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Assessing Hydrology, Biogeochemistry, and Organic Micropollutants in an Urban Stream-Aquifer System: An Interdisciplinary Data Set

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Abstract Urban expansion leads to increasing water pollution, impacting both human health and ecosystems. This decline in water quality often stems from insufficient wastewater treatment, along with runoff from both urban and agricultural areas. Water quality degradation challenges our efforts for sustainable water management and hinders progress toward the UN's Sustainable Development Goals (SDGs), particularly SDG6. Within aquatic environments, the hyporheic zone—the subsurface area where surface water and groundwater mix—plays a crucial role in facilitating pollutant turnover and overall aquatic health. Mixing between surface water and groundwater generates diverse microhabitats in the streambed with varying levels of oxygen, temperature, and chemical composition, which in turn allows diverse microbial communities to strive. The complexity of exchange flows within the hyporheic zone and associated turnover processes of pollutants and nutrients can only be assessed with detailed, cross-disciplinary data sets including data about hydrology, climatology, biogeochemistry, and the subsurface composition. However, integrated data sets of this kind are seldom available. As a result, the drivers behind pollutant dynamics in stream-aquifer systems are still not fully understood. Addressing this knowledge deficit, we present a comprehensive unique data set from an urban stream-aquifer system in Switzerland spanning over 6 months. Incorporating hydrometric, tracer, nutrient, microbial and organic micropollutant data, our data set can help to shed light on the intricate mechanisms governing hyporheic exchange flows, as well as nutrient and organic micropollutant cycling in urban environments.

Plain Language Summary Polluted water can have negative impacts on human health and other animals and organisms living in water. One of the main reasons for water pollution in urban areas is that wastewater is not always treated properly, and rain can wash harmful substances from cities and farms into streams and groundwater. However, nature has the capacity to clean up some of the pollution. Below rivers and lakes lies the hyporheic zone—an area where water from surface waters mixes with groundwater. The organisms living in this zone can naturally remove some of the pollution, which can improve the water quality. However, assessing how the self-cleaning of the hyporheic zone works is difficult because we rarely have all the data necessary to study it in detail. This data paper provides a detailed set of different kinds of data collected from an urbanized area in Switzerland over 6 months. We believe that the comprehensive data set presented here will help other scientists understand how the hyporheic zone works, especially in urban environments.

1. Introduction

Increasing urbanization, typically paired with a corresponding rise in water pollution, is a global concern (Rockström et al., 2023; Schwarzenbach et al., 2010). Degrading water quality has far-reaching socio-economic and ecological repercussions, posing substantial threats to the well-being of humans and ecosystems and challenging sustainable water resource management (e.g., Burri et al., 2019; Lintern et al., 2020; Rockström et al., 2023). The continued pollution of freshwater resources primarily stems from ineffective treatment or disposal of wastewater as well as from surface runoff from agricultural and urban areas (e.g., Burri et al., 2019; Kolpin et al., 2002; Schönenberger & Stamm, 2021). Addressing water pollution is vital to meeting the UN Sustainable Development Goals and ensuring a safe and equitable future on Earth (Rockström et al., 2023). Assessing water pollution
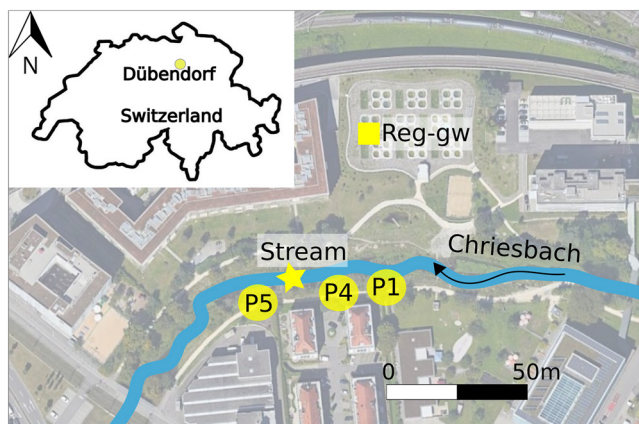
Figure 1. Overview of the study site with sampling locations, that is, the piezometers P1, P4, and P5 (circles), the stream (star), and the regional groundwater (Reg-gw; rectangle) highlighted in yellow. The map top left shows the approximate location of the study site, the city of Dübendorf in Switzerland.

dynamics requires an in-depth understanding of the nexus between climatology, hydrology, biogeochemistry, and subsurface composition. However, openly available, interdisciplinary data sets that allow studying these complex linkages, especially with a spatial and temporal resolution, remain scarce.

Recognizing these environmental challenges underscores the critical role of nature-based solutions (NRBs) such as stream restoration with the goal of reviving ecosystem functioning to enhance water quality (e.g., Lammers & Bledsoe, 2017). Central in the context of aquatic health is the hyporheic zone—the interface between surface water and groundwater—which plays a pivotal role in stream ecosystem functioning. Recognized as a hotspot for the transformation of pollutants through stream-aquifer interactions, enhancing hyporheic exchange flow through measures such as stream restoration is key to improving pollutant degradation and other vital ecosystem services (e.g., Boano et al., 2014; Boulton et al., 1998; Lewandowski et al., 2019). Thus, understanding how and when interactions between surface water and groundwater facilitate nutrient and pollutant turnover is fundamental for better managing water resources (Bencala, 1993; Boulton et al., 1998; Hester & Gooseff, 2010; Lewandowski et al., 2019). This understanding becomes particularly critical in urban environments, where anthropogenic influences such as wastewater treatment plants have pronounced impacts on the water quality by introducing substantial loads of nutrients and organic micropollutants to surface waters (Burri et al., 2019; Kolpin et al., 2002). Likewise, stream restoration projects in urban areas become more common. By deepening our understanding of the ecosystem services provided by hyporheic zones, future restoration efforts can be optimized to enhance water quantity and quality.

Hyporheic zones are highly dynamic in space and time: for instance, the hydraulic conductivity of the stream bed or bank can vary several orders of magnitude and can highly affect surface water-groundwater interactions and pollutant turnover (e.g., Naganna et al., 2017; Newcomer et al., 2016; Popp et al., 2020). Moreover, extreme flow events, temperature changes and the release of wastewater from treatment plants all considerably impact pollutant turnover at the interface of surface and groundwater systems, hampering the accurate quantification of the fate of pollutants (e.g., Barth et al., 2007; Krause et al., 2022). The inherent complexity of stream-aquifer systems and the variable spatiotemporal distribution of anthropogenic substances demand a comprehensive and integrated data set to assess the dynamics of surface water-groundwater interactions and associated pollutant turnover. However, existing databases often provide either tracer, nutrient, or organic micropollutant data, but rarely are interdisciplinary data sets combined and openly available. Spatiotemporally-resolved data that allow studying the intertwined hydrological and (bio-)geochemical dynamics of stream-aquifer systems are seldom, most likely due to the high costs associated with sampling and analyzing a wide range of parameters, especially for non-standard parameters such as organic micropollutants.

This data paper presents a spatiotemporally-resolved data set that spans a 6-month period and includes hydrometric, tracer, nutrient, and organic micropollutant data from an urban stream-aquifer system. This unique data set can help to better understand the interaction, feedback- and transport mechanisms of hyporheic exchange flow and nutrient and organic micropollutant dynamics in urban environments with potential insights relevant to water managers and environmental policymakers.

2. Methods

2.1. Field Site

The field site is located in northern Switzerland in the city of Dübendorf (Figure 1). We studied a reach of the stream "Chriesbach," which is a heavily urbanized, losing stream. With no sewer overflow occurring, about 30% of the stream's discharge consists of treated wastewater. 900 m of the stream, including the studied stream reach, have been restored in 2014. This restoration effort has been shown to considerably increase surface water-groundwater interactions (Kurth et al., 2015). Previous research has also shown that nutrient concentrations and turnover at the study site are highly variable in space and time (Popp et al., 2020). For a more detailed depiction of the site, we refer to Popp et al. (2020).

Table 1
Overview List of Parameters Obtained at the Study Site Between January and June 2018 (for Details See List Below)

Parameters	Location	Temporal resolution	Data access
Meteorological Data			
Air temperature and precipitation	Measurement station "Dübendorf-Empa" of the Swiss Federal Office for the Environment	Hourly	Data set S7 in Popp, Manning, et al. (2019)
Hydrological Data			
Water levels	Stream, P1 and P4	Quarter-hourly (i.e., every 15 min)	Data sets S5 (stream) and S6 (P1 and P4) in Popp, Manning, et al. (2019)
Hydraulic conductivity	P1, P4, P5	Discrete data	Data set S4 in Popp, Manning, et al. (2019)
Microbiological Data			
Total Cell Concentrations	Stream, P1, P4, P5	Sporadic sampling every few weeks	Data set S3 in Popp, Manning, et al. (2019)
Tracer and Hydrochemical Data			
Dissolved noble and reactive gases and derivatives	P1, P4, P5	Quasi-continuously, resolution <1 hr	Data sets S1-1 to S1-3 in Popp, Manning, et al. (2019)
Major ions and other hydrochemical data	Stream, P1, P4, P5, regional groundwater	~Weekly to quarter-hourly	Popp et al. (2023) (this work)
Nutrients	Stream, P1, P4, P5, regional groundwater	~Weekly	Popp et al. (2023) (this work)
Radioactive tracer (radon-222)	Stream, P1, P5, regional groundwater	Discrete data	Popp et al. (2023) (this work)
Organic micropollutant data			
Various industrial and pharmaceutical pollutants	Stream, P1, P4, P5, regional groundwater	Sporadic sampling	Popp et al. (2023) (this work)

2.2. Experimental Setup, Field Sampling, and Data

From January to June 2018, we sampled water from three 6 m deep piezometers (called "P1," "P4," and "P5") which are screened over their entire lengths and located in close approximation (0.5 m) from the stream (Figure 1). Additionally, we collected water samples from the Chriesbach stream and a 10 m deep well representing regional groundwater ("Reg-gw"; Figure 1). The water samples were analyzed for various parameters with different temporal resolutions (Table 1). Note that we did not assess aquifer stratification, as the aquifer is only up to 20 m deep and the subsurface is known to be homogeneous (Popp et al., 2020). Moreover, since the piezometers are shallow and screened over their entire length stratification and borehole clogging should not be an issue.

Table 1 provides information about the resolution and access to all available data newly (this paper) and previously published (Popp et al., 2020), encompassing

- meteorological data, that is, precipitation and air temperature;
- hydrological data, that is, water levels of the stream and piezometers (except for P5; Figure 2) and estimates of hydraulic conductivities of the streambank;
- tracers and hydrochemical parameters (Figure 3), that is, dissolved reactive and noble gases (N_2, O_2, He, Ar, Kr) and derivatives (i.e., excess air amount, groundwater recharge temperature, N_2 from denitrification), alkalinity, calcium, chloride, electrical conductivity (EC), dissolved organic carbon (DOC), magnesium, natrium, oxygen [O_2] including O_2 saturation, pH, potassium, radon-222, silica acid, sulfate, total inorganic carbon (TIC), total hardness, total organic carbon (TOC), water temperature;
- nutrients (Figure 4), that is, nitrate, nitrite, ammonium, total nitrogen, phosphate, total phosphorus;
- microbiological data, that is, total cell counts (TCC);
- organic micropollutants (Figure 5; International Chemical Identifiers [InChIKeys]) can be found in the readme file "3_micropollutant-readme" on Zenodo), that is,
  - pesticides: atrazine**, chloridazon-methyl-desphenyl**, DCPMU (3-(3,4-dichlorophenyl)-1-methyl urea; degradation product of diuron), diuron, terbutylazine;
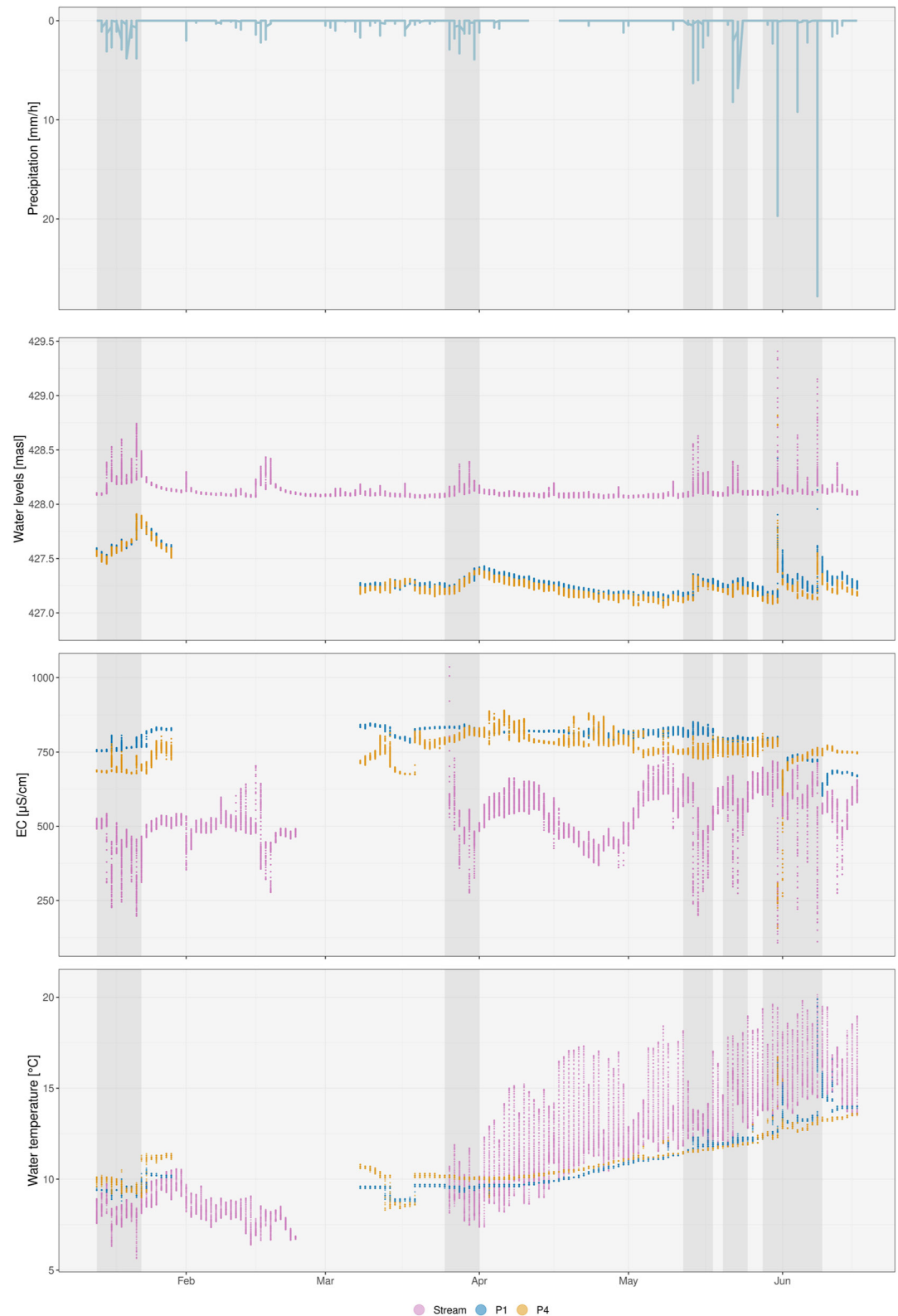
Figure 2. Hydrological and hydrochemical conditions for the duration of our experiment. Precipitation data provided by the Swiss Federal Office for the Environment (top column) and logger data (i.e., water level, EC, and water temperature) continuously recorded at P1, P4 and the stream; logger data from P5 are distorted due to logger malfunctioning and are therefore not included. Logger data from Reg-gw do not exist. Darker gray segments indicate precipitation events.

Figure 3. Example data: distribution of typical hydrologic tracers measured at P1, P4, P5, the regional groundwater (Reg-gw) and the Chriesbach (stream). Gray segments represent precipitation events.

- pharmaceuticals: atenolol, atenolol acid* (degradation product of atenolol), candesartan, carbamazepine*, carbamazepine 10,11 epoxide (degradation product of carbamazepine), diclofenac**, hy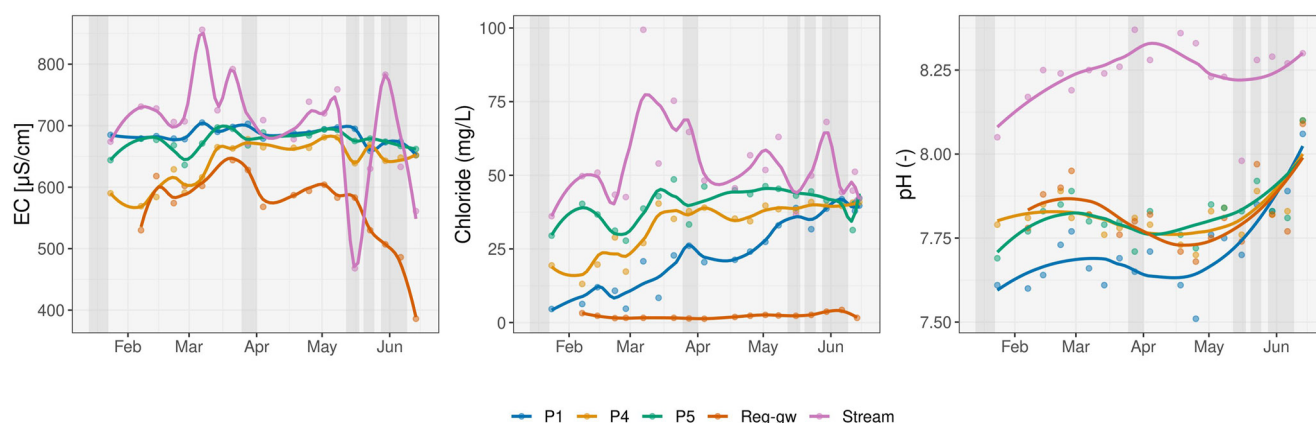drochlorothiazide**, lamotrigine**, N4 acetyl sulfamethoxazole** (degradation product of sulfamethoxazole), paracetamol, sulfamethoxazole**, valsartan**;
- anti-corrosion agents: 5-methyl-benzotriazole**, benzotriazole**;
- lifestyle product: caffeine.

We tested whether there were significant differences in parameters (i.e., organic micropollutants and tracers) between the different sampling locations. Note that differences between sampling locations are anticipated due to the various water sources of samples, which include surface water, very shallow groundwater, and regional groundwater. Moreover, the hydraulic conductivity in the streambank varies over two orders of magnitude and
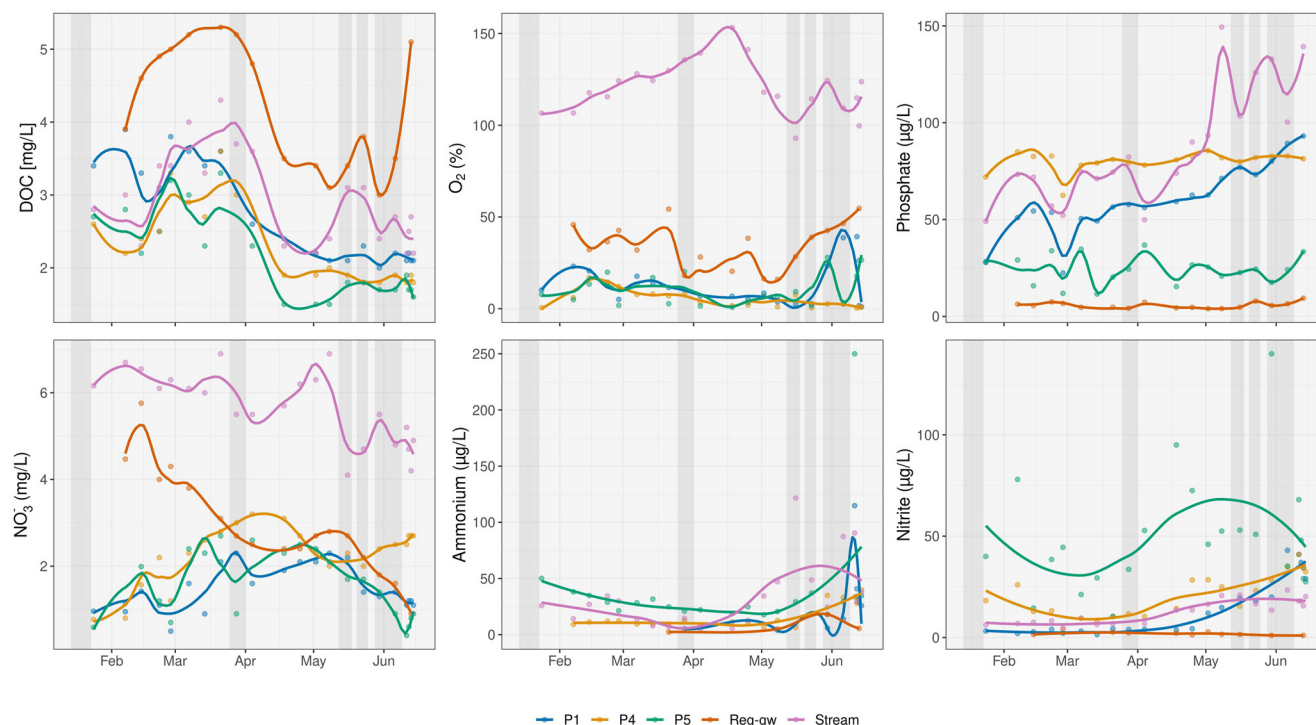

Figure 4. Example data: distribution of various nutrients and other biogeochemically relevant parameters measured at P1, P4, P5, the regional groundwater (Reg-gw) and the Chriesbach (stream). Gray segments represent precipitation events.
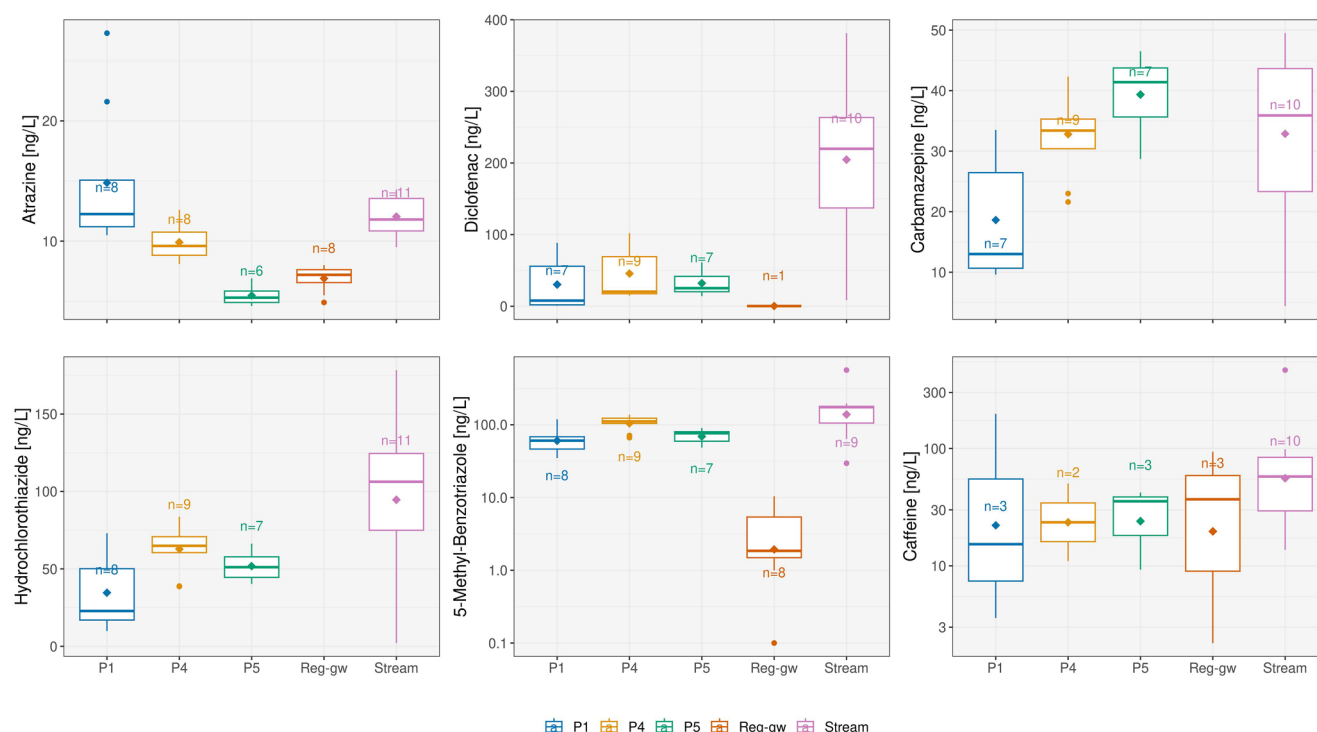
Figure 5. Example data: boxplots of various organic micropollutants with different origins, retention, adsorption and degradation behavior measured at P1, P4, P5, the regional groundwater (Reg-gw) and the Chriesbach (Stream); n indicates the number of samples plotted omitting samples where no concentrations were detected or where concentrations were below the limits of quantification. Hydrochlorothiazide and carbamazepine concentrations were not detectable in the regional groundwater well. Diamonds represent mean values.

greatly influences nutrient turnover, as demonstrated by Popp et al. (2020). Given that the majority of our data do not follow a normal distribution, we employed the Kruskal-Wallis Test, which is a non-parametric test that determines if there are statistically significant differences between two or more groups of an independent variable. Organic micropollutant compounds that are significantly different are marked with * (p-value < 0.05) and ** (p-value < 0.01) in the list above (parameters without an * are not significantly different between sampling locations or do not have data from more than one sampling location). We used R version 4.2.2 and RStudio version 2021.09.2 + 382 for the statistical analyses and data plotting; scripts for data analysis are provided in the linked data file (Popp et al., 2023).

For the water quality analyses (hydrochemical parameters and nutrients), we took water samples in 1 L Schott glass bottles. The bottles were cooled immediately after sampling and analyzed the following day at an accredited laboratory at Eawag (see data files for instruments used, units, and uncertainties). Only pH, O_2, EC and temperature were measured with a hand-held, calibrated HACH HQ40D portable multimeter. EC and temperature were also continuously measured with Ott CTD probes at all piezometers and with an STS multi-parameter probe (STS DL/N 70) in the stream. An EXO2 probe also continuously measured pH in the stream. Groundwater was sampled in the respective piezometers via fixed-installed pumps (Comet ECO-PLUS_20000; placed about 3 m below the groundwater table). Water from the piezometers was filtered using stainless-steel filters (Nussbaum) with a screen opening of 10 μm. We sampled regional groundwater using a peristaltic pump (Eijkelkamp) and streamwater by hand.

A total of 30 organic micropollutants were targeted for screening, 20 of which were included for final reporting (see list above) after removing unstable constituents (absolute recovery <0.5 or non-linear calibration curve). Micropollutants were selected to represent different pollution sources: Lifestyle products (i.e., caffeine) and pharmaceuticals represent wastewater, for example, paracetamol is well degraded in treatment plants and can indicate untreated wastewater (i.e., sewage overflow during rain events); anti-corrosion agents can also indicate wastewater as well as industrial sources; pesticides can indicate current and former agricultural activities, for example, atrazine indicates former input (most likely originating from regional groundwater) because it is no

longer allowed as plant protection product; similarly, terbutylazine, for example, represents more current input since its use is still legal in Switzerland.

Samples for targeted organic micropollutant screening were collected in standard 0.25 L glass bottles. Gloves were used to reduce the risk of cross-contamination, and samples were stored at −20°C for a short period (days to weeks) before the analysis. Measurements were carried out using online solid-phase extraction (SPE) liquid chromatography-tandem mass spectrometry (LC-MS/MS). Isotopically matching internal standards in connection with calibration standards were used for the quantification of all reported organic micropollutants. Quality control samples included laboratory standard solutions, laboratory blanks, field blanks, triplicate field samples, and field samples spiked with laboratory standards. Calibration curves using laboratory standards spanned 0.1–1,000 ng/L. Limits of quantification (LOQs) were determined with the calibration curve corrected for matrix factors. Relative recoveries were calculated to determine data quality following Huntscha et al. (2012).

Parts of the measured data were already used to study the spatiotemporal variability of denitrification by river-aquifer exchange (Popp et al., 2020). The quasi-continuously analyzed dissolved noble (helium, argon, krypton) and reactive gases (oxygen, nitrogen), total cell concentrations, parameters relevant for denitrification (e.g., NO_3^- and O_2 saturation), hydraulic conductivities of P1, P4, and P5 as well as hydro-meteorological data were released in Popp et al. (2020); we refer to this publication for details about measurement techniques, data analysis and parameter uncertainty. However, we believe further studies with the whole data set obtained during the study period can improve the understanding of water flow and transport within the hyporheic zone, especially with the release of the organic micropollutant data. Table 1 gives an overview of all data obtained during the study period and indicates which data have already been published. Parameter uncertainties such as LOQs and measurement uncertainties are provided in the respective links to the data.

3. Results and Brief Discussion of the Data

Not all organic micropollutant compounds are significantly different between sampling locations or do have data from more than one sampling location (see list above). All tracer data show statistically significant differences between sampling locations except for radon and water temperature.

Figure 2 shows the general hydrologic conditions for the duration of the experiment as well as logger data (EC and water temperature) observed at the stream, P1 and P4. The darker gray segments correspond to precipitation events, indicating wetter periods (i.e., the beginning of the sampling campaign in January, a couple of days end of March and the end of the sampling period in June), while the remaining time was impacted by only short and minor precipitation events.

To increase readability, we applied local polynomial regression fitting (i.e., LOESS) to all data sets shown in Figures 3 and 4. In our implementation of LOESS, we utilized a span of 0.3, which means that each local regression in the smoothing process incorporates 30% of the data points, selected based on their proximity to the point being estimated.

Figures 3 and 4 show tracer and key water quality parameters observed between January and June 2018 (Figures S1 and S2 in Supporting Information S1 show the same data as boxplots). The data reveal substantial spatiotemporal variations in parameters across different sampling locations. Gray segments shown in these figures represent the same precipitation events as highlighted in Figure 2. Generally, stream water shows for the most time the highest values across most parameters (except for DOC and nitrite) compared to shallow and regional groundwaters. For instance, the peaks in streamwater in EC concentrations can suggest episodes of high ionic concentration, possibly from urban runoff or point-source discharges. Logically, chloride levels followed a similar pattern, peaking concurrently with EC, further corroborating the influx of salts or other soluble components into the stream. Values of pH also notably differed among measurement locations, with stream water values being considerably different to those of the groundwater samples. Note that streamwater pH was also measured using a logger, however, we emphasize that the measurements with the hand-held instrument are more reliable since we calibrated the device before every measurement campaign.

Figure 4 shows an example of other nutrients and biogeochemical relevant parameters which are part of the data set. Most of these parameters also varied considerably in time and space, with some locations showing similar or contrasting trends. DOC concentrations fluctuated considerably, with the highest values observed at the regional

groundwater well. Conversely, the remaining locations demonstrated lower DOC levels, suggesting more dilution and/or degradation dynamics. Generally, DOC concentrations in groundwaters were decreasing over time. Oxygen saturations were relatively stable in the shallow groundwater and more dynamic in the stream and the regional groundwater. The highest O_2 saturations occurred in the stream, reflecting heightened photosynthetic activity. In contrast, groundwaters exhibited comparatively low saturations, with a general increase in oxygen levels observed toward the last weeks, possibly due to prolonged and high precipitation events followed by high discharge that potentially led to increased infiltration of oxygenated river water into the piezometers. Phosphate concentrations were highest in P4 and the stream, with a sharp increase in stream concentrations observed in May, which is not clearly attributable to an increased discharge event. Except for at P1 (where phosphate levels were increasing over time), the remaining sites exhibited relatively low and consistent phosphate levels, suggesting less influence from point source pollution or more effective nutrient cycling and retention within the aquatic system. Nitrate (NO_3^-) levels also varied distinctively across sites. The stream contained the highest NO_3^- concentrations, possibly due to wastewater inputs. This decreasing trend in the stream water may reflect plant uptake during the growing season or enhanced denitrification. Likewise, the decreasing trend observed within the groundwater systems can reflect increased denitrification rates as well as reduced input from the streamwater. Ammonium and nitrite concentrations were relatively low across all locations, yet both parameters showed an increasing trend toward the end of the study period. Also toward the end, P5 exhibited some distinct outliers. These trends are likely related to alterations in nitrogen cycling due to temperature-related changes in microbial activity or variations in stream-aquifer connectivity.

Figure 5 illustrates the differences in organic micropollutant concentrations across the sampling sites. For most compounds shown here, streamwater concentrations were elevated compared to those observed in the piezometers and the regional well, suggesting that the stream receives these pollutants from runoff or direct discharge of treated wastewater. At the same time, most concentrations of micropollutants also show great variability in stream concentrations (e.g., carbamazepine or hydrochlorothiazide). For some compounds, mean concentrations in the piezometers are higher than in the stream, for instance, atrazine concentrations in P1 or carbamazepine concentrations in P5. These differences can result from various conditions that can impact each other: for example, different locations along the streambank (i.e., piezometers) can be subject to differences in water source contributions from the stream and the regional groundwater. Moreover, there can be differences in pollutant turnover and retention due to differences in factors controlling microbial communities such as redox conditions, water temperature and water residence times (Figure S3 in Supporting Information S1). For an in-depth analysis and interpretation, one also needs to take into account the degradation and sorption dynamics of each specific micropollutant. Certain micropollutant concentrations sampled in the regional groundwater well were below the LOQ (e.g., carbamazepine), while for other contaminants reg-gw showed intermediate levels (e.g., caffeine), implying some degree of connectivity with surface contamination sources, but with less variation than observed in the stream. Overall, the spatial variation depicted across these sites highlights the impact of hydrogeological properties (e.g., differences in hydraulic conductivity), water source contributions and different degradation and sorption behavior of organic micropollutants.

The broad scope of this data set (Table 1), encompassing meteorological, hydro(geo)logical, tracer, nutrient, hydraulic, microbial, and organic micropollutant data, has the potential to facilitate a diverse range of applications that can contribute to an enhanced understanding of urban stream-aquifer systems and associated (bio-)geochemical cycling and pollutant turnover. We suggest the following potential research and applied usages of the data:

- Modeling of surface water-groundwater interactions or Multi-component Reactive Transport Models: The data can be leveraged to set up, calibrate, and validate hydrological models ranging from 1D to 3D, simulating surface water-groundwater interactions and reactive transport (e.g., Henzler et al., 2014; Prommer et al., 2002; Zheng & Bennett, 2002). Such models can be used for sensitivity analyses, examining how changes in data such as temperature and hydraulic conductivity influence water flow as well as the transport and turnover of major ions, nutrients, and organic micropollutants. Additionally, these models can be harnessed for scenario modeling, such as simulating increased temperatures due to global warming or changes in hydraulic conductivity resulting from potential streambed clogging or river restoration. Moreover, the data can be used for model calibration and validation by reducing parameter uncertainty and thereby improving the predictive capacity of the chosen model. Research has shown that hydraulic heads alone do not contain sufficient information to calibrate flow models (Moeck et al., 2020; Schilling et al., 2019), consequently, combining hydraulic

with hydrochemical data has great potential to further system understanding of surface water-groundwater interactions and associated biogeochemical cycling (Popp, Manning, & Knapp, 2021; Popp, Pardo-Alvarez, et al., 2021; Popp, Scheidegger, et al., 2019).

- Machine learning approaches: The data can serve as a foundation for the development and validation of machine learning models (e.g., Maier et al., 2010; Tyralis et al., 2019). Such models can be trained to identify patterns and relationships among various parameters (e.g., organic micropollutants) and can offer insights into pollutant turnover or key drivers of biogeochemical cycling.
- More parsimonious data analysis approaches: The data set can be efficiently utilized for standard statistical analysis techniques such as Principal Component Analysis or Bayesian models (Clark & Gelfand, 2006; Hastie et al., 2009). The data set can further be used to determine travel times of infiltrated river water by time-series deconvolution analysis of naturally varying tracers (e.g., temperature, EC) following Cirpka et al. (2007) and Vogt et al. (2010). The travel time can, in turn, provide important insights to quantify pollutant turnover.

By employing these methodologies, maybe also in combination, the data set can also enable a comparison of pollutant and nutrient cycling in other areas (e.g., reviews of Boano et al. (2014) and Lewandowski et al. (2019) and references therein), offering the ability to discern potential temporal and spatial drivers of nutrient and pollutant turnover. Insights gained from this data set can be valuable to water managers in decision-making processes, such as planning future river restoration projects where factors like shading, changes in river bed hydraulic conductivity, and enhanced hyporheic exchange flow have key impacts on ecosystem health and services.

4. Summary Statement

In this study, we present a comprehensive interdisciplinary and unique data set collected from January to June 2018 at an urban river-aquifer system in Switzerland. With the release of this data set, we aim (a) to facilitate the use of the provided data by other scientists and practitioners to enhance the understanding of biogeochemical cycling and pollutant turnover facilitated by hyporheic exchange and (b) to support Open Science by making data generated by public funding available to everyone (Hall et al., 2022).

Data Availability Statement

Data and R code used for the presented figures and statistical analysis can be accessed on Zenodo (Popp et al., 2023). Previously published data can be accessed via Popp, Manning, et al. (2019).

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