputs [14], resulting in more heterogeneous spatial patterns.

The sum concentrations in the dissolved phase in sampling campaign 4 are substantially higher than in sampling campaigns 1-3 in some locations with concentrations reaching 64572.99 ng/L.

Overall, this spatial pattern clearly identifies urban tributaries and WWTP effluents as the dominant pathways for TDC entry into the Danube River system in Vienna and highlights urban areas as sources of TDC, with increasing loads observed downstream of Vienna.

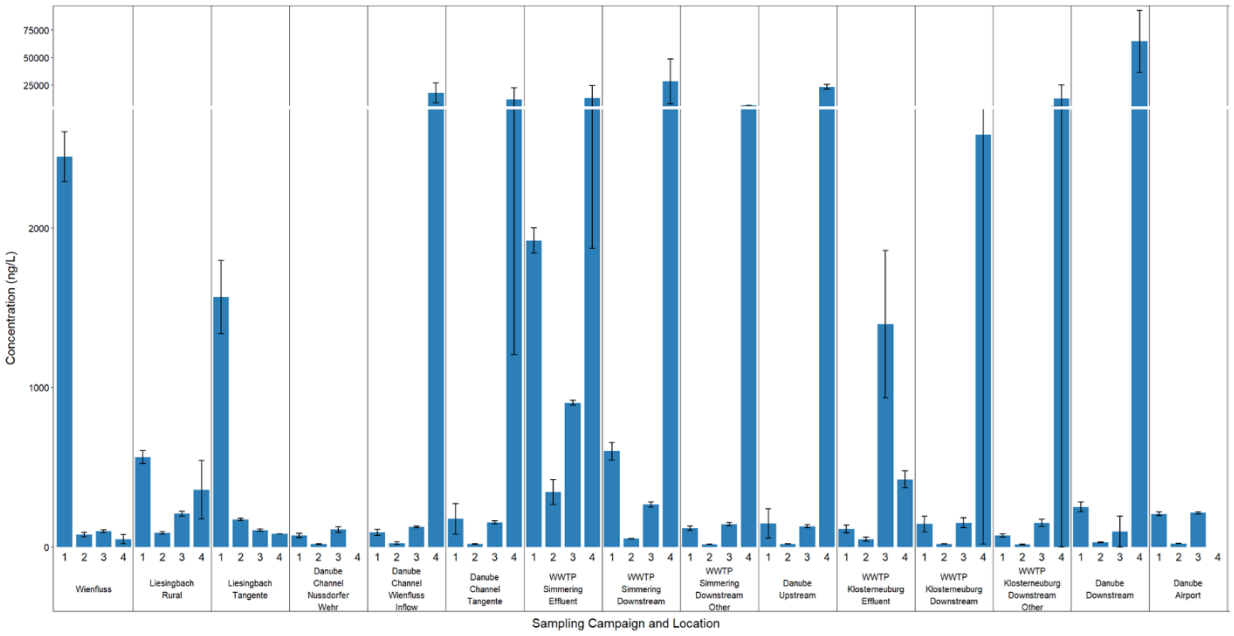

Fig. 3: Sum concentrations (ng/L) of all detected TDC in water samples across all sampling locations and sampling campaigns 1–4. Values represent the mean of duplicate samples.

Analysis of the compound profiles (Fig. 4) across the different sampling locations revealed a consistent pattern in the main Danube (upstream, downstream, Airport) and the Danube Channel (Nußdorf, Wienfluss, Tangente). In all sampling campaigns, these sites were dominated by 2-amino BTH, DPG, 5-Me BTR, DTG, HMMM, and AO2246. In addition, IPPD was detected once during sampling campaign 2 at the "Danube Cannel Wienfluss inflow", and 2-Me BTH was detected in sampling campaign 2 at the "Danube Channel Nußdorfer Wehr".

In contrast, tributaries and WWTP effluents exhibit a broader spectrum of compounds, with a wider range of additional substances detected alongside the dominant compounds mentioned above. In WWTP effluent samples, these include 2-OH BTH, BTH, Aniline, CBS, DPTU, and 2-S BTH. In the tributaries, additional compounds, including BTH, Aniline, IPPD, CPPD, and DPTU were identified. This broader compound spectrum suggests that tributaries and WWTP effluents act as direct input pathways of TDC in Vienna, reflecting source-specific compound signatures. In contrast, the main Danube and the Danube Canal integrate these inputs over larger spatial scales, where dilution and mixing processes result in a more homogenized profile dominated by the most abundant compounds. [53]

Furthermore, dilution processes likely explain why certain compounds detected in tributaries and WWTP effluents are not observed in the main river. Compounds present at lower concentrations in these input pathways may fall below detection limits after dilution in the larger water body, which does not mean that they are absent. This effect may be particularly relevant for substances with lower environmental persistence or lower initial concentrations. [53], [87]

Comparing upstream and downstream samples of the Danube, sum TDC concentrations increased in three out of four sampling campaigns, while the overall compound profiles remained largely unchanged. This indicates that urban inputs contribute to increased concentrations but do not substantially alter the relative composition of TDC in the Danube.

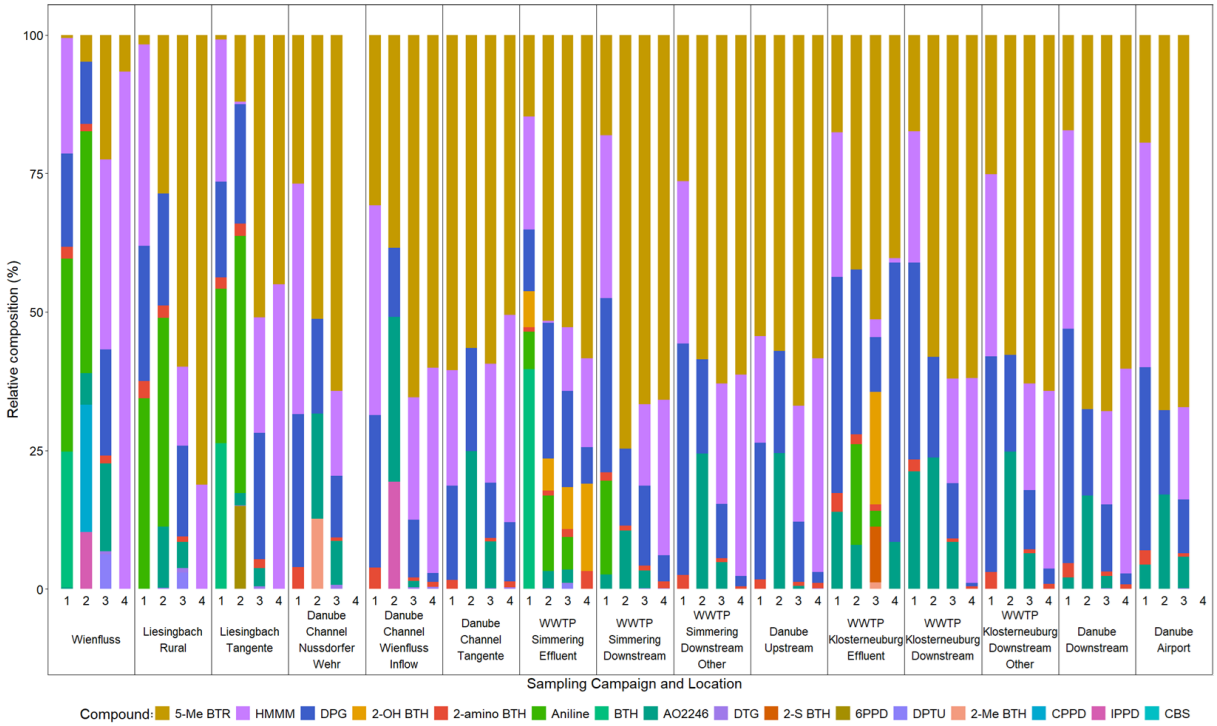

Fig. 4: Relative composition (%) of detected TDC in water samples across all sampling locations and campaigns. Bars represent the proportional contribution of individual compounds to the total concentration, based on mean values of duplicate samples.

5.3.2 No Consistent Spatial Pattern in SPM

Compared to the dissolved phase, the distribution of TDC in SPM does not show a clear spatial pattern across all sampling locations (Fig. 5). The highest sum concentrations were observed in both WWTP effluents. In sampling campaign 2, concentrations in the WWTP effluents reached 1973222.50 µg/kg in Simmering, and in sampling campaign 3, it reached 947724.32 µg/kg in Klosterneuburg. (Appendix 11) These elevated levels suggest that WWTP effluents represent significant pathways for SPM-associated TDC. The highest concentrations were also observed at WWTP effluents in the water samples, which indicates that WWTP effluents are a significant pathway for both dissolved and particle-associated TDC.

Apart from these pronounced peaks, concentrations at the remaining sampling locations were substantially lower (< 6.08×10^5 µg/kg) and did not exhibit a consistent spatial trend along the Danube or tributaries. No systematic increase or decrease in concentrations from upstream to downstream locations in the Danube was observed.

The difference of concentrations between tributaries compared to the bigger water bodies (main Danube and Danube Channel) also shows no clear pattern. Tributaries have higher concentrations with the exception of “Vienna Airport” in sampling campaign 1 and “Danube downstream” in sampling campaign 3. Sampling campaigns 2 and 4 show no spatial pattern.

As mentioned before, quantifying TDC in SPM is associated with considerable uncertainty due to the low mass of collected particles. Due to these low particle masses, small absolute differences in analyte concentrations may result in large variability when normalized to dry weight (µg/kg), increasing analytical uncertainty. This could be an additional reason for the absence of a clear spatial pattern in SPM-associated TDC concentrations.

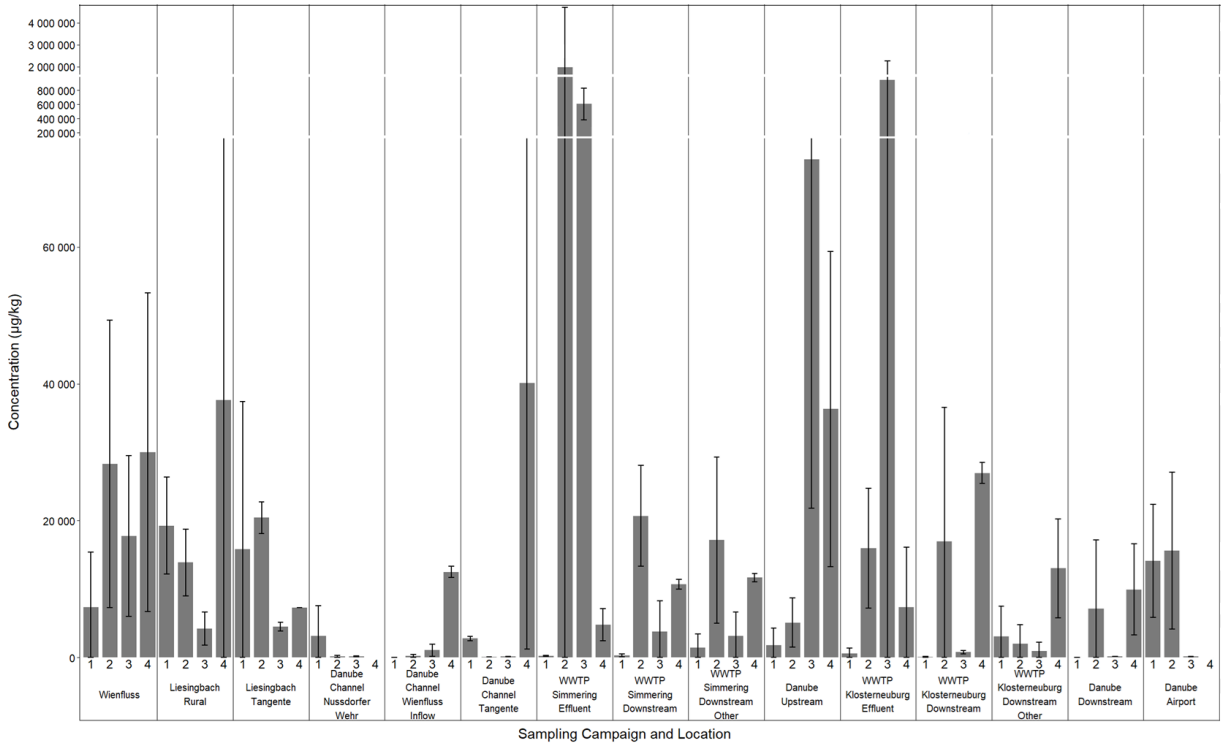

Fig. 5: Sum concentrations (µg/kg) of all detected TDC in SPM samples across all sampling locations and sampling campaigns 1–4. Values represent the mean of duplicate samples.

The compound profiles of the measured TDC in the SPM samples show no consistent spatial pattern across the different sampling locations. (Fig. 6) In contrast to the dissolved phase, where distinct spatial differences were observed, the composition of SPM samples varied strongly between sites and sampling campaigns.

AO2246 is the dominant compound, accounting for more than 80% of the total composition in 30 out of 58 samples across all sampling campaigns. This can be explained by its high $\log K_{ow}$ value of 7.1 (Tab. 1), indicating a strong hydrophobicity and a pronounced tendency to associate with suspended particulate matter. [48], [49] In addition, 5-Me BTR and DPG also contribute to the overall composition, although their relative importance varies between sampling locations. In

comparison to the water samples, where a clear difference between tributaries and the Danube in the compound profiles were observed, a pattern like this could not be detected in the SPM samples.

Patterns in up- and downstream samples in the Danube could also not be observed. While in the water samples compound profiles remained largely unchanged, SPM samples showed much more variation. For example, in sampling campaign 1 in "Danube upstream" AO2246 was the dominant compound with over 95% relative concentration while in "Danube downstream" 2-Me BTH was the only detected compound in both duplicates.

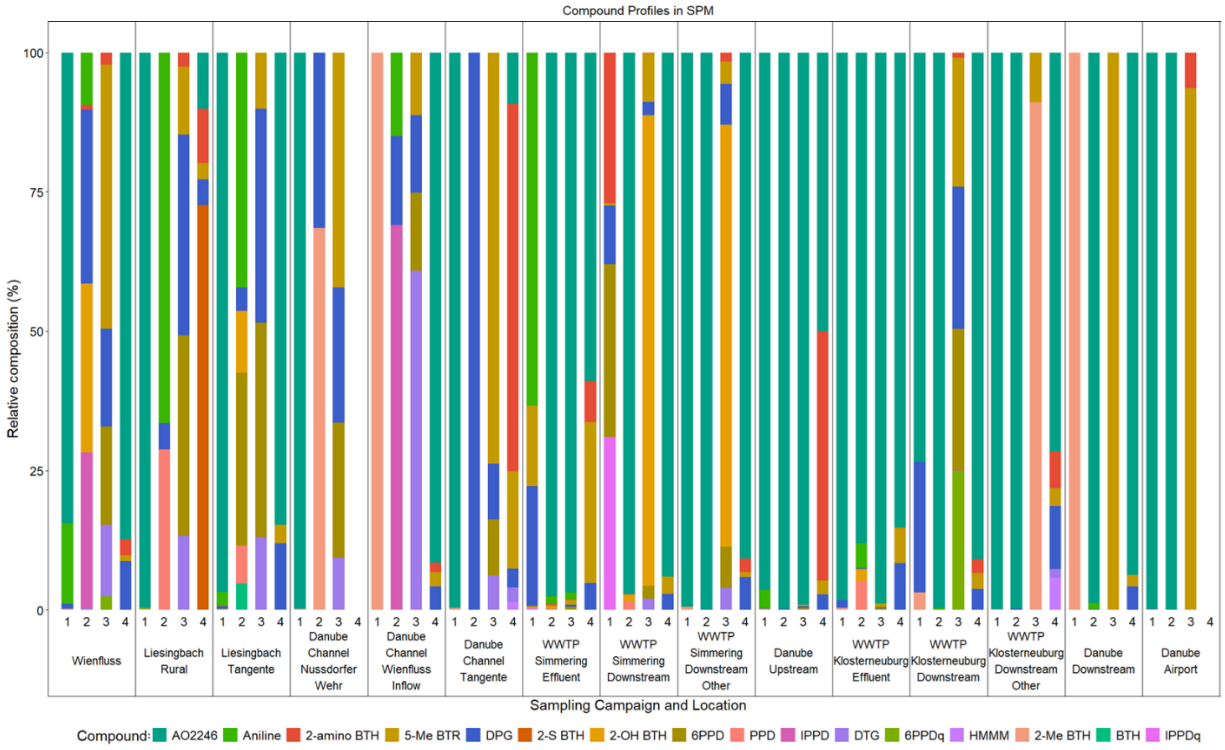

Fig. 6: Relative composition (%) of detected TDC in SPM samples across all sampling locations and campaigns. Bars represent the proportional contribution of individual compounds to the total concentration, based on mean values of duplicate samples.

5.3.3 TDC Accumulate in Sediment Samples Downstream of Vienna

Sediments samples were only collected at five locations, therefore comparison for spatial patterns can only be assessed for these locations. The sum concertation in the sediment samples (µg/kg) are shown in Fig. 7.

Similarly to the water samples, the sum TDC concentrations in sediment samples increased from Danube upstream to downstream in all campaigns where both sites were sampled. For sampling campaign 2 it increased from 0.62 to 2.74 µg/kg, in sampling campaign 3 from 557.94 to 12405.96 µg/kg and in sampling campaign 4 from 1412.16 to 2136.20 µg/kg. (Appendix 12) The consistent increase in both dissolved and sediment-associated TDC concentrations between upstream and

downstream locations suggests that contaminant loads in the Danube are influenced by urban inputs from Vienna.

Comparing Liesingbach rural and Tangente, a similar lack of consistency was observed in sediment samples, as was the case in SPM. TDC sum concentrations decreased from upstream to downstream in sampling campaign 1 (from 1295.57 to 23.95 µg/kg) but increased in sampling campaigns 2–4 (from 1.48 to 46.66 µg/kg, from 323.27 to 752.22 µg/kg, and from 1294.60 to 1702.02 µg/kg, respectively). This variability indicates that local factors, such as runoff events and site-specific emission sources, strongly influence smaller river systems.

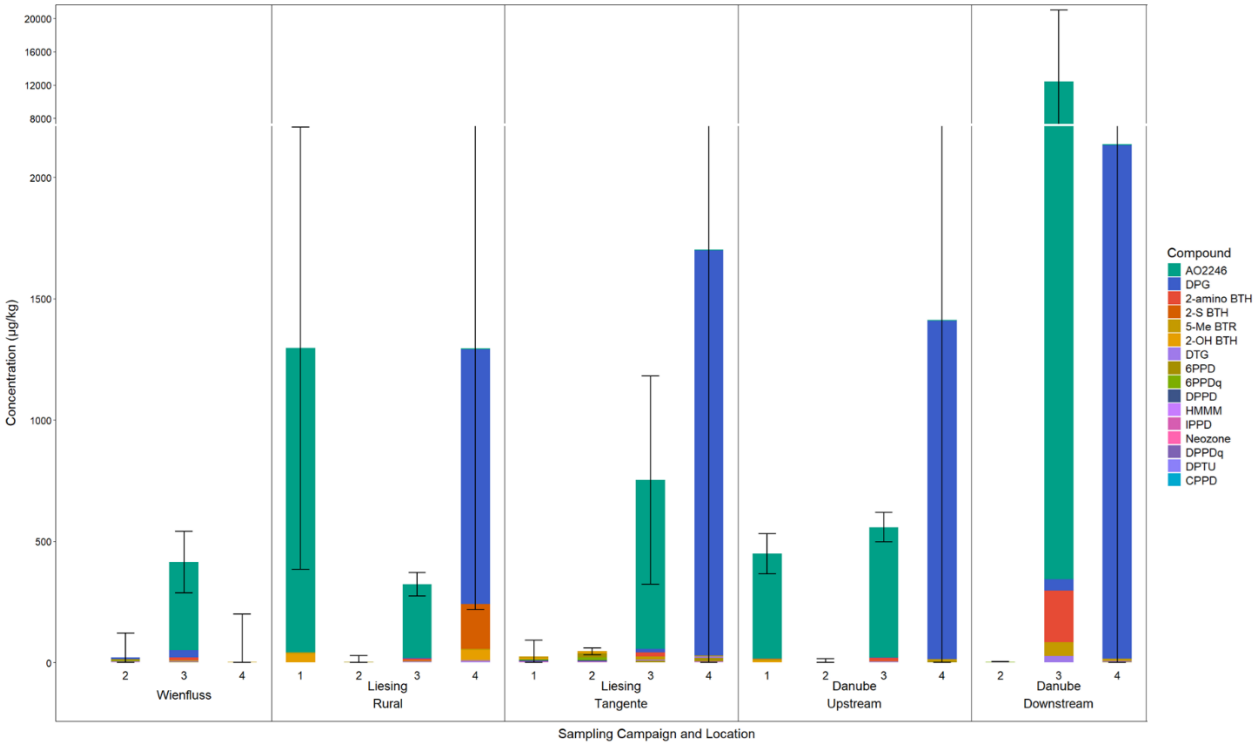

Fig. 7: Sum concentrations (µg/kg) of all detected TDC in sediment samples across all sampling locations and sampling campaigns 1–4. Values represent the mean of duplicate samples.

The compound profiles of the sediment samples show a variable pattern over the different sampling locations and campaigns. (Fig. 8) AO2246 is dominant in all five sampling locations in sampling campaign 3 (>85%), which can also be explained by its high $\log K_{ow}$ value of 7.1 (Tab. 1). DPG is dominant in sampling campaign 4 in all locations (>80%) except at "Wienfluss", where 5-Me BTR is the only detected compound. AO2246 and DPG have also been detected in water and SPM samples. This suggests that these compounds are the most dominant additives in the studied system.

For "Danube upstream" and "Danube downstream" the compounds profiles for sampling campaign 3 and 4 remained largely consistent. The same pattern was observed in sampling campaign 3 for both locations in Liesingbach. However, no fully consistent spatial trend between

upstream and downstream locations in the Danube or between tributaries and the main river can be identified. Instead, the compound composition in sediments appears to vary more strongly between sampling campaigns than between locations. This can likely be explained by the fact that sediments act as a sink for particle-associated contaminants and therefore reflect cumulative inputs over time. [48], [88] In addition, hydrodynamic processes such as flow velocity, sedimentation, and resuspension can strongly influence sediment composition by redistributing and mixing previously deposited material. [89] Furthermore, episodic inputs, such as rainfall events or wastewater discharges, can introduce pulses of contaminants with varying composition into the system. [7]

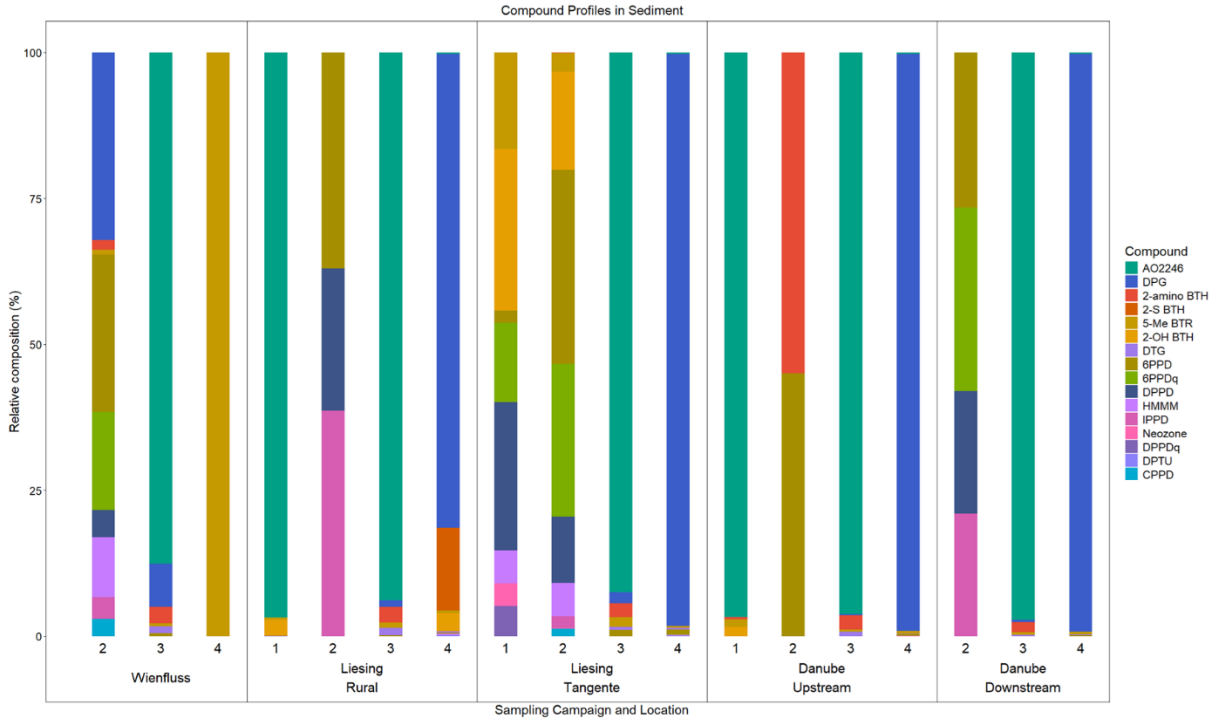

Fig. 8: Relative composition (%) of detected TDC in sediment samples across all sampling locations and campaigns. Bars represent the proportional contribution of individual compounds to the total concentration, based on mean values of duplicate samples.

5.4 Temporal Patterns Suggest Seasonal Influences on TDC Concentrations

5.4.1 TDC Concentrations in Water Peak during the Winter Campaign

The highest sum concentrations across the different sampling locations were observed during sampling campaign 4, with values reaching up to 64572.99 ng/L. (Appendix 10) In this campaign, the highest concentrations were recorded at 9 out of 13 sampling locations. (Fig. 3) Exceptions to this pattern were observed at the Wienfluss, both Liesingbach sites, where sampling campaign 1, and the WWTP Klosterneuburg effluent, where sampling campaign 3 showed highest sum

concentrations. The lowest sum concentrations in all locations were measured in sampling campaign 2.

A possible factor for higher concentrations in sampling campaign 4 could be a lower water level in the Danube, which lowers the dilution of the contaminants. However, for sampling campaign 4, a water level of 228 cm in the Danube and 280 cm in the Danube Channel was measured and is comparable to the water levels of sampling campaign 3, with 220 cm in the Danube and 283 cm in the Danube Channel. Water levels during sampling campaign 2 of 245 cm in the Danube and 285 cm in the Danube Channel were measured. This indicates that the dilution in the river is not the driving factor for the concentration elevations, rather point sources and event-driven inputs are responsible for the elevated concentrations.

Another possible explanation for the differing behavior observed in the tributaries is the sampling schedule. While most locations were sampled on December 2nd, 2025, the tributaries were sampled one day later, on December 3rd, 2025. This temporal offset may limit the direct comparability between these sites, particularly when assessing short-term variations.

During sampling campaign 4, precipitation levels were very low. On December 2nd, 2025, no precipitation was recorded at the monitoring stations in Schwedenplatz and Schwechat Flughafen, while only 0.3 mm and 0.1 mm were measured in Stammersdorf and Brunn am Gebirge, respectively. On December 3rd, 2025, no precipitation was recorded at Schwedenplatz, Schwechat Flughafen, and Brunn am Gebirge, and only 0.1 mm was measured in Stammersdorf. (Appendix 6). According to the Austrian Civil Protection Service (Zivilschutz Österreich), strong rainfall or storm events are defined as precipitation exceeding 25 mm per hour. [90] Upstream of Vienna, no storm events in Austria have been recorded. [82] The recorded precipitation during the sampling period was therefore negligible and does not qualify as a storm event.

Looking at the compounds detected of sampling campaign 4 (Fig. 4), the compounds HMMM and 5-Me BTR clearly dominate the sum concentrations in all locations. Highest concentrations have been measured at “Danube downstream” of 23832.47 ng/L and 38927.86 ng/L, respectively.

The compound profiles in the water samples show no temporal pattern.

5.4.2 No Consistent Temporal Pattern in SPM and Sediments

The sum concentrations in the sediment samples for all five locations are only comparable for sampling campaigns 2-4, since for campaign 1, only three out of the five locations have been sampled. Sampling 2 shows the lowest concentrations in all five locations. In sampling campaign 3 the highest sum concentrations have been detected at “Danube downstream”, reaching 12405.96 µg/kg, while sampling campaign 4 shows the highest concentrations at “Wienfluss”,

“Liesingbach Tangente”, and “Danube upstream”, and sampling campaign 1 at “Liesingbach rural”. This suggests that there is no clear temporal pattern for the sediment samples. (Appendix 12)

Looking at the compound profiles in the sediment samples (Fig. 8), the most consistent temporal pattern can be seen in sampling campaign 3, which shows very similar profiles at all locations, which are largely dominated by AO2246, followed by 2-amino BTH, 5-Me BTR, DPG, and DTG. Also sampling campaign 4 is dominated by DPG in all locations except for “Wienfluss”, where only 5-Me BTR has been detected.

The sum concentrations and compound profiles of TDC in SPM showed no temporal pattern.

6 Conclusion

In this study, the TDC concentrations in water, suspended particles, and sediment throughout Vienna's surface waters, including the Danube, Danube Channel, Wienfluss, and Liesingbach, were determined. The results show that TDC are continuously present in the Rivers of Vienna.

Water samples revealed a clear spatial pattern with WWTP effluents (reaching up to 13150.45 ng/L) and urban tributaries (reaching up to 2445.98 ng/L) being the primary entry pathways of TDC into the River system in Vienna. Large river systems such as the Danube act as integrators, where dilution and mixing processes govern the spatial distribution and composition of these compounds across different environmental compartments. [53] SPM samples also showed elevated concentrations in WWTP effluents (up to 1973222.50 µg/kg), further strengthening the pattern of WWTPs being one of the main pathways for TDC into surface waters.

For both water and sediment samples the concentrations increased from up- to downstream Danube. In water samples the compound profiles remained largely unchanged, the same pattern was observed in two sampling campaigns for sediment samples. The consistent increase in both dissolved and sediment-associated TDC concentrations between upstream and downstream locations suggests urban Vienna increases the loads of TDC in the Danube, while the relative compound composition remains largely unchanged. Such spatial patterns were not observed in SPM samples.

Danube and the Danube Channel were dominated by 2-amino BTH, DPG, 5-Me BTR, DTG, HMMM, and AO2246, and singular other TDC while Tributaries and WWTP effluents showed a broader spectrum of compounds in the dissolved phase. Compound profiles of sediment samples were largely dominated by AO2246, which can be explained by the high $\log K_{ow}$ value of 7.1 (Tab. 1).

Overall, no consistent temporal pattern was identified in water, SPM, and sediment samples. While sampling campaign 4 showed the highest concentrations in water at most locations, this could not be explained by dilution effects, as water levels were comparable to other campaigns, indicating that point sources or event-driven inputs are more likely responsible.

Since no stormwater event was caught in the four sampling campaigns, the influence of such events on concentration levels could not be evaluated.

Overall, TDC occurrence in the Danube and its tributaries in Vienna is characterized by continuous inputs and an uneven compound distribution, where a small number of compounds (5-Me BTR, AO2246, DPG, and 2-amino BTH) dominate concentrations and detection frequencies in dissolved, particulate and sediment phases.

7 Outlook

The targeted capture of stormwater events would provide valuable insights into the temporal dynamics of TDC. Previous studies have already highlighted that wet-season or storm-event sampling can cause short-term concentration peaks, which can substantially improve the understanding of occurrence patterns of these contaminants. [7] Additionally, elevated river flow can influence concentrations by dilution. [53]

To improve temporal resolution, passive sampling could be implemented as an additional approach to grab sampling. Passive samplers allow for time-integrated measurements and can capture fluctuations over shorter time intervals, which are often missed by discrete sampling campaigns. [61]

Environmental parameters such as water temperature and pH are known to influence the behavior and distribution of TDC in aquatic systems. A more detailed investigation of these parameters could therefore provide deeper insight into different processes, including partitioning and transport dynamics. [5]

Further insight into removal processes of TDC in WWTP could be achieved by analyzing both influent and effluent samples of WWTP Klosterneuburg and Simmering. This would enable the calculation of removal efficiencies for the compounds of interest and help to better assess the role of different wastewater treatments in Vienna in controlling TDC emissions. [32], [39]

Regarding the sampling design, certain locations, such as the "Danube Channel Nußdorfer Wehr" and "Danube Airport" showed limited influence on the overall findings in this study and could potentially be excluded in future campaigns to optimize sampling effort, which has already been done for sampling campaign 4. However, these sites may still become relevant during stormwater events, particularly if runoff inputs from the airport can occur under such conditions.

In terms of sediment analysis, additional sampling would be beneficial to further investigate the partitioning behavior of TDC between water and sediment phases. However, sampling in large rivers such as the Danube requires more extensive logistical effort and may therefore be more feasible within a larger-scale project.

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Appendix

A. Supplementary Data

Appendix 1: Compound names, CAS number and Vendor where the compound was bought.

Compound Name	CAS number	Vendor
Benzothiazole 96%	95-16-9	Merck, Darmstadt, Germany
2-aminobenzothiazole 97%	136-95-8	Merck, Darmstadt, Germany
2-methylbenzothiazole 99%	120-75-2	Merck, Darmstadt, Germany
2-mercaptobenzothiazole 97%	149-30-4	Merck, Darmstadt, Germany
2-hydroxybenzothiazole 98%	934-34-9	Merck, Darmstadt, Germany
5-methyl-1h-benzotriazole 98%	136-85-6	Merck, Darmstadt, Germany
p-Phenylenediamine 98%	106-50-3	Merck, Darmstadt, Germany
N-Isopropyl-N'-phenyl-p-phenylendiamin	101-72-4	HPC Standards, Borsdorf, Germany
2-[(1-Methylethyl)amino]-5-(phenylamino)-2,5-cyclohexadiene-1,4-dione	68054-73-9	HPC Standards, Borsdorf, Germany
N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylenediamine	793-24-8	Merck, Darmstadt, Germany
2-anilino-5-[(4-methylpentan-2-yl)amino]-cyclohexa-2,5-diene-1,4-dione	2754428-18-5	HPC Standards, Borsdorf, Germany
N-Cyclohexyl-N'-phenyl-p-phenylenediamine	101-87-1	HPC Standards, Borsdorf, Germany
2-(Cyclohexylamino)-5-(phenylamino)-2,5-cyclohexadiene-1,4-dione	68054-78-4	HPC Standards, Borsdorf, Germany
N,N'-Diphenyl-p-phenylenediamine 97%	74-31-7	Fisher Scientific, Wien, Austria
2,5-bis(phenylamino)cyclohexa-2,5-diene-1,4-dione	3421-08-7	HPC Standards, Borsdorf, Germany
Aniline	62-53-3	Merck, Darmstadt, Germany
N-Cyclohexyl-2-benzothiazolesulfenamide	95-33-0	Merck, Darmstadt, Germany
1,3-Diphenylguanidine 97%	102-06-7	Merck, Darmstadt, Germany
N,N'-Diphenylthiourea 98%	102-08-9	Merck, Darmstadt, Germany
1,3-Di-o-tolylguanidine	97-39-2	Merck, Darmstadt, Germany
Hexa(methoxymethyl)melamine	3089-11-0	TCI Chemicals, Eschborn, Germany
N-Phenyl-2-naphthylamine 95%	135-88-6	Merck, Darmstadt, Germany
2,2-Methylenebis(6-tert-butyl-4-methylphenol)		

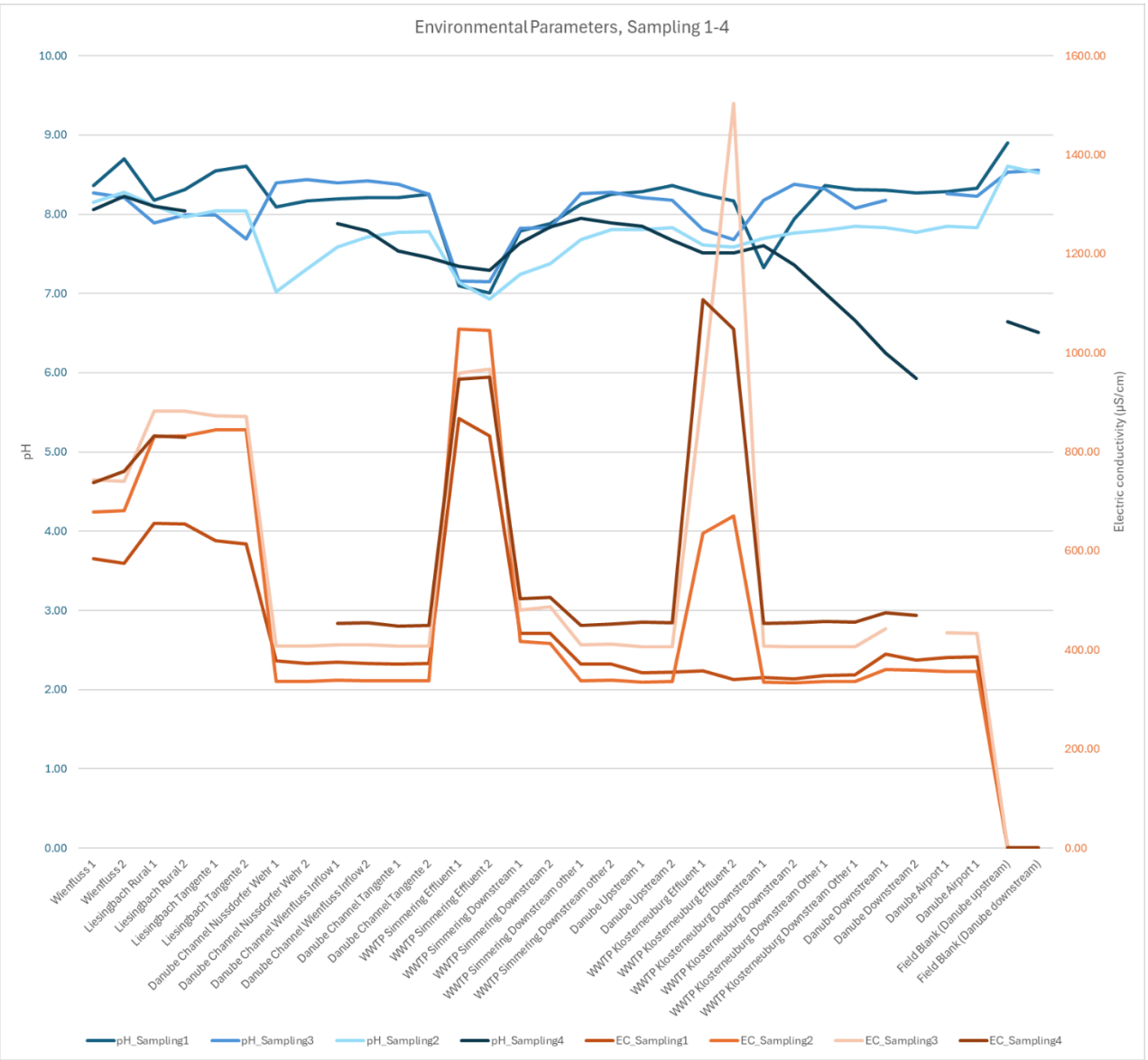
Butylated hydroxytoluene	128-37-0	Merck, Darmstadt, Germany
Butylated hydroxyanizole	25013-16-5	Merck, Darmstadt, Germany
Carbamazepine	298-46-4	Merck, Darmstadt, Germany
2-[(4-methylpentan-2-yl)amino]-5-{[(2,3,4,5,6-$^{2}H_{5}$)phenyl]amino}cyclohexa-2,5-diene-1,4-dione	2750119-14-1	HPC Standards, Borsdorf, Germany
benzo[d]thiazole-4,5,6,7-d4	194423-51-3	LGC Standards

Appendix 2: Sampling location names and coordinates, sampling date (DD.MM.) and time.

		Sampling 1		Sampling 2		Sampling 3		Sampling 4	
Location	**Coordinates**	**Date**	**Time**	**Date**	**Time**	**Date**	**Time**	**Date**	**Time**
Wienfluss	48°12'21.9"N 16°22'55.3"E	03.06.	12:00	17.07.	11:37	01.10.	12:10	03.12.	11:55
Liesingbach Rural	48°08'10.9"N 16°13'26.0"E	03.06.	13:35	17.07.	09:57	01.10.	13:20	03.12.	09:50
Liesingbach Tangente	48°09'04.2"N 16°20'51.0"E	03.06.	14:53	17.07.	10:47	01.10.	14:08	03.12.	10:40
Danube Channel Nussdorfer Wehr	48°15'17.2"N 16°22'14.8"E	05.06.	10:23	16.07.	12:04	30.09.	11:26	02.12.	-
Danube Channel Wienfluss Inflow	48°12'35.9"N 16°23'45.2"E	05.06.	11:21	16.07.	13:00	30.09.	12:28	02.12.	12:55
Danube Channel Tangente	48°11'22.8"N 16°25'19.7"E	05.06.	11:44	16.07.	13:27	30.09.	12:50	02.12.	13:32
WWTP Simmering Effluent	48°10'23.3"N 16°28'27.5"E	05.06.	12:23	16.07.	14:03	30.09.	13:25	02.12.	14:07
WWTP Simmering Downstream	48°10'03.9"N 16°29'18.4"E	05.06.	12:34	16.07.	15:15	30.09.	15:05	02.12.	14:23
WWTP Simmering Downstream other	48°10'04.9"N 16°29'19.0"E	05.06.	12:34	16.07.	15:15	30.09.	15:05	02.12.	14:23
Danube Upstream	48°17'58.7"N 16°20'32.2"E	04.06.	10:09	16.07.	10:20	30.09.	10:00	02.12.	10:30
WWTP Klosterneuburg Effluent	48°17'35.6"N 16°20'38.7"E	04.06.	10:31	16.07.	10:27	30.09.	10:09	02.12.	10:42
WWTP Klosterneuburg Downstream	48°16'22.1"N 16°21'37.6"E	04.06.	10:56	16.07.	10:47	30.09.	10:38	02.12.	11:26
WWTP Klosterneuburg Downstream Other	48°16'24.8"N 16°21'47.7"E	04.06.	11:21	16.07.	11:01	30.09.	10:38	02.12.	11:26
Danube Downstream	48°08'51.7"N 16°32'00.5"E	04.06.	15:48	16.07.	15:43	30.09.	15:05	02.12.	15:56
Danube Airport	48°07'49.1"N 16°37'13.0"E	04.06.	16:37	16.07.	16:37	30.09.	16:15	02.12.	-
Field Blank (Danube upstream)	48°17'58.7"N 16°20'32.2"E	04.06.	12:14	16.07.	10:15	30.09.	09:45	02.12.	10:15
Field Blank (Danube downstream)	48°08'51.7"N 16°32'00.5"E	-	-	16.07.	17:00	30.09.	16:54	02.12.	16:20

Appendix 3: Electric conductivity (µS/cm) and pH of all samples.

	pH				electric conductivity (µS/cm)			
Sample	Sampling 1	Sampling 2	Sampling 3	Sampling 4	Sampling 1	Sampling 2	Sampling 3	Sampling 4
1	8.36	8.15	8.27	8.06	585	679	744	738
2	8.70	8.28	8.21	8.23	575	681	741	761
3	8.18	8.11	7.89	8.10	656	831	882	832
4	8.31	7.97	7.99	8.04	655	832	883	830
5	8.55	8.04	7.99	-	621	845	873	-
6	8.61	8.04	7.69	8.02	614	844	871	854
7	8.09	7.02	8.40	-	378	336	408	-
8	8.17	7.31	8.44	-	373	336	408	-
9	8.19	7.59	8.40	7.88	375	339	410	454
10	8.21	7.71	8.42	7.79	373	338	411	455
11	8.21	7.77	8.38	7.54	371	338	408	448
12	8.25	7.78	8.25	7.45	373	338	408	450
13	7.10	7.14	7.16	7.34	867	1048	959	947
14	7.01	6.93	7.15	7.29	833	1045	967	951
15	7.79	7.24	7.82	7.64	434	417	481	503
16	7.88	7.38	7.83	7.84	433	413	487	506
17	8.13	7.68	8.26	7.95	372	338	411	449
18	8.25	7.81	8.28	7.89	372	339	412	452
19	8.29	7.81	8.21	7.85	354	335	406	457
20	8.36	7.83	8.18	7.67	355	337	406	455
21	8.25	7.61	7.81	7.51	358	635	930	1107
22	8.17	7.59	7.68	7.51	341	671	1504	1048
23	7.33	7.70	8.18	7.60	344	335	408	454
24	7.94	7.76	8.38	7.36	342	334	406	455
25	8.36	7.80	8.32	7.01	349	336	407	458
26	8.31	7.85	8.08	6.66	350	336	407	456
27	8.30	7.83	8.18	6.25	392	360	443	475
28	8.27	7.77	-	5.93	380	359	-	470
29	8.29	7.85	8.26	-	385	357	435	-
30	8.33	7.83	8.23	-	386	357	434	-
31	8.90	8.61	8.53	6.64	1.08	1.16	1.02	0.71
32	-	8.52	8.56	6.51	-	0.99	0.98	0.85



Appendix 4: Electric conductivity (EC) (µS/cm) and pH of all four sampling campaigns

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Appendix 5: Water level (cm), flow velocity (m/s) and volume flow rate (m^3/s) for all sampling campaigns in the Danube, Danube Channel, Wienfluss and at two sites in Liesingbach.

	Water Level (cm)			
	Sampling 1	**Sampling 2**	**Sampling 3**	**Sampling 4**
Danube (Korneuburg)	347	245	220	228
Danube Channel (Schwedenbrücke)	331	285	283	280
Wienfluss	-	-	-	-
Liesingbach Rural	-	-	-	-
Liesingbach Tangente	-	-	-	-
	Flow Velocity (m/s)			
	Sampling 1	**Sampling 2**	**Sampling 3**	**Sampling 4**
Danube (Korneuburg)	-	-	-	-
Danube Channel (Schwedenbrücke)	-	-	-	-
Wienfluss	0.40	0.23	0.22	0.27
Liesingbach Rural	0.71	0.20	0.28	0.43
Liesingbach Tangente	1.01	0.18	0.15	0.15
	Volume Flow Rate (m^3/s)			
	Sampling 1	**Sampling 2**	**Sampling 3**	**Sampling 4**
Danube (Korneuburg)	2.36	1.38	1.12	1.20
Danube Channel (Schwedenbrücke)	-	-	-	-
Wienfluss	-	-	-	-
Liesingbach Rural	-	-	-	-
Liesingbach Tangente	-	-	-	-

Appendix 6: Precipitation (24h sum) in mm for 4 locations across Vienna for all samplings on the sampling days (marked in red) and up to 30 days before. -1=no precipitation, 0=less than 1/10 mm.

	Precipitation (24h sum) (mm)			
Date	**Schwedenplatz**	**Stammersdorf**	**Brunn am Gebirge**	**Schwechat Flughafen**
Sampling 1				
07.05.2025	-1	-1	-1	-1
08.05.2025	0	-1	0.4	-1
09.05.2025	-1	-1	-1	-1
10.05.2025	-1	-1	-1	-1
11.05.2025	-1	-1	-1	-1
12.05.2025	-1	-1	-1	-1
13.05.2025	-1	-1	-1	-1
14.05.2025	-1	-1	-1	-1
15.05.2025	0.3	0	1	0.2
16.05.2025	0.2	0.7	0.2	1.9
17.05.2025	0.8	5.8	0.9	1.7
18.05.2025	2.8	4	15	2.4
19.05.2025	-1	-1	0.2	-1
20.05.2025	-1	-1	-1	-1
21.05.2025	0.1	-1	6.7	0.4
22.05.2025	4.3	5	5.9	3.6
23.05.2025	-1	-1	-1	-1
24.05.2025	-1	-1	-1	-1
25.05.2025	2.2	3.2	2.3	3.7
26.05.2025	7.2	10.7	2.4	4.2
27.05.2025	-1	-1	-1	-1
28.05.2025	4.3	3.6	5	1.9
29.05.2025	2	0.4	8.5	-1
30.05.2025	0	0.3	0.3	0.1
31.05.2025	-1	-1	-1	-1
01.06.2025	1	3.6	5.9	2.1
02.06.2025	18.4	9	20.6	17.2
03.06.2025	1.6	1.4	1.3	0.9
04.06.2025	-1	-1	-1	-1
05.06.2025	-1	-1	-1	-1
Sampling 2				
18.06.2025	-1	-1	-1	-1
19.06.2025	-1	-1	-1	-1
20.06.2025	-1	-1	-1	-1
21.06.2025	-1	-1	-1	-1
22.06.2025	-1	-1	-1	-1
23.06.2025	6.9	4.4	15.4	5.1
24.06.2025	-1	-1	-1	0
25.06.2025	-1	-1	-1	0
26.06.2025	0.6	0.7	2	2.1

27.06.2025	1.8	0.4	0.4	1.2
28.06.2025	-1	-1	-1	-1
29.06.2025	-1	-1	-1	-1
30.06.2025	-1	-1	-1	-1
01.07.2025	-1	-1	-1	-1
02.07.2025	-1	-1	-1	-1
03.07.2025	-1	0.7	0.6	-1
04.07.2025	0	0.1	0.4	-1
05.07.2025	-1	-1	-1	-1
06.07.2025	18.2	14.6	25.4	20.1
07.07.2025	11.8	7.5	19.6	8
08.07.2025	12.1	12.6	10.6	12.9
09.07.2025	-1	0	-1	-1
10.07.2025	3.9	5.2	5.8	8.1
11.07.2025	1.7	0.9	-1	0
12.07.2025	5.5	0.8	2.6	0.4
13.07.2025	-1	-1	-1	-1
14.07.2025	0	1.3	0.1	-1
15.07.2025	-1	-1	-1	-1
16.07.2025	0.6	5.8	5	1.9
17.07.2025	1.3	3	3.6	1.3
Sampling 3				
02.09.2025	21.6	11.3	27.4	0.2
03.09.2025	-1	-1	-1	-1
04.09.2025	-1	-1	-1	-1
05.09.2025	10.6	8.2	11.6	6.3
06.09.2025	-1	-1	-1	-1
07.09.2025	-1	-1	-1	-1
08.09.2025	-1	-1	-1	-1
09.09.2025	2.8	1.1	3.7	2.1
10.09.2025	17.7	17.7	32.1	25.8
11.09.2025	-1	0.2	-1	-1
12.09.2025	25.7	19.9	12.4	8.7
13.09.2025	0.1	2.1	1	0.6
14.09.2025	0.2	-1	0.1	0.5
15.09.2025	0	0.3	0	0.1
16.09.2025	-1	-1	-1	-1
17.09.2025	-1	-1	0.1	-1
18.09.2025	-1	0.1	-1	-1
19.09.2025	-1	-1	-1	-1
20.09.2025	-1	-1	-1	-1
21.09.2025	-1	-1	-1	-1
22.09.2025	-1	-1	-1	-1
23.09.2025	1.7	0.8	2.7	1.5
24.09.2025	15.2	17.1	23.4	13.9
25.09.2025	4.2	5.4	7	2.7

26.09.2025	2.8	4.3	5.2	2.5
27.09.2025	-1	-1	0.1	-1
28.09.2025	-1	-1	-1	-1
29.09.2025	-1	-1	-1	-1
30.09.2025	-1	-1	-1	-1
01.10.2025	0.2	-1	2.2	-1
Sampling 4				
04.11.2025	-1	-1	-1	-1
05.11.2025	-1	-1	-1	-1
06.11.2025	-1	-1	-1	-1
07.11.2025	-1	-1	-1	-1
08.11.2025	0.5	0.3	0.2	0.2
09.11.2025	0.4	0	0.9	0.4
10.11.2025	-1	-1	-1	-1
11.11.2025	-1	-1	-1	-1
12.11.2025	-1	0.1	-1	0.1
13.11.2025	0.2	0	-1	-1
14.11.2025	-1	0.5	0.1	0.9
15.11.2025	0.2	0.6	0.7	0.6
16.11.2025	1.1	0.7	1.3	0.8
17.11.2025	24.3	25.3	29.4	22
18.11.2025	-1	-1	0.1	-1
19.11.2025	-1	-1	-1	-1
20.11.2025	-1	-1	-1	-1
21.11.2025	0	0	0	-1
22.11.2025	1.9	5	0.6	0.4
23.11.2025	0	0.1	0	0
24.11.2025	1.5	0.8	0.8	2.1
25.11.2025	5.8	8.2	4.6	6.7
26.11.2025	0	0	0.1	-1
27.11.2025	-1	-1	-1	-1
28.11.2025	-1	-1	-1	-1
29.11.2025	-1	-1	-1	-1
30.11.2025	-1	-1	-1	-1
01.12.2025	0.2	0.2	-1	0.2
02.12.2025	-1	0.3	0.1	-1
03.12.2025	-1	0.1	-1	-1

Appendix 7: Mass of water sample (m_W) (kg), mass of SPM (m_P) (mg), total suspended Solids (TSS) and mean TSS for duplicates (mg/L).

	Sampling 1				Sampling 2			
Sample	m_W (kg)	m_P (mg)	TSS (mg/L)	Mean TSS (mg/L)	m_W (kg)	m_P (mg)	TSS (mg/L)	Mean TSS (mg/L)
1	1.00	40.63	40.77	36.03	1.05	-0.73	-0.70	-0.06
2	1.02	31.91	31.30		1.02	0.59	0.58	
3	1.02	36.36	35.76	35.02	0.96	1.71	1.77	2.44
4	0.99	33.90	34.27		0.91	2.83	3.12	
5	1.03	42.11	40.85	77.70	0.93	4.60	4.95	5.70
6	1.01	115.53	114.55		0.93	5.98	6.44	
7	0.97	48.58	49.91	54.16	1.05	27.09	25.78	25.41
8	1.00	58.40	58.41		1.08	27.01	25.05	
9	0.96	83.09	86.11	72.78	0.90	29.15	32.47	30.77
10	1.00	59.17	59.45		0.89	25.86	29.07	
11	1.04	52.69	50.74	54.45	1.04	28.04	26.95	28.11
12	1.03	59.80	58.15		1.04	30.46	29.26	
13	0.84	122.25	145.58	195.50	0.95	-0.06	-0.06	0.52
14	0.94	231.26	245.43		1.00	1.09	1.10	
15	0.89	20.27	22.68	9.32	1.01	30.26	29.87	28.97
16	0.96	-3.88	-4.04		1.00	28.07	28.06	
17	0.99	27.38	27.75	26.86	0.96	28.78	29.94	32.25
18	0.94	24.44	25.98		1.00	34.64	34.56	
19	1.01	132.38	130.76	115.04	1.00	28.78	28.73	26.92
20	1.01	100.51	99.32		0.99	24.88	25.10	
21	1.01	73.82	72.89	75.59	1.01	21.48	21.23	20.51
22	1.02	79.59	78.29		1.01	19.93	19.79	
23	1.01	70.29	69.41	69.91	1.01	24.85	24.56	24.51
24	1.02	71.51	70.41		1.01	24.73	24.46	
25	0.99	63.22	63.96	68.02	1.01	32.21	31.82	30.36
26	0.91	65.95	72.09		1.01	29.24	28.91	
27	1.01	56.94	56.31	56.69	1.01	26.24	25.96	27.46
28	1.01	57.64	57.08		1.01	29.28	28.96	
29	1.01	55.35	54.75	54.21	1.00	26.78	26.72	26.70
30	0.98	52.76	53.68		1.01	26.90	26.69	
31	1.03	33.37	32.56	32.56	0.98	0.15	0.15	0.08
32	-	-	-		0.93	0.01	0.01	
	Sampling 3				**Sampling 4**			
Sample	m_W (kg)	m_P (mg)	TSS (mg/L)	Mean TSS (mg/L)	m_W (kg)	m_P (mg)	TSS (mg/L)	Mean TSS (mg/L)
1	0.96	1.32	1.38	1.28	0.94	0.68	0.72	1.88
2	1.00	1.19	1.18		0.94	2.85	3.04	
3	1.01	5.09	5.04	4.12	1.02	1.00	0.98	45.36
4	0.98	3.14	3.20		1.00	90.11	89.74	
5	0.97	2.03	2.10	2.10	-	-	-	6.61
6	0.92	1.93	2.10		0.86	5.71	6.61	
7	1.00	7.46	7.45	18.03	-	-	-	-
8	0.19	5.45	28.61		-	-	-	

9	1.03	8.11	7.85	7.58	1.00	5.61	5.58	4.31
10	1.03	7.52	7.30		0.97	2.96	3.04	
11	1.04	8.77	8.41	8.03	1.01	3.25	3.21	22.32
12	0.99	7.55	7.66		1.01	41.99	41.43	
13	1.00	14.01	13.99	8.90	1.01	43.74	43.14	26.54
14	0.98	3.72	3.81		0.96	9.51	9.94	
15	1.02	7.22	7.09	7.61	1.01	2.54	2.51	3.28
16	1.04	8.46	8.14		1.00	4.06	4.06	
17	0.90	6.86	7.63	8.74	1.01	5.17	5.13	4.00
18	0.94	9.25	9.85		1.00	2.88	2.87	
19	1.01	6.98	6.90	6.85	0.95	1.88	1.97	2.19
20	1.00	6.83	6.80		0.92	2.21	2.40	
21	1.00	3.46	3.46	5.75	1.03	147.66	143.42	72.80
22	1.00	8.06	8.03		1.02	2.23	2.18	
23	1.00	7.80	7.79	7.40	0.98	2.03	2.07	1.52
24	1.01	7.06	7.01		0.94	0.90	0.96	
25	0.96	10.82	11.30	11.40	0.94	2.48	2.65	4.39
26	0.98	11.24	11.50		0.94	5.78	6.13	
27	1.01	8.85	8.76	8.76	0.94	3.27	3.46	3.66
28	-	-	-		1.04	4.00	3.86	
29	1.01	11.17	11.10	10.83	-	-	-	-
30	0.99	10.41	10.56		-	-	-	
31	1.00	0.56	0.56	0.68	0.96	0.52	0.54	0.83
32	0.95	0.76	0.80		0.94	1.05	1.11	

Appendix 8: Recovery rates (%) and standard deviations of the first recovery test with different solvents (ACN, MeOH and DCM), pre-conditioning and one glass cartridge.

	Recovery rates (%)								
Compound	**Pre-Cond. + ACN**	**std. dev.**	**ACN**	**std. dev.**	**MeOH**	**std. dev.**	**DCM**	**std. dev.**	**Glass**
BTH	95.75	0.94	102.28	5.04	110.52	8.77	83.06	5.86	92.92
2-amino BTH	99.08	0.20	106.51	3.81	318.08	15.96	161.06	5.08	103.66
2-Me BTH	91.79	2.49	93.62	0.10	110.20	6.25	86.10	7.08	91.43
2-S BTH	3.58	2.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-OH BTH	60.73	0.63	56.52	3.30	55.98	4.85	49.51	8.31	48.70
5-Me BTR	84.71	1.12	73.62	2.47	71.33	2.89	58.90	1.78	78.86
PPD	35.45	2.21	50.92	0.43	104.26	5.19	0.00	0.00	62.43
IPPD	80.25	1.85	72.28	3.50	90.35	1.75	214.36	30.38	62.87
IPPDq	78.22	3.12	58.40	0.29	59.54	2.02	91.60	8.06	61.17
6PPD	68.77	2.02	61.31	0.46	49.94	3.93	0.00	0.00	51.77
6PPDq	90.43	0.74	90.06	1.27	89.78	2.87	206.90	28.41	87.01
CPPD	72.19	1.47	64.22	2.12	49.06	2.46	27.89	7.99	51.44
CPPDq	84.96	2.41	83.73	1.28	79.28	2.68	156.66	22.21	81.20
DPPD	86.51	3.59	82.76	1.19	85.55	2.57	199.84	29.28	79.25
DPPDq	65.63	3.85	59.66	0.57	51.96	2.23	76.13	25.48	62.05
Aniline	20.99	0.55	24.52	2.69	37.04	3.12	20.19	1.35	22.81
CBS	141.01	35.09	122.08	4.58	126.96	8.73	120.92	5.30	114.15
DPG	24.36	3.45	50.80	2.72	170.07	8.17	1.24	0.00	60.42
DPTU	6.74	4.98	0.00	0.00	1.58	2.24	0.00	0.00	0.00
DTG	38.38	0.92	61.20	0.13	138.69	7.42	0.43	0.61	67.68
HMMM	123.05	32.55	108.20	2.03	113.99	5.42	109.08	6.57	102.38
Neozone	80.11	1.18	78.27	0.94	66.07	1.43	99.37	12.88	75.57
AO2246	69.84	0.79	68.99	4.49	66.73	10.02	65.56	2.84	76.99
BHT	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BHA	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Appendix 9: log(K_D) values of all compounds in all sampling locations and campaigns 1-4.

Location	Campaign	2-amino BTH	BHA	DPG	5-Me BTR	PPD	DTG	2-OH BTH	IPPD	BTH	2-S BTH	2-Me BTH	HMMM	CPPD	DPTU	Aniline	6PPD	IPPDq	DPPDq	CPPDq	BHT	6PPDq	DPPD	Neozone	CBS	AO2246
Wienfluss	1	-	-	2.20	-	-	-	-	-	-	-	-	-	-	-	3.10	-	-	-	-	-	-	-	-	-	6.01
	2	5.39	-	6.01	-	-	-	-	6.00	-	-	-	-	-	-	4.90	-	-	-	-	-	-	-	-	-	-
	3	5.44	-	5.22	5.58	-	6.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	-	-	-	4.98	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Liesingbach Rural	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.50	-	-	-	-	-	-	-	-	-	-
	2	-	-	4.57	-	-	-	-	-	-	-	-	-	-	-	5.44	-	-	-	-	-	-	-	-	-	-
	3	4.69	-	4.65	3.61	-	5.52	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	-	-	-	3.58	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Liesingbach Tangente	1	2.07	-	2.47	-	-	-	-	-	-	-	-	-	-	-	2.97	-	-	-	-	-	-	-	-	-	-
	2	-	-	4.36	-	-	-	-	-	-	-	-	-	-	-	5.03	5.39	-	-	-	-	-	-	-	-	-
	3	-	-	4.86	3.93	-	6.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	-	-	-	3.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Danube Channel Nussdorfer Wehr	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	2	-	-	4.17	-	-	-	-	-	-	-	4.64	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	3	-	-	3.54	3.02	-	4.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Danube Channel Wienfluss Inflow	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	2	-	-	4.10	-	-	-	-	4.55	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	3	-	-	4.05	3.16	-	6.35	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	3.14	-	3.26	1.47	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Danube Channel Tangente	1	2.37	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	2	-	-	4.35	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	3	-	-	2.94	3.04	-	4.77	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	5.30	-	3.04	3.07	-	4.59	-	-	-	-	-	2.11	-	-	-	-	-	-	-	-	-	-	-	-	-
	1	-	-	2.65	2.05	-	-	-	-	-	-	-	-	-	-	3.03	-	-	-	-	-	-	-	-	-	-

N

WWTP Simmering Effluent	2	6.25	-	4.33	4.81	-	6.89	5.52	-	-	-	-	-	-	-	6.05	-	-	-	-	-	-	-	-	-	8.56
	3	4.26	-	4.14	4.06	-	4.90	-	-	-	-	-	-	-	-	5.17	-	-	-	-	-	-	-	-	-	7.43
	4	2.93	-	2.43	2.25	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
WWTP Simmering Downstream	1	3.96	-	2.24	1.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	2	-	-	3.29	2.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.56
	3	3.10	-	3.36	3.27	-	5.39	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	-	-	2.36	1.25	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
WWTP Simmering Downstream Other	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	2	-	-	3.60	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.63
	3	4.68	-	4.22	3.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	3.96	-	3.75	1.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Danube Upstream	1	2.67	-	1.41	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	2	-	-	3.39	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.05
	3	-	-	4.17	3.53	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	8.03
	4	4.86	-	3.34	1.86	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
WWTP Klosterneuburg Effluent	1	-	-	2.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4.55
	2	3.55	-	3.33	-	-	-	-	-	-	-	-	-	-	-	4.61	-	-	-	-	-	-	-	-	-	6.56
	3	3.35	-	4.16	3.92	-	5.88	-	-	-	-	-	-	-	-	4.81	-	-	-	-	-	-	-	-	-	-
	4	-	-	3.46	3.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4.94
WWTP Klosterneuburg Downstream	1	-	-	2.50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3.22
	2	-	-	3.29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.57
	3	3.89	-	4.12	3.29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	4.76	-	4.78	2.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
WWTP Klosterneuburg Downstream Other	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	2	-	-	3.34	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5.73
	3	-	-	-	2.96	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	3.91	-	3.62	1.72	-	-	-	-	-	-	-	2.28	-	-	-	-	-	-	-	-	-	-	-	-	-
Danube Downstream	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	2	-	-	3.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.17
	3	-	-	-	3.41	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

	4	-	-	2.50	0.73	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Danube Airport	1	-	-	1.99	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.19
	2	-	-	3.36	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.63
	3	3.83	-	-	2.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Appendix 10: All mean concentrations and standard deviations (ng/L) for water samples and the sum of all TDC without Carbamazepine.

Sampling Location	Campaign	2-amino BTH		BHA		DPG		5-Me BTR		PPD		DTG		2-OH BTH		IPPD		BTH	
		Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
Wienfluss	1	51.49	7.39	0.00	0.00	411.85	34.46	14.08	2.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	600.89	82.39
	2	1.03	0.10	0.00	0.00	8.59	0.60	3.68	0.28	0.00	0.00	0.00	0.00	0.00	0.00	7.85	0.15	0.00	0.00
	3	1.36	0.15	0.00	0.00	18.94	2.02	22.14	1.35	0.00	0.00	0.51	0.18	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	3.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesingbach Rural	1	17.72	1.55	0.00	0.00	137.20	24.14	9.37	2.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	1.90	0.05	0.00	0.00	17.82	1.72	25.17	1.87	0.00	0.00	0.17	0.01	0.00	0.00	0.00	0.00	0.00	0.00
	3	2.16	0.60	0.00	0.00	34.19	1.45	124.85	5.66	0.00	0.00	1.69	0.62	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	291.24	167.98	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesingbach Tangente	1	31.94	3.16	0.00	0.00	270.21	81.04	12.26	7.86	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	411.40	100.19
	2	3.77	0.41	0.00	0.00	37.21	0.62	20.72	1.48	0.00	0.00	0.16	0.01	0.00	0.00	0.00	0.00	0.00	0.00
	3	1.65	0.09	0.00	0.00	23.95	3.86	53.50	0.18	0.00	0.00	0.49	0.09	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	37.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Channel Nussdorfer	1	2.81	0.31	0.00	0.00	19.63	0.43	19.07	10.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	2.98	0.07	8.91	0.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.69	0.16	0.00	0.00	12.07	0.05	69.43	2.47	0.00	0.00	0.77	0.81	0.00	0.00	0.00	0.00	0.00	0.00
	4																		
Danube Channel Wienfluss	1	3.46	0.58	0.00	0.00	25.15	4.62	28.04	7.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	2.94	0.04	9.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	4.54	6.42	0.00	0.00
	3	0.84	0.00	0.00	0.00	13.19	0.70	82.57	4.76	0.00	0.00	0.29	0.13	0.00	0.00	0.00	0.00	0.00	0.00
	4	156.94	121.65	0.00	0.00	289.45	113.63	10634.42	7512.07	0.00	0.00	61.34	60.33	0.00	0.00	0.00	0.00	0.00	0.00
Danube Chan	1	2.89	0.37	0.00	0.00	29.77	4.85	106.28	95.81	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	3.22	0.14	9.76	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

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	3	0.94	0.15	0.00	0.00	15.32	0.28	91.04	8.79	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	131.57	186.07	0.00	0.00	1253.22	1746.02	5935.54	8323.62	0.00	0.00	26.70	37.76	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Effluent	1	15.05	0.00	0.00	0.00	212.86	39.58	283.23	36.73	0.00	0.00	0.00	0.00	126.54	19.00	0.00	0.00	761.67	42.15
	2	3.03	0.00	0.00	0.00	84.48	70.61	177.49	1.72	0.00	0.00	0.28	0.01	19.84	28.06	0.00	0.00	0.00	0.00
	3	13.29	0.00	0.00	0.00	157.07	3.01	476.69	2.54	0.00	0.00	1.26	0.13	68.06	8.12	0.00	0.00	0.00	0.00
	4	413.72	0.00	0.00	0.00	863.26	1106.94	7678.68	10432.04	0.00	0.00	3.35	0.00	2084.04	2947.28	0.00	0.00	0.00	0.00
WWTP Simmering Downstream	1	9.13	0.64	0.00	0.00	188.56	47.50	108.66	11.66	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.44	0.01	0.00	0.00	7.29	0.18	39.11	0.72	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	2.38	0.03	0.00	0.00	38.46	4.53	177.30	15.05	0.00	0.00	0.30	0.10	0.00	0.00	0.00	0.00	0.00	0.00
	4	350.55	421.22	0.00	0.00	1349.06	1556.36	18615.09	18548.78	0.00	0.00	26.39	37.32	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Downstream	1	2.92	0.22	0.00	0.00	48.91	12.00	30.80	3.37	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	2.78	0.06	9.54	0.87	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	1.05	0.03	0.00	0.00	14.02	0.66	89.90	2.79	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	31.62	0.00	0.00	0.00	121.23	0.00	3994.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Upstream	1	2.43	0.61	0.00	0.00	36.26	13.27	79.89	89.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	3.37	0.90	10.42	1.56	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.92	0.06	0.00	0.00	14.11	0.48	86.79	9.42	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	223.00	123.68	0.00	0.00	456.61	127.81	13602.64	1283.68	0.00	0.00	27.79	39.30	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Effluent	1	3.81	0.00	0.00	0.00	43.89	5.61	19.72	5.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.84	0.00	0.00	0.00	14.33	0.93	20.37	1.16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	16.16	0.00	0.00	0.00	138.40	45.26	717.20	237.89	0.00	0.00	0.67	0.34	283.19	336.70	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	213.80	1.48	170.69	11.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Downstream	1	3.06	0.24	0.00	0.00	51.13	20.64	25.04	8.84	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	3.46	0.07	11.05	0.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.91	0.18	0.00	0.00	15.13	4.85	93.77	22.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	11.42	16.15	0.00	0.00	17.03	7.71	1599.71	2179.16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Downstream	1	2.19	0.42	0.00	0.00	28.21	4.18	18.21	4.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	2.63	0.66	8.68	1.53	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	1.06	0.21	0.00	0.00	16.08	5.65	95.02	16.88	0.00	0.00	0.07	0.10	0.00	0.00	0.00	0.00	0.00	0.00
	4	106.33	150.38	0.00	0.00	352.76	453.77	7982.33	11172.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Danube Downstream	1	6.47	0.34	0.00	0.00	106.14	26.84	43.20	4.83	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	4.41	0.42	19.17	1.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.79	1.12	0.00	0.00	11.74	16.60	65.59	92.76	0.00	0.00	0.09	0.13	0.00	0.00	0.00	0.00	0.00	0.00
	4	500.21	451.62	0.00	0.00	1304.41	907.30	38927.86	22824.50	0.00	0.00	8.03	11.35	0.00	0.00	0.00	0.00	0.00	0.00
Danube Airport	1	5.47	0.18	0.00	0.00	68.56	0.44	40.36	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	3.22	0.19	14.36	0.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	1.37	0.11	0.00	0.00	20.74	0.36	143.38	1.65	0.00	0.00	0.14	0.01	0.00	0.00	0.00	0.00	0.00	0.00
	4																		
Field Blanks	1	9.41	0.00	0.00	0.00	3.51	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	8.21	0.32	0.00	0.00	7.35	0.14	0.00	0.00	0.00	0.00	8.40	0.31	0.00	0.00	0.00	0.00	0.00	0.00
	3	22.20	0.96	0.00	0.00	14.93	0.87	3.17	0.11	0.00	0.00	9.48	0.44	0.00	0.00	0.00	0.00	0.00	0.00
	4	37.68	3.15	0.00	0.00	30.66	0.09	29.08	7.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		2-S BTH		**2-Me BTH**		**HMMM**		**CPPD**		**DPTU**		**Aniline**		**6PPD**		**IPPDq**		**DPPDq**	
Sampling Location	**Campaign**	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
Wienfluss	1	0.00	0.00	0.00	0.00	509.31	63.86	0.00	0.00	0.00	0.00	852.32	110.40	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	17.66	12.49	0.00	0.00	33.48	0.08	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	33.73	0.47	0.00	0.00	6.16	0.59	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	45.04	27.93	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesingbach Rural	1	0.00	0.00	0.00	0.00	204.44	23.07	0.00	0.00	0.00	0.00	193.46	22.95	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	33.17	0.95	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	29.74	2.13	0.00	0.00	6.15	0.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	67.60	67.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesingbach Tangente	1	0.00	0.00	0.00	0.00	402.90	123.60	0.00	0.00	0.00	0.00	437.82	142.39	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.88	1.25	0.00	0.00	0.00	0.00	80.17	4.22	25.80	0.03	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	21.85	0.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	45.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Donau	1	0.00	0.00	0.00	0.00	29.64	8.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

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	2	0.00	0.00	2.21	3.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	16.61	12.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4																		
Danube Channel Wienfluss	1	0.00	0.00	0.00	0.00	34.43	16.89	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	27.88	2.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	6558.05	4963.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Channel Tangente	1	0.00	0.00	0.00	0.00	36.69	1.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	32.84	2.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	4392.39	6211.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Effluent	1	0.00	0.00	0.00	0.00	391.64	34.14	0.00	0.00	0.00	0.00	129.23	6.63	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	1.16	0.00	0.00	0.00	0.00	0.00	46.98	15.31	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	103.62	9.85	0.00	0.00	8.25	0.00	53.04	5.17	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	2107.41	2916.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Downstream	1	0.00	0.00	0.00	0.00	175.96	16.28	0.00	0.00	0.00	0.00	101.60	2.73	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	39.11	5.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	7923.28	8071.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Downstream	1	0.00	0.00	0.00	0.00	34.26	4.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	31.01	1.69	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	2366.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Upstream	1	0.00	0.00	0.00	0.00	28.30	9.74	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	27.11	3.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	8994.23	1722.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg	1	0.00	0.00	0.00	0.00	29.39	6.60	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8.73	12.35	0.00	0.00	0.00	0.00	0.00	0.00
	3	140.26	198.36	16.36	23.13	44.66	8.00	0.00	0.00	0.00	0.00	39.41	6.29	0.00	0.00	0.00	0.00	0.00	0.00

	4	0.00	0.00	0.00	0.00	3.14	4.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Downstream	1	0.00	0.00	0.00	0.00	34.01	11.74	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	28.53	7.43	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	953.83	1348.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Downstream	1	0.00	0.00	0.00	0.00	23.78	8.35	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	29.04	6.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	3989.13	5625.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Downstream	1	0.00	0.00	0.00	0.00	89.94	13.67	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	16.32	23.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	23832.47	16621.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Airport	1	0.00	0.00	0.00	0.00	84.30	1.88	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	35.55	0.79	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4																		
Field Blanks	1	0.00	0.00	0.00	0.00	2.88	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	181.53	11.10	0.00	0.00	32.87	0.57	8.05	0.03	0.00	0.00	130.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		CPPDq		**BHT**		**6PPDq**		**DPPD**		**Neozone**		**CBS**		**AO2246**		**Carbamazepine**		**Σ TDC**	
Sampling Location	**Campaign**	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
Wienfluss	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.04	8.54	69.55	11.78	2445.98	156.13
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.39	3.19	6.01	0.10	76.69	12.91
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	15.65	8.12	35.36	0.55	98.48	8.52
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	40.75	16.39	48.24	27.93

Liesingbach Rural	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	46.56	11.33	562.20	40.61
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9.71	7.60	13.47	0.58	87.95	8.07
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9.74	13.78	125.01	7.24	208.51	15.14
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	163.06	94.60	358.84	180.94
Liesingbach Tangente	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	12.13	11.81	1566.53	228.54
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.92	3.88	3.20	0.13	172.63	6.09
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.48	4.93	47.44	0.15	104.92	6.27
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	45.86	0.00	82.56	0.00
Danube Channel Nussdorfer	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	71.14	13.29
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.30	1.45	2.05	0.18	17.40	3.52
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8.55	12.09	4.40	6.23	108.11	17.40
	4																		
Danube Channel Wienfluss	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.11	7.23	91.07	18.87
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.96	5.23	2.14	0.10	23.44	8.28
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.49	2.10	13.40	1.26	126.25	5.74
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3347.79	2836.58	17700.20	9005.25
Danube Channel Tangente	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	11.69	1.44	175.63	95.95
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.30	2.65	1.98	0.00	17.28	2.66
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	13.02	3.11	15.81	1.77	153.30	9.59
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1945.23	2739.03	11739.43	10533.45
WWTP Simmering Effluent	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	566.95	100.02	1920.81	79.14
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	10.65	3.55	21.61	0.20	343.91	77.61
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	21.70	3.56	148.41	7.24	902.97	14.77
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3232.14	4413.53	13150.45	11280.34
WWTP Simmering Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	15.63	22.10	108.01	12.25	599.55	56.16
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.52	1.29	8.07	0.07	52.37	1.49
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8.39	4.86	57.99	5.77	265.94	17.23
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8739.93	7744.96	28264.36	20293.18
WWTP Sim	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.78	3.48	116.89	13.16
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.98	2.29	2.05	0.16	16.31	2.45

	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.90	9.76	16.21	1.84	142.87	10.31
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1161.80	0.00	6513.29	0.00
Danube Upstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.32	8.40	146.88	91.30
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.48	0.20	1.92	0.21	18.28	1.81
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.68	0.96	13.55	2.60	129.61	10.28
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3480.83	998.84	23304.27	2155.69
WWTP Klosterneubur g Effluent	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	15.68	22.18	6.72	6.82	112.49	24.36
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.83	0.67	13.24	1.07	48.11	12.46
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	135.74	36.58	1396.31	460.42
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	35.78	50.61	56.68	7.88	423.42	52.03
WWTP Klosterneubur g Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	30.49	43.12	10.12	7.74	143.72	50.01
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.51	1.58	1.99	0.04	19.03	1.65
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	12.82	18.13	14.53	3.89	151.15	30.03
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	541.84	754.24	2581.99	2562.93
WWTP Klosterneubur g Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.20	4.52	72.40	10.24
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.72	1.21	1.67	0.12	15.03	2.05
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9.66	10.93	14.30	4.03	150.94	22.03
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1975.37	2778.57	12430.56	12517.52
Danube Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.22	7.38	38.62	9.06	250.96	31.39
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.79	1.41	4.00	0.05	28.37	1.80
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.11	2.99	18.47	26.11	96.64	97.07
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	16902.25	9235.21	64572.99	28253.36
Danube Airport	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9.03	12.77	27.40	0.42	207.72	12.92
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.62	0.15	1.62	0.60	21.20	0.94
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	12.16	7.50	29.43	8.68	213.34	7.73
	4																		
Field Blanks	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	125.32	0.00	0.00	0.00	141.12	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.06	0.30	0.00	0.00	26.03	0.56
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	43.14	10.70	0.00	0.00	92.92	10.78
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	21.13	1.34	7.58	1.79	471.63	13.71

Appendix 11: All mean concentrations and standard deviations (µg/kg) for SPM samples and the sum of all TDC without Carbamazepine.

Sampling Location	Campaign	2-amino BTH		BHA		DPG		5-Me BTR		PPD		DTG		2-OH BTH		IPPD		BTH	
		Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
Wienfluss	1	0.00	0.00	0.00	0.00	64.64	36.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	252.47	357.05	0.00	0.00	8820.42	12473.95	0.00	0.00	0.00	0.00	86.45	122.27	8563.35	12110.41	7905.82	11180.52	0.00	0.00
	3	375.45	530.97	0.00	0.00	3122.92	1917.25	8407.25	11254.62	0.00	0.00	2273.91	1839.17	0.00	0.00	0.00	0.00	0.00	0.00
	4	858.77	1214.48	0.00	0.00	2626.51	2426.96	307.42	287.56	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesingbach Rural	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	660.43	235.68	0.00	0.00	3991.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	106.68	27.30	0.00	0.00	1519.13	1657.03	512.14	80.64	0.00	0.00	561.64	686.78	0.00	0.00	0.00	0.00	0.00	0.00
	4	3645.10	5154.95	0.00	0.00	1751.43	2465.70	1113.86	1546.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesingbach Tangente	1	3.72	5.26	0.00	0.00	78.88	97.86	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	855.35	528.79	0.00	0.00	1376.13	0.00	0.00	0.00	2278.09	491.79	0.00	0.00	971.34	1373.68
	3	0.00	0.00	0.00	0.00	1734.40	114.93	452.04	48.01	0.00	0.00	585.75	651.07	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	871.37	0.00	236.69	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Channel Nussdorfer Wehr	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	43.78	13.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	42.25	59.74	73.37	24.60	0.00	0.00	16.29	11.58	0.00	0.00	0.00	0.00	0.00	0.00
	4																		
Danube Channel Wienfluss Inflow	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	37.01	7.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	161.14	227.88	0.00	0.00
	3	0.00	0.00	0.00	0.00	148.52	64.96	120.27	21.66	0.00	0.00	650.18	868.27	0.00	0.00	0.00	0.00	0.00	0.00
	4	218.95	309.65	0.00	0.00	526.60	112.27	316.91	77.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Channel Tangente	1	0.68	0.96	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	72.44	1.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	13.42	18.98	98.78	24.32	0.00	0.00	8.30	11.73	0.00	0.00	0.00	0.00	0.00	0.00
	4	26445.94	37348.01	0.00	0.00	1381.25	1854.58	7015.13	9821.48	0.00	0.00	1030.92	1457.93	0.00	0.00	0.00	0.00	0.00	0.00

WWTP Simmering Effluent	1	0.00	0.00	0.00	0.00	47.48	67.15	31.91	2.51	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	5362.86	0.00	0.00	0.00	904.72	1279.46	5689.97	8046.84	2401.86	0.00	1077.20	1523.39	6521.65	9223.00	0.00	0.00	0.00	0.00
	3	242.51	183.95	0.00	0.00	2149.84	2189.70	5482.14	3992.28	0.00	0.00	99.30	70.48	0.00	0.00	0.00	0.00	0.00	0.00
	4	353.75	0.00	0.00	0.00	231.39	145.66	1381.22	949.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Downstream	1	83.60	118.23	0.00	0.00	32.71	46.26	1.34	1.89	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	14.33	5.64	6.69	9.16	307.88	0.00	0.00	0.00	267.70	378.58	0.00	0.00	0.00	0.00
	3	2.97	4.20	0.00	0.00	88.78	69.98	331.35	16.09	0.00	0.00	73.12	56.05	3190.99	4512.74	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	306.26	286.71	334.36	101.95	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Downstream Other	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	11.02	6.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	50.10	70.85	0.00	0.00	233.17	161.85	127.92	0.00	0.00	0.00	126.26	147.61	2414.18	3414.17	0.00	0.00	0.00	0.00
	4	285.32	403.50	0.00	0.00	688.57	434.86	102.77	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Upstream	1	1.14	1.61	0.00	0.00	0.92	1.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	8.26	6.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	206.67	65.57	196.52	0.00	0.00	0.00	63.60	29.02	0.00	0.00	0.00	0.00	0.00	0.00
	4	16238.06	22964.09	0.00	0.00	1001.41	641.71	916.48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Effluent	1	0.00	0.00	0.00	0.00	7.99	6.41	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	1.48	2.09	0.00	0.00	30.97	6.61	0.00	0.00	830.27	0.00	0.00	0.00	330.42	467.29	0.00	0.00	0.00	0.00
	3	18.01	25.48	0.00	0.00	2004.49	2161.90	5975.10	5431.28	0.00	0.00	252.33	356.85	0.00	0.00	0.00	0.00	0.00	0.00
	4	3.19	4.51	0.00	0.00	619.08	843.25	464.76	632.58	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Downstream	1	0.00	0.00	0.00	0.00	16.22	22.93	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	6.71	2.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	7.06	9.98	0.00	0.00	198.96	182.55	181.43	7.01	0.00	0.00	0.76	1.08	0.00	0.00	0.00	0.00	0.00	0.00
	4	658.21	930.85	0.00	0.00	1017.38	1046.58	764.63	565.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	5.82	8.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	86.20	21.68	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	858.89	1214.65	0.00	0.00	1468.70	1906.35	420.69	442.31	0.00	0.00	193.85	274.14	0.00	0.00	0.00	0.00	0.00	0.00
Danube Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	5.58	3.87	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	3	0.00	0.00	0.00	0.00	0.00	0.00	167.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	417.22	18.31	206.69	92.69	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Airport	1	0.00	0.00	0.00	0.00	6.69	9.47	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	7.35	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	9.17	12.97	0.00	0.00	0.00	0.00	135.35	20.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4																		
Field Blanks	1	59.77	0.00	0.00	0.00	43.65	0.00	18.24	0.00	0.00	0.00	0.00	0.00	1155.38	0.00	0.00	0.00	894.68	0.00
	2	450407.26	554433.69	0.00	0.00	388563.85	0.00	0.00	0.00	0.00	0.00	447363.31	554216.54	0.00	0.00	0.00	0.00	250436.86	0.00
	3	27305.30	6292.07	0.00	0.00	22923.08	0.00	5069.25	1252.49	0.00	0.00	12204.14	3257.43	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	601.66	0.00	474.87	62.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

		2-S BTH		2-Me BTH		HMMM		CPPD		DPTU		Aniline		6PPD		IPPDq		DPPDq	
Sampling Location	Campaign	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
Wienfluss	1	0.00	0.00	11.53	1.06	0.00	0.00	0.00	0.00	0.00	0.00	1066.20	267.02	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2655.98	3756.13	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3122.92	1917.25	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesingbach Rural	1	0.00	0.00	24.18	2.40	0.00	0.00	0.00	0.00	0.00	0.00	61.01	86.29	2.84	4.02	2.84	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9223.36	4860.93	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1519.13	1657.03	0.00	0.00	0.00	0.00
	4	27340.07	38664.70	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesingbach Tangente	1	0.00	0.00	15.26	21.59	0.00	0.00	0.00	0.00	0.00	0.00	406.86	512.06	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8615.06	1585.01	6328.11	638.64	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1734.40	114.93	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Channel Nussdorfer Wehr	1	0.00	0.00	6.65	7.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	95.54	135.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	42.25	59.74	0.00	0.00	0.00	0.00
	4																		

Danube Channel Wienfluss Inflow	1	0.00	0.00	1.56	2.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	35.00	49.50	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	148.52	64.96	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Channel Tangente	1	0.00	0.00	8.75	3.28	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	13.42	18.98	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	561.10	793.51	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Effluent	1	0.00	0.00	0.46	0.65	0.00	0.00	0.00	0.00	0.00	0.00	139.81	31.74	0.53	0.74	0.53	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	26390.88	37322.35	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7784.67	4963.13	2149.84	2189.70	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	96.13	135.95	96.13	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	88.78	69.98	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Simmering Downstream Other	1	0.00	0.00	7.96	2.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	233.17	161.85	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Upstream	1	0.00	0.00	3.27	0.15	0.00	0.00	0.00	0.00	0.00	0.00	59.41	84.02	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	206.67	65.57	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Effluent	1	0.00	0.00	1.88	0.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	717.66	28.33	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1283.60	1815.28	2004.49	2161.90	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg	1	0.00	0.00	2.15	0.26	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	50.83	71.89	0.00	0.00	0.00	0.00	0.00	0.00

	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	198.96	182.55	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WWTP Klosterneuburg Downstream	1	0.00	0.00	3.05	4.32	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	876.56	1239.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	759.74	1074.43	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Downstream	1	0.00	0.00	1.09	1.55	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	83.46	118.03	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Airport	1	0.00	0.00	14.72	3.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4																		
Field Blanks	1	272.72	0.00	20.70	0.00	0.00	0.00	0.00	0.00	0.00	0.00	307.36	0.00	40.00	0.00	40.00	0.00	66.89	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	773065.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	22923.08	6676.94	0.00	0.00	0.00	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	53.00	0.00	0.00	0.00

		CPPDq		BHT		6PPDq		DPPD		Neozone		CBS		AO2246		Carbamazepine		Σ TDC	
Sampling Location	**Campaign**	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
Wienfluss	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6234.75	8051.61	0.00	0.00	7377.11	8056.12
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3913.88	5535.07	28284.51	21012.30
	3	0.00	0.00	0.00	0.00	432.47	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	17734.93	11733.83
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	26200.10	23108.28	297.39	320.12	29992.79	23268.87
Liesingbach Rural	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	19186.48	7105.47	0.00	0.00	19277.36	7105.99
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	567.00	202.20	13875.71	4866.64
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4218.73	2443.45
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3790.75	5128.38	239.75	330.43	37641.22	39450.01

AA

BB

Liesingbach Tangente	1	0.00	0.00	0.00	0.00	9.27	0.00	0.00	0.00	0.00	0.00	0.00	0.00	15288.73	21621.53	0.00	0.00	15802.73	21627.83
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	128.67	77.13	20424.07	2308.37
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4506.59	672.77
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6164.83	0.00	38.31	0.00	7272.90	0.00
Danube Channel Nussdorfer Wehr	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3126.42	4421.42	0.00	0.00	3133.07	4421.43
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	40.51	20.00	139.33	135.82
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	174.15	88.76
	4																		
Danube Channel Wienfluss Inflow	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.56	2.21
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	18.62	1.09	233.15	233.30
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1067.49	873.38
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	11450.83	754.60	0.00	0.00	12513.30	826.96
Danube Channel Tangente	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2753.55	312.95	0.00	0.00	2762.99	312.97
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	15.32	3.61	72.44	1.08
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	133.92	38.07
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3670.40	3662.01	0.00	0.00	40104.74	38870.82
WWTP Simmering Effluent	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	220.72	74.33
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1924873.35	2722182.00	1500.81	2122.47	1973222.50	2722466.08
	3	0.00	0.00	0.00	0.00	1014.58	0.00	0.00	0.00	0.00	0.00	0.00	0.00	589064.30	225698.49	189.95	268.63	607987.17	225809.67
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2819.85	2123.41	333.92	311.42	4786.21	2330.38
WWTP Simmering Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	309.91	186.02
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	20099.17	7344.18	17.86	0.53	20695.77	7353.94
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3776.00	4514.20
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	10064.48	650.46	0.00	0.00	10705.10	718.11
WWTP Simmering Downstream Other	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1422.20	2011.29	0.00	0.00	1430.16	2011.30
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	17159.21	12133.39	9.27	10.22	17170.23	12133.40
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3184.80	3425.75
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	10593.16	211.24	0.00	0.00	11669.83	629.71
Danube Upstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1737.51	2457.21	0.00	0.00	1802.24	2458.65
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5074.85	3588.46	6.14	6.35	5083.11	3588.46

CC

	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	72139.62	51010.42	0.00	0.00	72813.08	51010.51
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	18143.97	1366.49	0.00	0.00	36299.93	23013.66
WWTP Klosterneuburg Effluent	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	557.95	789.05	0.00	0.00	567.82	789.08
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	14051.12	8763.36	20.21	0.06	15961.91	8775.86
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	936186.30	1323967.37	0.00	0.00	947724.32	1323983.33
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6278.59	8683.60	149.82	206.47	7365.61	8747.35
WWTP Klosterneuburg Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	50.76	71.79	0.00	0.00	69.13	75.36
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	16917.81	19541.12	8.81	6.66	16975.35	19541.25
	3	0.00	0.00	0.00	0.00	194.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	781.81	258.45
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	24521.48	153.20	140.41	198.57	26961.70	1518.41
WWTP Klosterneuburg Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3093.27	4374.55	0.00	0.00	3096.33	4374.55
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1993.74	2819.57	2.61	3.58	1999.56	2819.58
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	962.76	1239.83
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9319.21	6759.99	0.00	0.00	13021.07	7227.18
Danube Downstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.09	1.55
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7082.38	10015.99	3.73	1.51	7171.41	10016.69
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	167.29	0.00
	4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9318.72	6667.87	0.00	0.00	9942.63	6668.54
Danube Airport	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	14091.17	8282.32	0.00	0.00	14112.58	8282.33
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	15602.85	11439.47	28.02	15.41	15610.19	11439.47
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	144.52	23.94
	4																		
Field Blanks	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	35888.00	0.00	0.00	0.00	38807.39	0.00
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	82364607.79	96141232.13	5161.47	5266.00	84674444.71	96144428.17
	3	0.00	0.00	0.00	0.00	11296.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	14299346.85	6890126.20	0.00	0.00	14401067.79	6890133.19
	4	0.00	0.00	0.00	0.00	1404.36	0.00	0.00	0.00	0.00	0.00	0.00	0.00	20519.77	24364.08	0.00	0.00	23053.66	24364.16

Appendix 12: All mean concentrations and standard deviations (µg/kg) for sediment samples and the sum of all TDC.

		PPD		6PPD		6PPDq		DPPD		DPPDq		IPPD		IPPDq		CPPD		CPPDq		Neozone		BTH		2-amino BTH	
Sampling Location	**Campaign**	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
Wienfluss	2	0.00	0.00	5.40	2.69	3.38	1.00	0.93	0.62	0.00	0.00	0.76	0.03	0.00	0.00	0.59	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.00
	3	0.00	0.00	2.18	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	11.66	4.91
	4	0.00	0.00	0.00	6.59	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liesing Rural	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.70	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.39	0.63
	2	0.00	0.00	0.55	0.06	0.00	0.00	0.36	0.16	0.00	0.00	0.57	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8.72	3.44
	4	0.00	0.00	2.16	2.61	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.69	0.00	0.00	0.00	0.00	0.00
Liesing Tangente	1	0.00	0.00	0.49	0.44	3.26	0.00	6.10	0.00	1.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.94	0.00	0.00	0.00	0.00	0.00
	2	0.00	0.00	15.52	9.44	12.21	2.23	5.29	5.94	0.00	0.00	0.92	0.15	0.00	0.00	0.59	0.00	0.00	0.00	0.08	0.03	0.00	0.00	0.03	0.04
	3	0.00	0.00	7.57	1.78	0.00	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	17.69	10.33
	4	0.00	0.00	14.04	5.05	0.92	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Danube Upstream	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.73	0.00
	2	0.00	0.00	0.28	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.34	0.36
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	13.49	2.34
	4	0.00	0.00	4.82	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.54	0.00	0.00	0.00	0.00	0.00
Danube Downstream	2	0.00	0.00	0.73	0.02	0.86	0.02	0.58	0.67	0.00	0.00	0.57	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	213.06	147.10
	4	0.00	0.00	2.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00

		2-OH BTH		2-Me BTH		2-S BTH		5-Me BTR		Aniline		HMMM		DPTU		CBS		DPG		DTG		AO2246		Σ TDC	
Sampling Location	**Campaign**	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
Wienfluss	2	0.00	0.00	0.00	0.00	0.00	0.00	0.17	1.19	0.00	0.00	2.06	0.82	0.00	0.00	0.00	0.00	6.44	9.19	0.00	0.00	0.00	101.75	20.07	102.22
	3	0.00	0.00	0.00	0.00	0.00	0.00	2.33	2.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	30.29	24.35	4.65	0.84	362.64	123.77	413.74	126.27
	4	0.00	0.00	0.00	0.00	0.00	0.00	2.54	0.12	0.00	0.00	0.00	1.39	0.00	0.00	0.00	0.00	0.00	6.57	0.00	0.27	0.00	196.64	2.54	196.86

Liesing Rural	1	35.20	25.94	0.00	0.00	0.00	0.00	5.21	5.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1254.07	910.85	1295.57	911.24
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	26.07	1.48	26.08
	3	0.00	0.00	0.00	0.00	0.00	0.00	3.03	1.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.58	2.77	4.11	0.24	303.42	48.02	323.27	48.26
	4	40.91	0.00	0.00	0.00	183.28	0.00	5.44	8.98	0.00	0.00	3.69	0.00	1.44	0.00	0.00	0.00	1050.97	2.12	2.41	0.97	3.62	1076.48	1294.60	1076.53
Liesing Tangente	1	6.65	6.22	0.00	0.00	0.00	0.00	3.95	1.64	0.00	0.00	1.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	67.71	23.95	68.02
	2	7.85	0.80	0.00	0.00	0.00	0.00	1.50	0.33	0.00	0.00	2.67	0.68	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.94	46.66	13.92
	3	0.00	0.00	0.00	0.00	0.00	0.00	12.58	13.35	0.00	0.00	0.00	2.65	0.00	0.00	0.00	0.00	14.12	10.86	4.40	0.48	695.87	428.76	752.22	429.24
	4	0.00	0.00	0.00	0.00	0.00	0.00	4.57	1.63	0.00	0.00	3.10	1.63	0.40	0.00	0.00	0.00	1668.73	4.15	6.19	0.78	4.09	2250.93	1702.02	2250.94
Danube Upstream	1	7.09	6.20	0.00	0.00	0.00	0.00	5.72	11.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	434.36	81.58	448.90	82.56
	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	15.12	0.62	15.13
	3	0.00	0.00	0.00	0.00	0.00	0.00	2.14	1.72	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.42	1.18	4.14	0.27	536.76	60.28	557.94	60.36
	4	0.00	0.00	0.00	0.00	0.00	0.00	6.39	0.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1395.47	0.07	1.20	0.18	3.76	1774.22	1412.16	1774.22
Danube Downstream	2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.27	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.97	2.74	1.21
	3	0.00	0.00	0.00	0.00	0.00	0.00	57.15	40.84	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	45.94	37.58	26.29	19.03	12063.52	8586.91	12405.96	8588.37
	4	0.00	0.00	0.00	0.00	0.00	0.00	9.38	0.62	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2115.56	0.06	4.21	0.48	4.53	2394.32	2136.20	2394.32

EE

B. AI Usage Disclaimer

During the preparation of this thesis, ChatGPT (OpenAI, GPT-5.5 version) and Google Gemini (Google LLC, Gemini 3.5 Flash) were used for language revision to improve readability and clarity. R code was developed with coding assistance provided by ChatGPT. After using these tools, all generated content was carefully reviewed, revised where necessary, and verified by the author. The author takes full responsibility for the content of this thesis.