Supplementary Materials

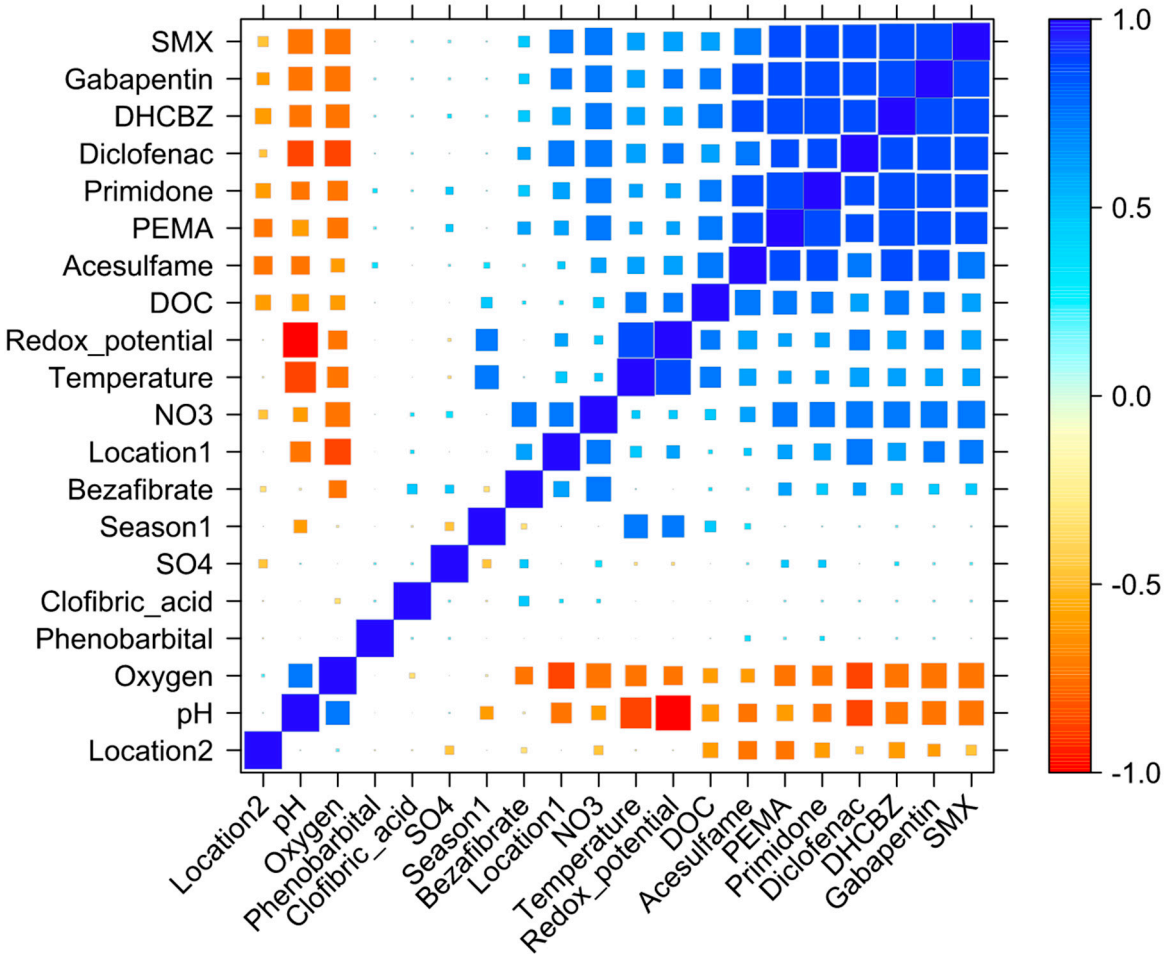

Figure S1. Pearson correlation of measured environmental variables.

The environmental variables provide redundant information. Hence, the variance inflation factor (VIF) was calculated on variables to select valid environmental variables for downstream statistical analysis. The variable with the highest VIF was removed from the set of variables, and the process was iterated on the reduced set until all VIF ≤ 5. These grouping variables were retained in the selection process, and the following variables were selected for downstream statistical analysis:

- Bezafibrate
- Clofibric acid
- Location
- Phenobarbital
- Season
- SO_4^{2-}

Table S1. Sediment characteristics of the sampling sites PuBG and PoBG in the Panke.

Sediment [a, b]		
	Sampling Site PuBG	**Sampling Site PoBG**
Gravel (%)	n.d.	n.d.
Coarse sand (%)	41.9	7.6
Medium sand (%)	53	63.3
Fine sand (%)	3.8	27.1
Silt & clay (%)	1.4	2.1
C (%)[c]	0.539 ± 0.0043	0.974 ± 0.0023
N (%)[c]	0.0215 ± 0.0003	0.0265 ± 0.00025
Ignition loss [c, d]	1.12 ± 0	1.44 ± 0
Mean porosity [e]	0.51	n.d.

[a] Grab sediment samples at sampling site P1 and P2 were taken in 16 June 2016, [b] grain-size classifications based on the norm DIN/ISO 11277, [c] data represent mean ± standard deviation values within measured duplicates, [d] the ignition loss was categorized by the norm DIN 18128 (550 °C). No classification of organic content feasible by the norm DIN 14688-2:2005 + A1:2013; both sediments can be classified into the inorganic sediments, [e] value represent measurements in triplicates; n.d. not detected.

Table S2. Water characteristics in the Panke.

Water			
	Average	**Min**	**Max**
Sampling Site PuBG—October 2016			
EC [a] (μS cm^{-1})	1173.83 ± 0.90	1172	1175
Redoxpotential[a] (mV)	−49.5 ± 5.53	−40	−55
Sampling Site PoBG—October 2016			
EC [a] (μS cm^{-1})	879.33 ± 9.2	860	886
Redoxpotential[a] (mV)	−67.83 ± 1.77	−64	−69
Sampling Site PvLg—October 2016			
EC [a] (μS cm^{-1})	802.83 ± 3.24	799	807
Redoxpotential[a] (mV)	−64 ± 0	−64	−64
Sampling Site PuBG—June 2017			
EC [a] (μS cm^{-1})	n.d.	n.d.	n.d.
Redoxpotential[a] (mV)	−19.17 ± 0.37	−19	−20
Sampling Site PoBG—June 2017			
EC [a] (μS cm^{-1})	n.d.	n.d.	n.d.
Redoxpotential[a] (mV)	−48.17 ± 0.9	−47	−49
Sampling Site PvLg—June 2017			
EC [a] (μS cm^{-1})	n.d.	n.d.	n.d.
Redoxpotential[a] (mV)	−38.67 ± 0.75	−37	−39

[a] Measurements were done at every sampling site. All water quality data represent mean ± standard deviation values within two sampling campaigns, n.d.: not detected, EC: electrical conductivity.

Table S3. Micropollutant concentrations (μg L^{-1}) in the Panke obtained from three different sampling sites during two seasons (autumn 2016 and summer 2017). All water quality data represent mean ± standard deviation values. If not different stated all means represent values from triplicates.

Sampling Sites **Date** **Sample Number**	**PuBG** **12 October 16** **n = 3**	**PoBG** **12 October 16** **n = 3**	**PvLg** **13 October 16** **n = 3**	**PuBG[1]** **26 June 17** **n = 3**	**PoBG[1]** **27 June 17** **n = 3**	**PvLg[1]** **26 June 17** **n = 3**
			Micropollutants (μg L^{-1})			
Acesulfame	0.82 ± 0.03	0.36 ± 0.10	LOD	1.8 ± 0.08	0.85 ± 0.33	0.10[2]
Bezafibrate	0.06 ± 0	LOD	LOD	0.10 ± 0.02	0.01 ± 0	LOD
Clofibric acid	0.25[2]	LOD	LOD	0.02	LOD	LOD
DHCBZ[+]	0.60 ± 0.03	0.06 ± 0.02	LOD	0.85 ± 0.03	0.29 ± 0.02	LOD
Diclofenac	0.95 ± 0.1	0.02 ± 0.01	0.02 ± 0.01[1]	1.3 ± 0.14	0.14 ± 0.02	0.31 ± 0.25[1]
Gabapentin	1 ± 0	0.08 ± 0.03	LOD	1.60 ± 0.16	0.29 ± 0.05	LOD
Phenobarbital	0.03 ± 0.02[1]	0.03 ± 0.02[1]	0.05 ± 0.01	0.05 ± 0.01	0.05 ± 0.02	0.05[2]
PEMA[+]	0.08 ± 0.01	0.02 ± 0	0 01 ± 0	0.09 ± 0.01	0.05 ± 0	LOD
Primidone	0.1 ± 0	0.02 ± 0.01	0.03 ± 0	0.14 ± 0	0.06 ± 0.01	0.01[2]
SMX[+]	0.09 ± 0	LOD	LOD	0.14 ± 0.01	0.02 ± 0.01[1]	LOD

[+] Abbreviations: DHCBZ: 11-dihydroxy-10, 11-dihydro-carbamazepine, PEMA: phenylethylmalonamide, SMX: sulfamethoxazole, LOD: limit of detection. [1] one value under detection limit, and [2] two values under detection limit.

Table S4. Micropollutant concentrations (μg L^{-1}) in the Panke obtained from three different sampling sites during one season (autumn 2016 or summer 2017). All water quality data represent mean ± standard deviation values.

Sampling Sites **Date** **Sample Number**	**PuBG** **12 October 16** **n = 3**	**PoBG** **12 October 16** **n = 3**	**PvLg** **13 October 16** **n = 3**	**PuBG[1]** **26 June 17** **n = 3**	**PoBG[1]** **27 June 17** **n = 3**	**PvLg[1]** **26 June 17** **n = 3**
			Micropollutants (μg L^{-1})			
Candesartan	-	-	-	1.33 ± 0.09	0.31 ± 0.03	LOD
Carbendazim	-	-	-	0.02 ± 0	LOD	LOD
Carbamazepine	0.46 ± 0.04	0.05 ± 0.02	0.71[2]	-	-	-
Coffein	-	-	-	0.15 ± 0.07[2]	LOD	0.13 ± 0.1′
FAA[+]	2.43 ± 0.31	0.13 ± 0.05	0.04±0	-	-	-
Gaba-Lactam	-	-	-	0.26 ± 0.06	0.1 ± 0.02	LOD
Irbesartan[#]	-	-	-	2.15 ± 0.15	0.38 ± 0.09	LOD
Losartan	-	-	-	0.31 ± 0.08	0.04 ± 0	0.02 ± 0.02
MCPA[+]	-	-	-	0.03 ± 0	LOD	LOD
Mecoprop	-	-	-	0.17 ± 0.03	0.03 ± 0	0.05 ± 0.01
Metformin	-	-	-	0.85 ± 0.05	0.06 ± 0.02	0.05 ± 0
Metoprolol	0.71 ± 0.02	0.02 ± 0.01	0.01 ± 0[1]	-	-	-
NASMX[+]	-	-	-	0.02 ± 0.02	LOD	LOD
Olmesartan				0.97 ± 0.02	0.21 ± 0.02	LOD
Oxipurinol[#]	-	-	-	N.E.	0.23 ± 0.02	LOD
Pregabalin	-	-	-	0.31 ± 0.03	0.01 ± 0.01[1]	LOD
p-TSA + *o*-TSA[+]	-	-	-	0.26 ± 0.05	0.30 ± 0.02	0.24 ± 0.10
Valsartan	-	-	-	9.07 ± 0.97	3.17 ± 0.24	0.02 ± 0.01
X2PSS[+]	-	-	-	LOD	0.02[1]	LOD

[+] Abbreviations: FAA: flavone acetic acid, MCPA: 2-(4-chloro-2-methylphenoxy)acetic acid, NASMX: N-acetyl sulfamethoxazole, *p*-TSA: *para*-toluene sulphonamide, *o*-TSA: *ortho*-toluene sulphonamide, X2PSS: Phenylsulfonylsarcosin, LOD: limit of detection, N.E.: not evaluable, -: not measured during this sampling campaign, [#] two replicates were measured, [1] one value under detection limit, and [2] two values under detection limit.

Table S5. Terms of the overall alpha diversity generalized least square model GLS model. Significance of terms in the final model was determined by Wald's Chi-Square Test with type II sums of squares. *p*-values were adjusted (* $p \leq 0.05$; ** $p \leq 0.01$; *** $p \leq 0.001$; . not statistically significant).

Term	Degrees of Freedom	Wald χ^2	*p*-Value	Significance
Location	2	1165.40	<0.001	***
Season	1	104.06	<0.001	***
Phenobarbital	1	4.61	0.032	*
SO_4^{2-}	1	25.04	<0.001	***
Clofibric acid	1	28.77	<0.001	***
Bezafibrate	1	43.12	<0.001	***
Location:Season	2	75.40	<0.001	***
Location:Phenobarbital	2	66.31	<0.001	***
Location:SO_4^{2-}	2	133.76	<0.001	***
Season:SO_4^{2-}	1	64.08	<0.001	***
Season:Clofibric acid	1	38.33	<0.001	***
Location:Season:SO_4^{2-}	2	271.03	<0.001	***

Table S6. The highest interaction terms of variables in the final RDA model of the beta diversity on the DNA level. *p*-values were adjusted (* $p \leq 0.05$; ** $p \leq 0.01$; *** $p \leq 0.001$; . not statistically significant).

Term	Degrees of Freedom	F statistic	*p*-Value	Significance
Location:Phenobarbital	2	1.99	0.036	*
Season:Bezafibrate	1	3.41	0.022	*
Location:Season: SO_4^{2-}	2	4.19	0.011	*

Table S7. Effect size and significance of SO_4^{2-} within location and season and phenobarbital within location for individual OTUs with high log_2(fold-change). Conditions are shown levels for variables were grouped and missing levels did not yield significant results. The ID of the OTU and the class of bacteria is given; base mean: mean of the occurred OTUs in the library; log_2(fold-change): size-factor normalized OTU counts; lfcSE: log_2(fold-change) standard error; *p*-value: adjusted *p*-value; padj: false discovery rate (Benjamini–Hochberg adjusted *p*-value).

Condition	OTU	Class of Bacteria	Base Mean	Log_2 (Fold-Change)	lfcSE	*p*-Value	Padj
			SO_4^{2-}				
PvLg:S2	452	*Anaerolineae*	0.007	−1.0177	2.93×10^{-1}	5.02×10^{-4}	2.81×10^{-3}
	514	*Sphingobacteriia*	0.007	−1.0144	2.93×10^{-1}	5.24×10^{-4}	2.84×10^{-3}
	582	*Anaerolineae*	0.009	−1.0109	2.93×10^{-1}	5.48×10^{-4}	2.91×10^{-3}
	636	*Actinobacteria*	0.007	−1.0168	2.93×10^{-1}	5.09×10^{-4}	2.81×10^{-3}
	2253	*Alphaproteo-bacteria*	0.007	−1.0151	2.93×10^{-1}	5.20×10^{-4}	2.84×10^{-3}
			Pheno-barbital				

PvLg	274	*Deltaproteo-bacteria*	0.938	2.2505	8.78×10^{-2}	7.07×10^{-245}	1.41×10^{-242}
	1558	*Blastocatellia*	0.311	9.0384	4.05×10^{-1}	1.77×10^{-110}	2.65×10^{-108}
	2455	*Deltaproteo-bacteria*	0.345	17.215	4.05×10^{-1}	0.0	0.0
	7929	*Nitrospira*	0.307	30.0	4.05×10^{-1}	0.0	0.0

Table S8. Individual OTUs belonging to the order *Syntrophobacteriales, Desulfuromonadales*, and *Desulfobacterales*.

OTU	Order	PuBG:S1 (OTU Counts)	PuBG:S2 (OTU Counts)	Pobg:S1 (OTU Counts)	PoBG:S2 (OTU Counts)	PvLg:S1 (OTU Counts)	PvLg:S2 (OTU Counts)
125	*Syntrophobacterales*	38	78	847	560	2226	294
171	*Syntrophobacterales*	82	61	1406	358	1103	170
438	*Syntrophobacterales*	36	14	1117	206	20	26
459	*Syntrophobacterales*	44	33	715	277	156	102
540	*Syntrophobacterales*	0	8	967	73	30	16
732	*Syntrophobacterales*	3	7	194	40	127	26
774	*Syntrophobacterales*	14	14	223	121	307	60
927	*Syntrophobacterales*	47	10	346	125	60	26
1048	*Syntrophobacterales*	0	6	67	31	119	29
1054	*Syntrophobacterales*	2	14	148	43	266	34
1056	*Syntrophobacterales*	46	18	319	86	44	14
1983	*Syntrophobacterales*	5	3	45	20	29	3
2151	*Syntrophobacterales*	0	1	56	18	14	3
2244	*Syntrophobacterales*	6	6	109	35	12	10
2728	*Syntrophobacterales*	0	1	17	4	35	7
3231	*Syntrophobacterales*	9	2	36	12	34	6
3291	*Syntrophobacterales*	2	2	22	22	32	12
3354	*Syntrophobacterales*	2	1	34	7	1	1
3758	*Syntrophobacterales*	0	4	54	19	4	0
5311	*Syntrophobacterales*	8	0	32	2	2	0
6308	*Syntrophobacterales*	0	0	27	0	2	0
6672	*Syntrophobacterales*	4	0	12	12	0	0
8195	*Syntrophobacterales*	0	0	0	17	0	2
23,740	*Syntrophobacterales*	0	0	0	0	0	0
45,686	*Syntrophobacterales*	0	0	0	2	0	0
45,699	*Syntrophobacterales*	0	0	0	2	0	0
163	*Desulfuromonadales*	401	31	389	108	138	143
270	*Desulfuromonadales*	196	24	126	159	111	143
285	*Desulfuromonadales*	235	39	171	101	96	90
461	*Desulfuromonadales*	500	2	6	0	0	0
503	*Desulfuromonadales*	63	10	169	89	75	56
758	*Desulfuromonadales*	76	17	48	37	72	32
826	*Desulfuromonadales*	2	5	291	48	0	4
841	*Desulfuromonadales*	158	4	19	13	36	21
847	*Desulfuromonadales*	71	10	51	59	34	27
993	*Desulfuromonadales*	45	8	54	61	78	26
1003	*Desulfuromonadales*	37	5	77	26	33	30
1959	*Desulfuromonadales*	71	1	2	4	0	3
2292	*Desulfuromonadales*	2	0	40	23	0	2
5228	*Desulfuromonadales*	1	1	4	8	6	1
12,690	*Desulfuromonadales*	0	0	0	0	1	1
14,732	*Desulfuromonadales*	1	0	0	2	0	0
17,294	*Desulfuromonadales*	0	0	0	0	0	1

17,296	*Desulfuromonadales*	1	1	0	1	0	0
20,923	*Desulfuromonadales*	0	1	0	1	0	0
30	*Desulfobacterales*	115	83	2072	1368	170	179
35	*Desulfobacterales*	61	22	2658	425	24	24
38	*Desulfobacterales*	38	54	1372	488	762	267
56	*Desulfobacterales*	220	45	1175	833	51	222
106	*Desulfobacterales*	39	16	777	199	240	100
113	*Desulfobacterales*	55	24	101	40	890	140
122	*Desulfobacterales*	114	28	697	318	157	119
147	*Desulfobacterales*	26	30	485	188	215	87
150	*Desulfobacterales*	105	24	1132	329	95	72
238	*Desulfobacterales*	10	6	1052	114	19	13
258	*Desulfobacterales*	30	21	563	129	278	86
261	*Desulfobacterales*	8	7	509	100	8	12
262	*Desulfobacterales*	272	6	606	142	24	44
278	*Desulfobacterales*	10	12	136	37	348	47
295	*Desulfobacterales*	23	15	328	84	82	40
312	*Desulfobacterales*	7	3	429	76	16	19
318	*Desulfobacterales*	153	11	207	162	26	58
336	*Desulfobacterales*	27	6	322	101	29	35
354	*Desulfobacterales*	16	8	307	124	18	29
380	*Desulfobacterales*	92	7	287	149	5	10
386	*Desulfobacterales*	72	6	268	180	8	12
441	*Desulfobacterales*	14	1	137	82	0	1
505	*Desulfobacterales*	93	7	202	58	16	27
528	*Desulfobacterales*	14	7	248	65	29	25
552	*Desulfobacterales*	12	9	35	83	83	53
556	*Desulfobacterales*	1	8	131	111	35	17
578	*Desulfobacterales*	2	8	215	76	0	6
625	*Desulfobacterales*	9	7	142	100	7	21
628	*Desulfobacterales*	9	7	160	76	41	35
701	*Desulfobacterales*	6	7	99	27	76	31
709	*Desulfobacterales*	1	1	58	35	28	8
765	*Desulfobacterales*	24	5	153	40	3	14
792	*Desulfobacterales*	5	12	51	44	12	80
828	*Desulfobacterales*	7	3	131	48	1	11
851	*Desulfobacterales*	4	6	133	61	16	6
882	*Desulfobacterales*	4	5	63	19	67	26
913	*Desulfobacterales*	4	3	79	46	38	20
926	*Desulfobacterales*	8	5	55	34	65	16
1070	*Desulfobacterales*	3	4	51	21	56	17
1152	*Desulfobacterales*	10	4	51	38	10	6
1183	*Desulfobacterales*	16	1	53	34	4	9
1365	*Desulfobacterales*	1	4	18	10	63	12
1420	*Desulfobacterales*	6	4	59	31	10	8
1454	*Desulfobacterales*	9	4	21	27	28	18
2129	*Desulfobacterales*	3	2	29	16	4	9
2494	*Desulfobacterales*	10	4	33	3	4	17
3216	*Desulfobacterales*	7	0	13	13	0	1
4276	*Desulfobacterales*	0	0	8	6	5	3
5197	*Desulfobacterales*	7	1	1	6	0	2
6905	*Desulfobacterales*	0	0	2	1	5	1
8524	*Desulfobacterales*	1	1	3	1	2	1
10,504	*Desulfobacterales*	1	0	3	2	0	0
10,703	*Desulfobacterales*	0	0	0	4	0	0
10,787	*Desulfobacterales*	0	0	1	2	0	0
18,218	*Desulfobacterales*	0	0	1	0	1	0
18,264	*Desulfobacterales*	0	0	1	0	0	0

18,275	*Desulfobacterales*	0	0	1	0	1	0
18,338	*Desulfobacterales*	0	0	0	1	1	0
23589	*Desulfobacterales*	0	0	0	0	0	0
23,620	*Desulfobacterales*	0	0	0	0	0	0
24,068	*Desulfobacterales*	0	0	1	0	0	0
24,077	*Desulfobacterales*	0	0	0	0	0	0
24,227	*Desulfobacterales*	0	1	0	0	0	0
24,237	*Desulfobacterales*	0	0	1	1	0	0
24,246	*Desulfobacterales*	0	0	1	0	0	0
24,247	*Desulfobacterales*	0	0	0	0	0	0
24,250	*Desulfobacterales*	0	1	0	0	0	0
24,296	*Desulfobacterales*	0	0	0	0	0	0
Sum of OTUs		3992	5000	26,167	9640	9479	3537