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# Compilation of transformation rates, sorption parameters and key microbes

## **Dissemination Level of Deliverable:**

PU	Public	х
СО	Confidential, only for the members of the	
	consortium (including the Commission Services)	

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# Compilation of transformation rates, sorption parameters and key microbes

## 1. Introduction

At this stage of HypoTRAIN a lot of data on transformation rates, sorption parameters, key microbes and other features related to hyporheic processes have been generated. These data result from a variety of experimental and applied field and lab works which were conducted in order to understand mechanisms of biogeochemical turnover in hyporheic zones.

The resulting data are jointly collected and stored on the internal communication platform Mondo (D7.2) to make them available for every ESR, PI and associated partners and external experts involved in HypoTRAIN.

Based on these data the ESRs are now writing their manuscripts for scientific journals which will be the core of their doctoral theses. Regular meetings with their supervisors and co-authors (either personally or via Skype) facilitate a maximum effectiveness of this process. Since many ESRs have been collaborating in different studies and experiments a number of manuscripts is expected to have HypoTRAIN ESRs and PIs as co-authors.

Below we describe an example for studies on attenuation of selected target organic micropollutants in aquatic sediment by sorption or microbial processes. The presented studies were carried out in lab-based microcosm (bottle) experiments. The results of such studies will contribute to transformation rate calculations.

#### 2. Sorption parameters

To understand sorption mechanisms, parameters such as sorption coefficient ( $K_d$ ), organic carbon sorption coefficient ( $K_{oc}$ ), and kinetics and isotherms of compounds in focus were considered. The sorption experiment was conducted based on OECD 106 guidelines for studying pharmaceutical attenuation by sorption processes using the model compounds Carbamazepine (CBZ), Ibuprofen (IBU) and Sulfamethoxazole (SMX) (Fig. 1). The micropollutant concentration sorbed onto the sediment matrix was then calculated, and the constants  $K_d$  as well as  $K_{oc}$ determined. Results from sorption kinetic experiments showed that the sorption equilibrium of CBZ, IBU and SMX was reached within 24 hours, respectively (Fig. 2).



Figure 1. Isotherm batch experiment using various water/sediment ratios based on the method of the OECD 106 guideline.

The role of organic matter, considered the main factor in regulating sorption coefficient values of micropollutants, was evaluated. Higher sorption capacities of micropollutants were found to be correlated with higher organic carbon (OC) content (8.65%) in the sediments of our model river Erpe. Moreover, the sorption of CBZ, IBU and SMX was negligible when using quartz sand and Erpe sediment cleared from OC as a sorbent. As for this, the  $K_{oc}$  for each micropollutant was calculated in order to normalize the values of  $K_d$  to the content of organic carbon in the sediment samples. Results showed that CBZ has a higher sorption coefficient ( $K_d$ ) than SMX and IBU for Erpe sediment. Furthermore, other parameters such as pH were found to affect the sorption capacities of the organic micropollutants onto Erpe sediment. Sorption experiments with solution of pH 5, 7 and 9 were conducted and resulting  $K_d$  values decreased with an increase in pH. At pH 9 the lowest  $K_d$  values were found compared to pH 5 and pH 7 for the all three pharmaceuticals studied. Based on these results and ongoing experiments, an in-depth understanding of the contribution of sorption to hyporheic attenuation processes of micropollutants will be developed that potentially can be used to better manage ecosystems surface-water groundwater interaction.



Figure 2. Sorption kinetics experiment.

## 3. Key microbes

Using sediment and water samples from the well at site 4 at the Erpe River (see D1.2), the role of biodegradation in removal of pharmaceutical compounds such as Ibuprofen (a non-steroidal anti-inflammatory drug), and metoprolol (beta-blocker) was investigated under both aerobic and anaerobic conditions. Furthermore, cognizant of the occurrence of most organic micropollutants as mixtures in the aquatic environment, the degradation of compounds with various physicochemical properties (Metoprolol, Propranolol, Bezafibrate, Carbamazepine, Acesulfame, Diclofenac, Furosemide, Ibuprofen, 1H-Benzotriazole, Hydrochlorothiazide, Ketoprofen, Clofibric acid, and Naproxen) was also investigated. Biodegradation was determined to be a major attenuation mechanism of most compounds. The potential microbial degraders were investigated using biological molecular techniques such as qPCR and Next Generation sequence analyses. The key taxa associated with Ibuprofen degradation and compounds with similar physicochemical characteristics are as shown in table 1.

Table 1. Potentia	I pharmaceutica	l microbial d	legraders in	the aquati	c sediment.
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Таха	Approx. relative abundance (%)
Proteobacteria	28-47
Chloroflexi	11-19
Actinobacteria	12-16
Acidobacteria	7-14
Bacterioidetes	3-18
Firmicutes	1-7
Others	2-4