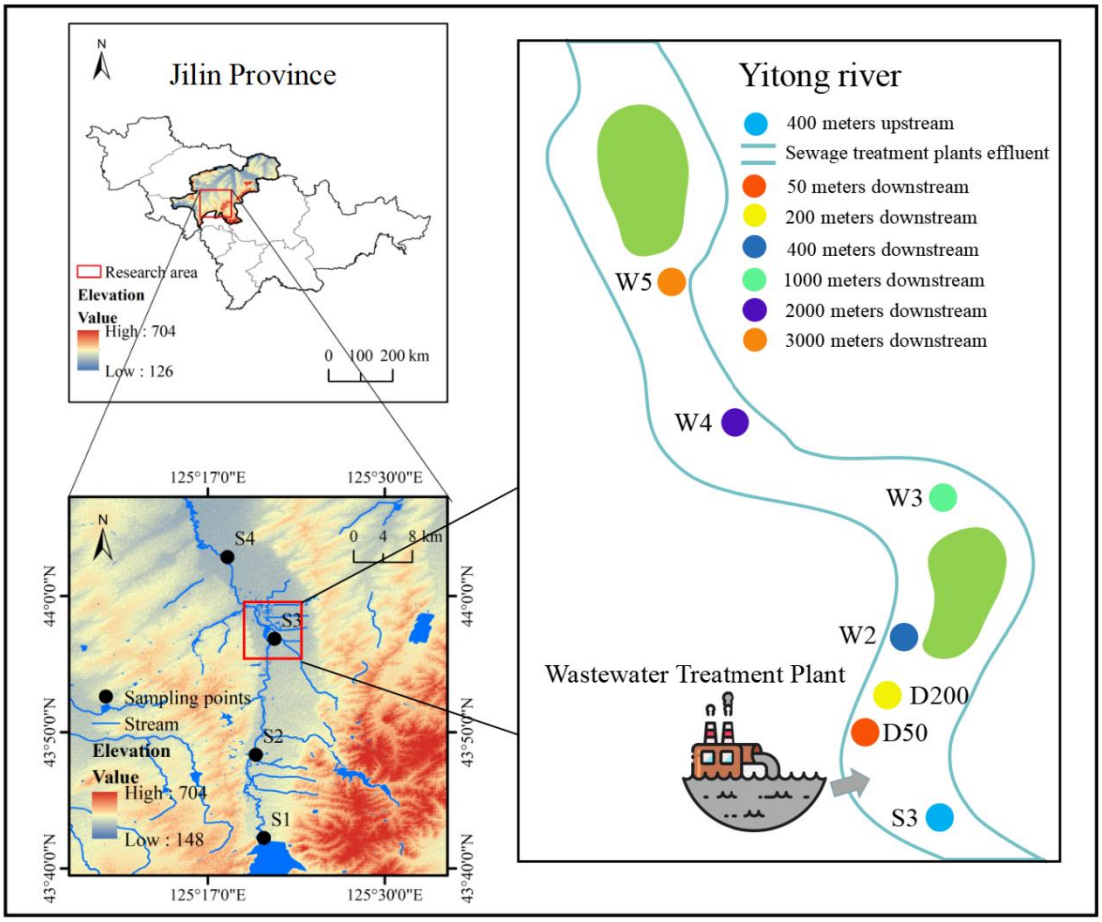


Figure S1. Setup of sampling point locations.

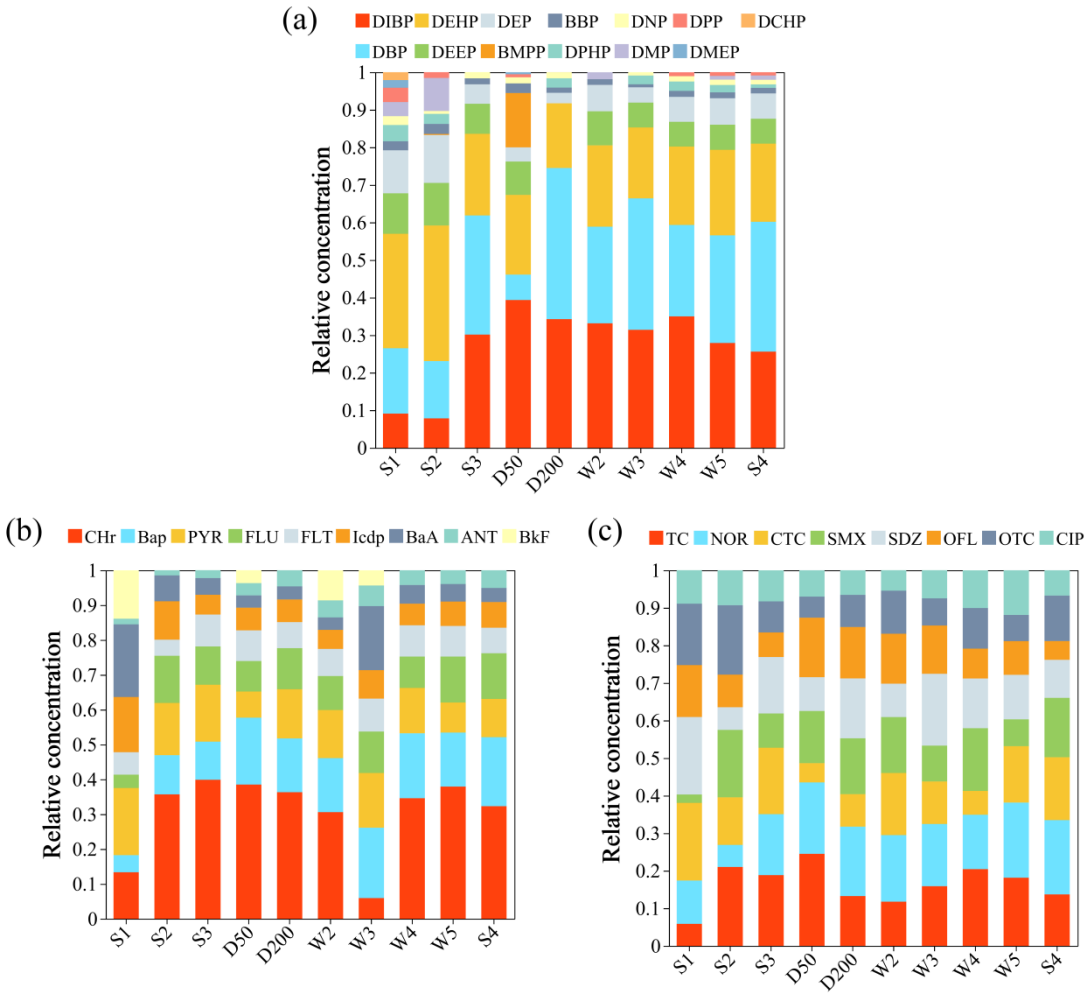


Figure S2. Relative concentrations of (a) PAEs, (b) PAHs and (c) antibiotics.

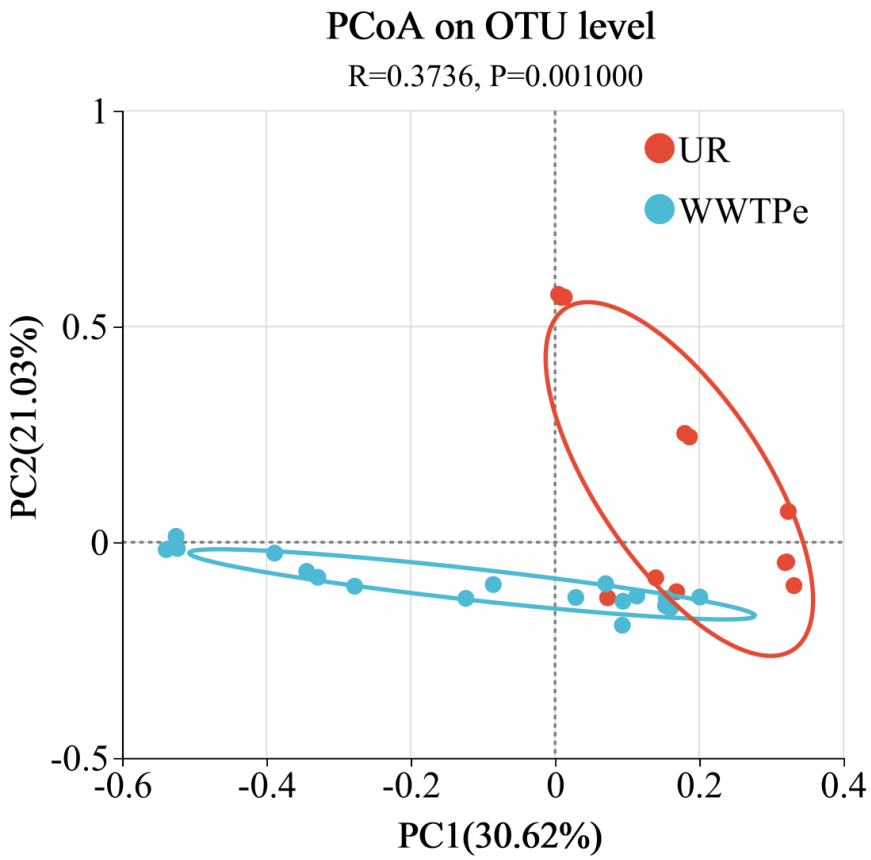


Figure S3. Principal coordinate analysis of microbial communities at the genus level in urban streams and wastewater plants impacting watersheds.

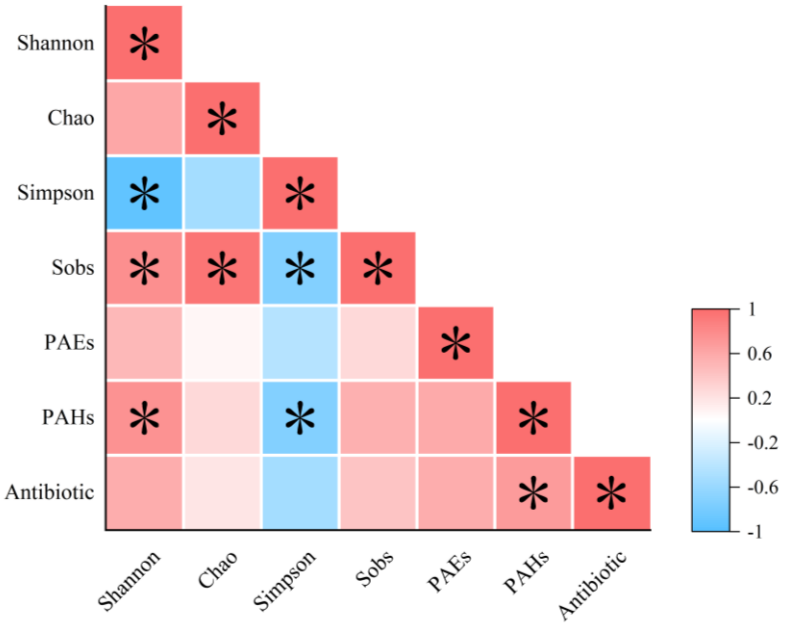
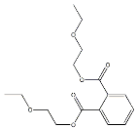
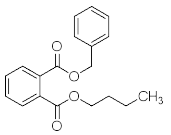
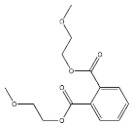
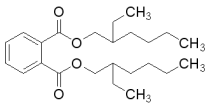
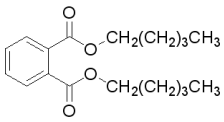
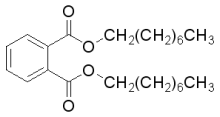
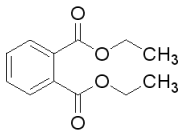
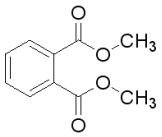
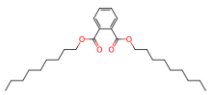
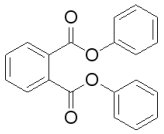
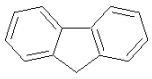
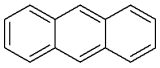
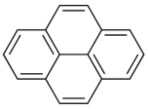
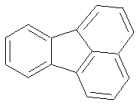
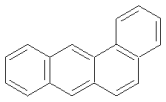
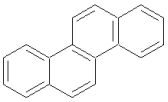
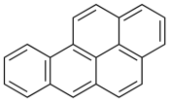
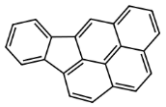
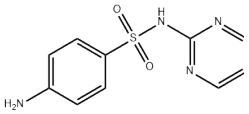
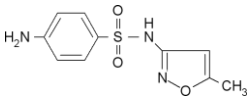
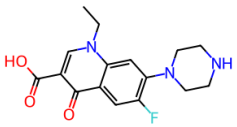
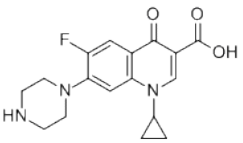
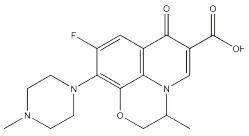
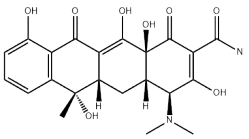


Figure S4. Heat map of correlation between organic pollution and microbial diversity indices. * $p \leqslant 0.05$.

Table S1. Compound Information

Compound	Abbreviation	Chemical formula	Molecular weight	CAS	Structured
Diethyl phthalate	DEP	$C_{12}H_{14}O_4$	222.24	605-54-9	
Dimethyl phthalate	DMP	$C_{10}H_{10}O_4$	194.18	85-68-7	
Dibutyl phthalate	DIBP	$C_{16}H_{22}O_4$	278.34	117-82-8	
Diisobutyl phthalate	DBP	$C_{16}H_{22}O_4$	278.34	117-81-7	
Di-N-pentyl phthalate	DPP	$C_{18}H_{26}O_4$	306.4	131-18-0	
Di (2-ethylhexyl) phthalate	DEEP	$C_{16}H_{22}O_6$	310.34	117-84-0	
Benzyl butyl phthalate	BBP	$C_{19}H_{20}O_4$	312.36	84-66-2	
Dimethyl phthalate	DEHP	$C_{24}H_{38}O_4$	390.56	131-11-3	
Diphenyl phthalate	DPHP	$C_{20}H_{14}O_4$	318.32	84-76-4	
Dinonyl phthalate	DNP	$C_{26}H_{42}O_5$	418.61	84-62-8	
Fluorene	FLU	$C_{13}H_{10}$	166.22	86-73-7	

Anthracene	ANT	$C_{14}H_{10}$	178.23	120-12-7	
Pyrene	PYR	$C_{16}H_{10}$	202.25	129-00-0	
Fluoranthene	FLT	$C_{16}H_{10}$	202.25	206-44-0	
Benz[a]anthracene	BaA	$C_{18}H_{12}$	228.29	56-55-3	
Chrysene	CHr	$C_{18}H_{12}$	228.29	218-01-9	
Benzo[a]pyrene	Bap	$C_{20}H_{12}$	252.31	50-32-8	
Indeno[1,2,3-cd]pyrene	Icdp	$C_{22}H_{12}$	276.33	193-39-5	
Sulfadiazine	SDZ	$C_{10}H_{10}N_4O_2S$	310.34	68-35-9	
Sulfamethoxazole	SMX	$C_{10}H_{11}N_3O_3S$	306.4	723-46-6	
Norfloxacin	NOR	$C_{16}H_{18}FN_3O_3$	319.34	70458-96-7	
Ciprofloxacin	CIP	$C_{17}H_{18}FN_3O_3$	344.45	85721-33-1	
Ofloxacin	OFL	$C_{18}H_{20}FN_3O_4$	282.29	82419-36-1	
Tetracycline	TC	$C_{22}H_{24}N_2O_8$	444.44	60-54-8	

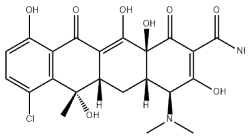
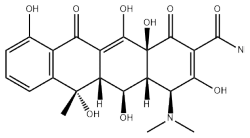
Aureomycin	OTC	$C_{22}H_{23}Cl_1N_2O_8$	478.89	57-62-5	
Oxytetracycline	CTC	$C_{22}H_{24}N_2O_9$	278.34	79-57-2	

Table S2. Toxicity analysis (ECOSAR prediction)

Compound	Acute toxicity (mg/L)			Chronic toxicity (ChV) (mg/L)		
	Fish LC_{50} (96 h)	Daphnid LC_{50} (48 h)	GreenAlgae EC_{50} (96 h)	Fish LC_{50}	Daphnid LC_{50}	GreenAlgae EC_{50}
DEP	36.427	74.941	31.409	2.685	49.834	8.308
DMP	0.911	1.397	0.379	0.038	0.421	0.425
DIBP	124.138	283.693	138.920	11.244	250.228	26.713
DBP	0.010	0.010	0.00157	0.00019	0.0011	0.003
DPP	0.327	0.463	0.111	0.012	0.113	0.092
DEEP	0.000	0.000	0.00124	0.00015	0.000053	0.003
BBP	12.471	24.192	9.295	0.819	13.793	2.938
DEHP	40.822	87.973	39.492	3.295	66.266	9.875
DPHP	0.002	0.002	0.0027	3.52E-005	0.000166	0.000803
DNP	2.538	4.215	1.287	0.123	1.577	0.625
FLU	2.114	1.446	2.325	0.257	0.237	0.922
ANT	1.147	0.809	1.475	0.145	0.144	0.625
PYR	0.386	0.287	0.656	0.052	0.060	0.314
FLT	0.386	0.287	0.656	0.052	0.060	0.314
BaA	0.129	0.101	0.290	0.019	0.024	0.157
CHr	0.129	0.101	0.290	0.019	0.024	0.157
Bap	0.042	0.035	0.125	0.006	0.010	0.076
Icdp	0.014	0.012	0.054	0.002	0.004	0.037
SDZ	1516	1.884	10.254	8.953	0.148	14.888
SMX	410.76	1.872	6.615	2.223	0.086	10.402
NOR	20081	1830	2567	2647	115.88	702.54
CIP	13131	1240	1621	1553	81.27	455.22
OFL	19352	1786	2444	2456	114.42	674.87
TC	13128	1062	1885	2486	59.921	473.56
OTC	5335	465	712	804	28.233	188.79
CTC	1.39E+005	2435.21	23848	45535	447	5265

Table S3.Water quality parameters

Parameter/Site	S1	S2	S3	D50	D200	W2	W3	W4	W5	S4
pH	8.35	7.79	7.49	7.40	7.30	7.52	7.72	7.62	7.44	7.40
EC (μs/cm)	234	432	758	842	663	801	932	751	895	643
WT (°C)	3.50	8.90	11.70	11.80	13.30	13.20	17.40	16.10	15.90	12.90
TP (ng/L)	0.07	0.08	0.06	0.10	0.09	0.09	0.13	0.16	0.21	0.17
DO (mg/L)	6.72	12.47	4.91	4.02	9.87	12.9	10.15	15.23	7.21	10.86
Chl-a (mg/L)	0.43	0.76	1.17	0.09	0.06	0.47	0.68	0.93	1.65	0.33
TN (mg/L)	2.70	3.85	3.57	11.61	10.24	4.25	8.71	10.20	9.61	8.72
NH_4^+-N (mg/L)	0.825	1.642	0.701	1.663	2.592	1.625	4.261	5.628	4.013	1.193
NO_3^--N (mg/L)	1.85	1.73	2.84	9.06	7.25	2.00	3.85	3.79	4.42	6.69
COD_{Cr} (mg/L)	36.12	40.64	33.86	39.88	42.14	38.38	51.92	57.94	54.93	42.89
COD_{Mn} (mg/L)	4.47	6.21	4.24	4.64	4.93	8.40	7.92	8.00	8.32	8.16
LC_{mix} (Fish)	0.0433	0.0678	0.0607	0.1520	0.0372	0.0775	0.0379	0.0495	0.0519	0.0537
LC_{mix} (Daphnid)	0.0419	0.0629	0.0583	0.1356	0.0360	0.0734	0.0369	0.0475	0.0497	0.0516

Method S1: Methods for the detection of microbial diversity

The total genomic DNA of the microbial community was extracted according to the instructions of the E.Z.N.A.® soil DNA kit (Omega Bio-tek, Norcross, GA, U.S.), and the quality of the extracted genomic DNA was checked by agarose gel electrophoresis with 1% agarose, and the concentration and purity of the DNA were determined by NanoDrop2000 (Thermo Scientific, USA). The quality of the extracted genomic DNA was determined by agarose gel electrophoresis (1%), and the DNA concentration and purity were determined by NanoDrop2000 (Thermo Scientific).

The above extracted DNA was used as a template for PCR amplification of the V3-V4 variable region of the 16S rRNA gene using upstream primer 33 8F (ACTCCTACGGGGAGGCAGCAG) and downstream primer 806R (GGACT ACHVGGGGTWTCTAAT) [51], and the PCR products were recovered on a 2% agarose gel. The PCR products were recovered on a 2% agarose gel, cut with the AxyPrepDNA Gel Recovery Kit (AXYGEN), and quantified by Qubit 4.0 (Thermo Fisher Scientific, USA).

The purified PCR products were library constructed using NEXTFLEX Rapid DNA-Seq Kit. Sequencing was performed using the Illumina PE300 platform (Shanghai Meiji Biomedical Technology Co., Ltd.).

The double-ended raw sequenced sequences were quality controlled using fastp [52] (https://github.com/OpenGene/fastp, version 0.19.6) software and spliced using FLASH [53] (http://www.cbcb.umd.edu/software/flash, the version 1.2.11) software for splicing. Operational taxonomic unit (OTU) clustering and chimera removal were performed on the QC spliced sequences based on 97% similarity using UPARSE v7.1 [54,55] software (http://drive5.com/uparse/). The OTU species taxonomy was annotated using the RDP classifier [56] (http://rdp.cme.msu.edu/, version 2.11) compared to the Silva 16S rRNA gene database (v138) with a confidence threshold of 70%, and the community composition of each sample was counted at different species classification levels. 16S functional prediction analyses were performed using PICRUSt2 [57] (version 2.2.0) software.

References:

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