Supporting Information

Table S1 Summary of existing screening methods for indicator PPCPs in potential pollution sources.

Indicator PPCPs	Substrate	Screening criteria						Reference
		Concentration	Detection frequency	Detection ratio [a)]	Fate and transport	Source-specificity	Representativeness	
Carbamazepine, clofibric acid, diclofenac, etc.	Treated municipal wastewater		√	√				(Dickenson et al., 2011)
Caffeine	Domestic wastewater	√	√					(Daneshvar et al., 2012)
Carbamazepine	Treated municipal wastewater							
Acetaminophen, caffeine	Domestic wastewater	√	√			√		(Fenech et al., 2013)
Acetaminophen, caffeine	Domestic wastewater	√	√					(Madoux-Humery et al., 2013)
Carbamazepine	Treated municipal wastewater							
Acetaminophen, caffeine, ibuprofen, naprofen	Domestic wastewater	√	√					(Lv et al., 2014)
Carbamazepine, diclofenac acid, mefenamic acid, metoprolol	Treated municipal wastewater							
Carbamazepine, gabapentin, primidone	Treated municipal wastewater		√	√	√			(Jekel et al., 2015)

Sulfamethazine, sulfadiazine	Livestock wastewater						
Acetaminophen, caffeine, methyl paraben	Domestic wastewater	√	√				(Sun et al., 2016)
Acetaminophen, caffeine, ethyl paraben, methyl paraben, propyl paraben, salicylic acid	Domestic wastewater		√	√		√	(Yang et al., 2017)
Caffeine	Domestic wastewater	√					(Cantwell et al., 2018)
Caffeine, crotamiton, DEET, triclocarban, triclosan	Domestic wastewater	√	√	√			(Tran et al., 2019)
Carbamazepine, crotamiton	Treated municipal wastewater						
Lincomycin	Livestock wastewater	√	√				(Wu et al., 2021)
Albendazole	Landfill leachate						

Notes: a) Detection ratio: measured concentration divided by the limit of quantification.

Table S2 Information about investigated WWTPs in this study.

WWTPs	Treatment process	Average flow (m^3/day)	Proportion of domestic wastewater
WWTPs-A	A^2/O [a] system	20×10^3	90.2%
WWTPs-B	SBR [b] system	30×10^3	100%
WWTPs-C	A^2/O system	95×10^3	95.2%
WWTPs-D	Oxidation ditch	10×10^4	99.5%
WWTPs-E	SBR system	50×10^2	100%
WWTPs-F	A^2/O system	15×10^3	100%

Notes: a) A^2/O: anaerobic/Anoxic/Oxic biological treatment; b) SBR: sequencing batch reactor activated sludge process.

Table S3 Information about investigated CAFOs in this study.

CAFOs	Sampling campaign	Animal type	Treatment process	Average flow (m^3/day)
CAFOs-A	May 2019	Cow	AD [a] system	50 – 60
CAFOs-B	October 2020	Cow	AD system	20 – 30
CAFOs-C	May 2019	Swine	A/O [b] system	150 – 200
CAFOs-D	November 2020	Swine	AD system	200
CAFOs-E	November 2019	Swine	AD system	70 – 100
CAFOs-F	October 2020	Swine	AD system	100 – 150
CAFOs-G	October 2020	Swine	AD system	70 – 100

Notes: a) AD: anaerobic digestion; b) A/O: anoxic/aerobic biological treatment.

S1 Description of the isotopically labeled internal standards (ILISs) and analytical methods using HPLC-MS/MS

Twelve ILISs of high purity grade (>98%) were purchased from the following suppliers: atrazine-^{5}D and mecoprop-^{3}D from CDN Isotopes (Quebec, Canada); ciprofloxacin-$^{13}C_3^{15}N$, gemfibrozil-^{6}D and phenacetin-^{13}C from Cambridge Isotope Laboratories (Andover, MA, USA); sulfamethazine-^{13}C from Sigma-Aldrich (St. Louis, MO, USA); chloramphenicol-^{5}D, DEET-^{7}D, fenbendazole-^{3}D, ofloxacin-^{6}D, roxithromycin-^{7}D and tetracycline-^{6}D from Toronto Research Chemicals (Toronto, Canada).

Ultra-high performance liquid chromatograph (UHPLC) equipped with electrospray ionization (ESI) and tandem mass spectrometry modules (LCMS-8050, Shimadzu, Japan) operated in multiple reaction monitoring (MRM) mode, was used to quantify the target PPCPs. The injection volume was 10 μL, and the column temperature was 40℃.

Pure water with 0.1% (v/v) formic acid (mobile phase A) and acetonitrile with 0.1% (v/v) formic acid (mobile phase B) were used. The analyses were conducted on a Shim-pack GIST C_{18} UHPLC column (100 mm × 2.1 mm i.d., 2 μm particle size) with a flow rate of 0.40 mL/min. The elution gradient was held at 10% B for 0.5 min, increased to 100% within 5 min, held for 7 min, then reset to 10% B at 7.1 min and kept for 10 min for reequilibration of the column.

Table S4 Method detection limits (MDLs), method quantification limits (MQLs) and recoveries of PPCPs.

PPCPs	MDL (ng/L)	MQL (ng/L)	Recovery (%)			
			Landfill leachates	WWTP influents	WWTP effluents	Livestock wastewater
ATM	0.53	1.59	78.0 ± 7.8	63.2 ± 10.7	84.1 ± 20.6	66.1 ± 4.2
CTM	0.73	2.18	101.9 ± 8.9	107.7 ± 14.5	110.1 ± 20.2	122.2 ± 0.8
ETM	0.35	1.06	108.7 ± 8.2	95.0 ± 12.3	88.9 ± 2.8	95.3 ± 4.0
LEM	0.26	0.79	103.0 ± 6.3	107.7 ± 7.2	117.0 ± 6.0	94.8 ± 6.4
RTM	0.27	0.82	61.0 ± 6.8	118.1 ± 9.6	135.1 ± 21.3	79.5 ± 18.4
TYL	0.46	1.37	113.3 ± 14.7	101.8 ± 19.0	99.2 ± 11.5	92.2 ± 29.7
FQ	0.53	1.58	112.6 ± 22.5	117.4 ± 19.0	133.1 ± 19.6	114.0 ± 25.0
OA	0.23	0.70	105.2 ± 21.2	143.7 ± 18.1	145.1 ± 14.6	109.8 ± 9.0
CLX	0.45	1.35	95.2 ± 3.3	111.7 ± 9.1	98.3 ± 15.2	111.8 ± 16.7
CPX	1.00	3.01	95.8 ± 18.9	91.8 ± 24.8	100.9 ± 10.2	83.0 ± 16.9
DAX	0.36	1.08	111.1 ± 8.1	65.2 ± 11.3	67.1 ± 5.1	153.5 ± 11.6
DIX	0.52	1.56	133.7 ± 14.8	134.2 ± 2.0	119.4 ± 15.1	136.7 ± 8.1
EFX	0.41	1.23	116.0 ± 4.8	108.2 ± 14.5	112.1 ± 23.1	88.4 ± 7.2
LFX	0.83	2.49	95.7 ± 9.2	143.1 ± 25.4	92.9 ± 12.0	88.7 ± 6.1
MAX	0.67	2.01	78.2 ± 14.5	74.2 ± 8.3	100.9 ± 10.9	130.4 ± 5.8
NFX	0.33	1.00	118.0 ± 11.5	98.5 ± 20.5	87.9 ± 8.4	101.1 ± 7.4
OFX	1.35	4.05	96.1 ± 21.2	107.2 ± 8.8	79.5 ± 2.4	85.5 ± 16.0
PFX	0.33	0.98	92.7 ± 4.2	65.2 ± 8.3	72.3 ± 10.5	75.2 ± 6.4
SFX	0.85	2.54	88.0 ± 11.1	125.0 ± 17.3	122.3 ± 13.5	102.2 ± 21.5
SPX	0.24	0.72	97.1 ± 20.0	133.6 ± 21.1	88.8 ± 13.6	129.9 ± 15.8
SC	0.32	0.95	117.5 ± 28.4	106.7 ± 14.8	118.3 ± 4.7	92.0 ± 15.1
SD	0.51	1.52	85.3 ± 13.5	56.1 ± 1.3	84.9 ± 6.0	73.7 ± 4.6
SDM	0.30	0.90	77.5 ± 18.9	131.0 ± 16.1	111.1 ± 9.7	74.1 ± 5.0
SF	0.52	1.55	95.8 ± 9.1	90.0 ± 8.7	100.6 ± 4.8	107.1 ± 4.1
SG	0.48	1.43	74.9 ± 18.0	111.6 ± 12.7	52.6 ± 4.7	79.4 ± 9.1
SIM	0.53	1.59	90.6 ± 6.7	92.2 ± 8.4	63.5 ± 4.2	75.8 ± 4.3
SIX	0.17	0.51	90.0 ± 5.7	108.7 ± 7.4	118.7 ± 7.8	72.1 ± 7.8
SMR	0.39	1.17	81.1 ± 16.7	73.1 ± 4.9	89.5 ± 5.6	104.4 ± 4.0
SMT	0.13	0.38	93.4 ± 9.0	93.4 ± 6.1	63.1 ± 6.8	82.1 ± 1.8
SMX	0.23	0.70	90.6 ± 6.5	107.4 ± 11.1	118.0 ± 5.9	94.0 ± 5.9
SMZ	0.15	0.46	85.5 ± 18.8	117.6 ± 2.4	114.7 ± 10.9	82.6 ± 9.4
SPZ	0.35	1.04	52.2 ± 8.0	114.2 ± 7.1	111.9 ± 13.3	60.7 ± 7.2
SQX	0.26	0.78	65.1 ± 20.4	102.9 ± 24.8	119.8 ± 18.1	64.9 ± 10.0

PPCPs	MDL (ng/L)	MQL (ng/L)	Recovery (%)			
			Landfill leachates	WWTP influents	WWTP effluents	Livestock wastewater
STZ	0.47	1.40	94.7 ± 8.8	83.5 ± 10.3	112.9 ± 4.3	107.4 ± 4.5
CTC	0.47	1.41	81.0 ± 1.8	123.2 ± 14.6	139.1 ± 10.7	76.3 ± 5.2
DMC	0.63	1.90	98.4 ± 8.9	114.6 ± 8.0	112.7 ± 15.9	79.1 ± 14.1
DTC	0.25	0.75	86.4 ± 3.2	86.8 ± 10.6	104.5 ± 7.8	97.5 ± 18.2
OTC	0.69	2.08	126.7 ± 11.4	87.7 ± 18.4	97.9 ± 8.7	76.5 ± 12.8
TC	0.37	1.12	98.7 ± 15.8	102.2 ± 6.8	122.5 ± 15.2	87.7 ± 13.1
CP	0.29	0.87	115.5 ± 5.7	99.5 ± 12.5	106.5 ± 10.2	96.4 ± 1.8
FF	0.57	1.71	88.6 ± 13.0	88.8 ± 6.9	81.3 ± 6.4	73.1 ± 9.5
LIN	0.43	1.28	67.8 ± 23.1	65.6 ± 4.5	74.1 ± 5.5	111.3 ± 1.5
TIA	0.40	1.21	88.8 ± 10.3	123.2 ± 21.5	107.3 ± 18.5	118.8 ± 7.8
TP	0.35	1.04	89.1 ± 4.4	61.1 ± 9.9	95.7 ± 10.0	75.4 ± 3.7
SAL	0.31	0.94	94.0 ± 8.8	66.5 ± 5.8	127.4 ± 8.2	73.5 ± 7.0
CIM	0.53	1.60	107.1 ± 1.8	61.4 ± 5.3	63.3 ± 4.2	118.0 ± 18.7
ABZ	0.49	1.47	94.2 ± 27.5	124.0 ± 8.8	117.4 ± 14.6	90.4 ± 30.6
FBZ	0.08	0.23	83.0 ± 7.6	127.1 ± 10.3	120.1 ± 13.1	82.2 ± 8.1
THP	0.57	1.72	148.2 ± 20.4	89.0 ± 11.1	77.5 ± 17.3	98.3 ± 6.6
TCS	0.69	2.06	97.1 ± 21.3	64.0 ± 3.5	94.8 ± 6.6	104.8 ± 21.0
WAR	0.22	0.66	115.5 ± 8.6	79.3 ± 1.8	82.2 ± 2.4	103.3 ± 5.2
FLU	0.59	1.76	109.1 ± 25.0	97.1 ± 6.8	120.2 ± 13.4	82.7 ± 18.1
SP	0.34	1.02	84.7 ± 1.9	63.0 ± 11.1	83.6 ± 7.4	113.6 ± 4.4
DIL	1.21	3.63	112.0 ± 15.5	83.3 ± 12.4	82.3 ± 12.7	80.0 ± 19.7
CRO	0.33	1.00	91.3 ± 17.4	122.3 ± 7.4	139.6 ± 12.3	111.0 ± 2.0
CBZ	0.26	0.79	107.8 ± 4.9	73.7 ± 4.0	66.5 ± 3.3	75.0 ± 2.2
GLI	0.24	0.72	105.1 ± 10.2	124.2 ± 3.8	122.9 ± 14.5	103.1 ± 10.3
GLY	0.22	0.66	102.7 ± 22.0	93.1 ± 7.1	93.1 ± 3.1	107.5 ± 2.8
TOL	0.37	1.10	66.4 ± 15.5	91.8 ± 6.8	87.0 ± 2.8	111.9 ± 19.5
DEET	0.16	0.49	96.8 ± 9.0	94.8 ± 12.4	100.5 ± 11.0	96.4 ± 6.1
BF	0.36	1.08	73.0 ± 11.1	60.3 ± 1.7	88.9 ± 4.7	80.0 ± 13.5
GF	0.30	0.90	100.9 ± 10.6	80.9 ± 5.6	95.9 ± 11.1	103.5 ± 7.8
ACE	0.64	1.92	110.9 ± 7.4	71.9 ± 12.8	60.2 ± 1.4	103.7 ± 7.4
DCF	0.26	0.79	67.4 ± 3.8	87.9 ± 3.2	108.8 ± 6.0	67.7 ± 8.2
NAP	0.93	2.79	104.1 ± 19.5	98.0 ± 7.0	112.1 ± 17.4	113.1 ± 19.0
CF	0.60	1.80	91.5 ± 7.0	104.9 ± 25.3	127.9 ± 6.3	128.8 ± 8.6
ATE	0.44	1.32	88.8 ± 17.5	62.5 ± 8.7	74.2 ± 4.5	87.2 ± 8.7
MTP	0.43	1.29	122.1 ± 9.7	64.6 ± 4.7	73.0 ± 7.6	90.9 ± 8.2

Table S5 The persistence, transportability and bioaccumulation of PPCPs.

PPCPs	CAS	half-life* (days)	log K_{oc}*	log K_{ow}
ATM	83905-01-5	0.97	4.64	4.02
CTM	81103-11-9	1.20	4.66	3.16

PPCPs	CAS	half-life* (days)	log K_{oc}*	log K_{ow}
ETM	114-07-8	1.24	4.65	3.06
LEM	8025-81-8	/	4.49	3.24*
RTM	80214-83-1	1.01	4.50	2.75*
TYL	1401-69-0	1.41	4.50	1.63
FQ	42835-25-6	/	2.99	1.6
OA	14698-29-4	2.59	2.91	0.94
CLX	105956-97-6	14.1	2.71	1.15
CPX	85721-33-1	1.92	2.48	0.28
DAX	112398-08-0	1.58	2.68	0.44*
DIX	98106-17-3	1.08	2.69	1.28
EFX	93106-60-6	1.58	2.68	0.70*
LFX	98079-51-7	1.46	3.25	−0.30
MAX	115550-35-1	1.76	2.67	−0.33*
NFX	70458-96-7	1.94	2.48	−1.03
OFX	82419-36-1	3.36	2.68	−0.39
PFX	70458-92-3	1.63	2.66	0.27
SFX	98105-99-8	1.39	3.40	1.07*
SPX	110871-86-8	1.24	2.58	2.50
SC	80-32-0	3.36	2.46	0.94*
SD	68-35-9	2.51	2.06	−0.09
SDM	122-11-2	2.26	1.72	1.36
SF	651-06-9	2.39	2.24	0.41
SG	57-67-0	2.59	1.21	−1.22
SIM	515-64-0	3.36	2.16	−0.33
SIX	127-69-5	2.32	2.30	1.01
SMR	127-79-7	2.40	2.29	0.14
SMT	57-68-1	2.30	2.16	0.89
SMX	723-46-6	2.43	1.96	0.89
SMZ	144-82-1	2.39	2.17	0.54
SPZ	526-08-9	3.36	2.88	1.52
SQX	59-40-5	2.40	2.94	0.84
STZ	72-14-0	2.50	2.43	0.05
CTC	57-62-5	1.53	3.18	−0.62
DMC	127-33-3	1.89	2.75	−1.14
DTC	564-25-0	2.11	2.75	−0.02
OTC	79-57-2	1.94	2.43	−0.90
TC	60-54-8	1.82	2.75	−1.30
CP	56-75-7	2.23	2.06	1.14
FF	73231-34-2	2.17	1.70	0.16*
LIN	154-21-2	2.62	1.78	0.56
TIA	55297-95-5	1.49	5.14	4.75
TP	738-70-5	2.04	2.06	0.91
SAL	18559-94-9	2.59	2.03	1.40

PPCPs	CAS	half-life* (days)	log K_{oc}*	log K_{ow}
CIM	51481-61-9	2.57	2.19	0.40
ABZ	54965-21-8	3.54	2.75	2.70
FBZ	43210-67-9	5.24	3.43	3.60*
THP	58-55-9	4.27	1.58	−0.02
TCS	3380-34-5	1.94	4.35	4.76
WAR	81-81-2	1.50	−0.39	2.60
FLU	54910-89-3	1.99	3.63	4.05
SP	15676-16-1	2.08	2.84	0.57
DIL	34933-06-7	2.06	3.18	2.79
CRO	483-63-6	2.62	2.16	2.73*
CBZ	298-46-4	2.67	2.74	2.45
GLI	21187-98-4	3.36	3.06	2.12
GLY	10238-21-8	1.71	4.86	3.75*
TOL	64-77-7	3.36	2.21	2.34
DEET	134-62-3	2.65	2.28	2.18
BF	41859-67-0	2.16	4.14	4.25
GF	25812-30-0	2.59	2.33	4.77*
ACE	103-90-2	2.87	1.68	0.46
DCF	15307-86-5	2.29	3.76	4.51
NAP	22204-53-1	2.92	2.74	3.18
CF	58-08-2	2.77	1.79	−0.07
ATE	29122-68-7	2.61	2.48	0.16
MTP	51384-51-1	2.65	3.11	1.88

Notes: * data modeled from QSAR model.

Table S6 The concentrations (median) and PNECs of PPCPs in landfill leachates.

Chemicals	Concentration (μg/L)	Detection frequency (%)	NOEC[a)] (μg/L)	EC_{50}/LC_{50}[a)] (μg/L)	AF	PNEC (μg/L)
ATM	4.98	100	0.20	/	10	0.020
CTM	1.90	20	0.84	/	10	0.084
ETM	4.72	100	/	22	1000	0.022
LEM	< MQL[b)]	0.0	/	5.0	1000	0.0050
RTM	0.533	40	10	/	100	0.10
TYL	0.746	20	/	950	1000	0.95
FQ	< MQL	0.0	5.0×10^3	/	10	5.0×10^2
OA	0.843	20	/	180	1000	0.18
CLX	17.0	80	0.98	/	10	0.098
CPX	17.2	40	5.0×10^2	/	100	5.0
DAX	4.40	60	$5.0 \times 10^{4*}$	/	10	5.0×10^3
DIX	6.03	40	$1.9 \times 10^{4*}$	/	10	1.9×10^3
EFX	4.37	60	19	/	100	0.19

Chemicals	Concentration (μg/L)	Detection frequency (%)	NOEC[a)] (μg/L)	EC_{50}/LC_{50}[a)] (μg/L)	AF	PNEC (μg/L)
LFX	3.24	40	1.0×10^4	/	50	2×10^2
MAX	2.80	40	/	$6.2 \times 10^{4*}$	1000	62
NFX	9.35	40	1.2×10^2	/	1000	0.12
OFX	< MQL	0.0	21	/	10	2.1
PFX	4.59	40	$9.2 \times 10^{4*}$	/	10	9.2×10^3
SFX	4.90	40	/	15	1000	0.015
SPX	2.80	60	$8.3 \times 10^{4*}$	/	10	8.3×10^3
SC	< MQL	0.0	/	/	/	/
SD	3.56	100	10	/	100	0.10
SDM	0.305	100	/	2.3×10^3	1000	2.3
SF	1.18	100	$1.6 \times 10^{2*}$	/	10	16
SG	3.43	40	/	3.4×10^3	1000	3.4
SIM	1.19	94	5.3×10^2	/	100	5.3
SIX	0.112	71	/	1.9×10^4	1000	19
SMR	0.377	82	/	1.2×10^4	1000	12
SMT	1.22	100	/	2.0×10^4	1000	20
SMX	0.577	94	/	1.5×10^4	1000	1.5
SMZ	3.40	94	/	2.5×10^4	1000	25
SPZ	1.65	60	2.6×10^2	/	100	2.6
SQX	0.824	53	/	246	1000	0.25
STZ	2.23	82	/	1.3×10^4	1000	13
CTC	5.35	20	5.0×10^2	/	100	5.0
DMC	36.6	40	3.3	/	10	0.33
DTC	7.72	60	/	316	1000	0.32
OTC	2.20	20	/	1.0×10^4	1000	1.0
TC	8.78	20	0.0050	/	10	5.0×10^{-4}
CP	0.431	88	2.0×10^3	/	10	2.0×10^2
FF	1.29	20	2.5×10^3	/	10	2.5×10^2
LIN	13.5	100	8.1	/	10	0.81
TIA	0.600	40	/	4.0×10^4	1000	40
TP	0.297	94	1.6×10^2	/	10	16
SAL	< MQL	0.0	/	1.0×10^5	1000	1.0×10^2
CIM	5.73	100	/	1.0×10^5	1000	1.0×10^2
ABZ	5.76	100	22.	/	50	0.44
FBZ	1.80	80	0.63	/	50	0.013
THP	2.92	40	/	1.7×10^5	1000	1.7×10^2
TCS	< MQL	0.0	0.20	/	10	0.020
WAR	3.87	60	/	34	1000	0.034
FLU	< MQL	0.0	0.32	/	10	0.032
SP	7.42	100	0.16	/	10	0.016
DIL	< MQL	0.0	/	8200	1000	8.2

Chemicals	Concentration (μg/L)	Detection frequency (%)	NOEC[a)] (μg/L)	EC_{50}/LC_{50}[a)] (μg/L)	AF	PNEC (μg/L)
CRO	2.86	100	53*	/	10	5.3
CBZ	0.660	94	0.50	/	10	0.050
GLI	2.02	100	/	1335	1000	1.3
GLY	1.24	60	1.7×10^{-4}	/	10	1.7×10^{-5}
TOL	< MQL	0.0	/	/	/	/
DEET	41.1	100	0.60	/	10	0.060
BF	0.733	94	0.034	/	50	6.8×10^{-4}
GF	2.46	100	0.38	/	10	0.038
ACE	16.3	20	1.0	/	10	0.10
DCF	12.6	100	0.36	/	10	0.036
NAP	15.8	40	0.020	/	10	0.0021
CF	2.45	94	0.010	/	10	0.001
ATE	7.83	20	20	/	50	0.40
MTP	1.53	94	5.0	/	100	0.050

Notes: a) data collected from ECOTOX database and references (Lützhøft et al., 1999; Jones et al., 2002; Eguchi et al., 2004; Kim et al., 2007; Comenges et al., 2010; De Liguoro et al., 2010; Białk-Bielińska et al., 2011; González-Pleiter et al., 2013; Huang et al., 2014; Kolar et al., 2014; Baumann et al., 2015; Deng et al., 2016; Li et al., 2019; Tell et al., 2019; Xu et al., 2019; Jurado et al., 2020; Peng et al., 2020; Han et al., 2021). b) < MQL: the concentration is below the method quantification limits. * data from model prediction.

S2 Calculation of risk quotient (RQ)

Risk quotient (RQ) was calculated following European technical guidance (EC, 2003), as shown in Eqs. (S1) and (S2).

$$\text{PNEC}=\frac{\text{NOEC or } EC_{50}/LC_{50}}{\text{AF}} \quad , \qquad \text{(S1)}$$

$$\text{RQ}=\frac{\text{MEC}}{\text{PNEC}} \quad , \qquad \text{(S2)}$$

where PNEC is predicted no effect environmental concentration, AF is assessment factor, and MEC is measured environmental concentration. The NOEC was utilized preferentially and EC_{50}/LC_{50} was employed only when NOEC was unavailable. According to EC (2003), AF values were assigned as 10, 50 or 100 if the NOEC data were available from three, two, or one trophic level, respectively. If only EC_{50} or LC_{50} values were available, the AF value was set to be 1000.

Table S7 Normalization of data for each index and individual normalized scores of PPCPs for three criteria.

PPCPs	Occurrence			Exposure potential			Ecological effect		
	U(DF)	U(DC)	PC1 (67.6%)	U(P)	U(T)	PC1 (52.8%)	U(B)	U(E)	PC1 (58.9%)
ATM	1.00	0.64	0.79	0.00	0.09	0.00	0.88	0.70	0.85
CTM	0.20	0.48	0.36	0.04	0.09	0.03	0.73	0.58	0.69
ETM	1.00	0.63	0.79	0.05	0.09	0.04	0.72	0.70	0.75
LEM	0.00	0.00	0.00	1.00	0.12	0.69	0.75	0.00	0.36
RTM	0.40	0.26	0.32	0.00	0.12	0.03	0.67	0.50	0.61
TYL	0.20	0.32	0.27	0.09	0.12	0.09	0.48	0.40	0.44
FQ	0.00	0.00	0.00	1.00	0.39	0.93	0.48	0.00	0.20
OA	0.20	0.34	0.28	0.37	0.40	0.53	0.37	0.50	0.42
CLX	0.80	0.85	0.83	1.00	0.44	0.97	0.40	0.68	0.56
CPX	0.40	0.85	0.66	0.21	0.48	0.49	0.26	0.48	0.35
DAX	0.60	0.62	0.61	0.13	0.44	0.40	0.29	0.05	0.11
DIX	0.40	0.68	0.56	0.01	0.44	0.32	0.43	0.12	0.23
EFX	0.60	0.62	0.61	0.13	0.44	0.40	0.33	0.58	0.45
LFX	0.40	0.57	0.50	0.11	0.34	0.30	0.16	0.21	0.13
MAX	0.40	0.55	0.49	0.18	0.45	0.43	0.16	0.25	0.15
NFX	0.40	0.75	0.60	0.22	0.48	0.49	0.04	0.64	0.31
OFX	0.00	0.00	0.00	0.55	0.44	0.68	0.15	0.00	0.00
PFX	0.40	0.63	0.53	0.14	0.45	0.41	0.26	0.02	0.08
SFX	0.40	0.64	0.54	0.09	0.31	0.26	0.39	0.72	0.57
SPX	0.60	0.55	0.57	0.05	0.46	0.36	0.63	0.00	0.29
SC	0.00	0.00	0.00	0.55	0.48	0.72	0.37	0.00	0.13
SD	1.00	0.59	0.76	0.35	0.56	0.65	0.20	0.60	0.38
SDM	1.00	0.17	0.52	0.29	0.62	0.66	0.44	0.31	0.36
SF	1.00	0.40	0.66	0.32	0.52	0.60	0.28	0.28	0.25
SG	0.40	0.58	0.50	0.37	0.71	0.79	0.01	0.42	0.16
SIM	0.94	0.40	0.63	0.55	0.54	0.77	0.16	0.34	0.20
SIX	0.71	0.00	0.30	0.31	0.51	0.58	0.38	0.18	0.24
SMR	0.82	0.21	0.47	0.33	0.52	0.59	0.24	0.23	0.19
SMT	1.00	0.41	0.66	0.30	0.54	0.60	0.36	0.27	0.29
SMX	0.94	0.28	0.56	0.33	0.57	0.65	0.36	0.36	0.34
SMZ	0.94	0.58	0.73	0.32	0.54	0.61	0.30	0.31	0.28
SPZ	0.60	0.46	0.52	0.55	0.41	0.65	0.46	0.39	0.42
SQX	0.53	0.34	0.42	0.33	0.40	0.49	0.35	0.48	0.40
STZ	0.82	0.51	0.64	0.35	0.49	0.59	0.22	0.32	0.23
CTC	0.20	0.65	0.46	0.12	0.35	0.32	0.11	0.42	0.22
DMC	0.40	0.98	0.73	0.21	0.43	0.44	0.03	0.66	0.31
DTC	0.60	0.72	0.67	0.26	0.43	0.47	0.21	0.58	0.38
OTC	0.20	0.50	0.37	0.22	0.49	0.50	0.07	0.46	0.22
TC	0.20	0.74	0.51	0.19	0.43	0.43	0.00	0.93	0.45
CP	0.88	0.23	0.51	0.29	0.56	0.60	0.40	0.10	0.21

PPCPs	Occurrence			Exposure potential			Ecological effect		
	U(DF)	U(DC)	PC1 (67.6%)	U(P)	U(T)	PC1 (52.8%)	U(B)	U(E)	PC1 (58.9%)
FF	0.20	0.41	0.32	0.27	0.62	0.65	0.24	0.18	0.16
LIN	1.00	0.81	0.89	0.38	0.61	0.71	0.31	0.56	0.43
TIA	0.40	0.28	0.33	0.11	0.00	0.00	1.00	0.18	0.62
TP	0.94	0.17	0.50	0.24	0.56	0.57	0.36	0.21	0.25
SAL	0.00	0.00	0.00	0.37	0.56	0.66	0.44	0.00	0.18
CIM	1.00	0.67	0.81	0.37	0.53	0.64	0.28	0.27	0.24
ABZ	1.00	0.67	0.81	0.60	0.43	0.70	0.66	0.55	0.63
FBZ	0.80	0.47	0.61	1.00	0.31	0.86	0.81	0.67	0.79
THP	0.40	0.55	0.49	0.77	0.64	1.00	0.21	0.21	0.16
TCS	0.00	0.00	0.00	0.22	0.14	0.19	1.00	0.00	0.51
WAR	0.60	0.60	0.60	0.11	1.00	0.87	0.64	0.66	0.69
FLU	0.00	0.00	0.00	0.23	0.27	0.32	0.88	0.00	0.44
SP	1.00	0.71	0.83	0.25	0.42	0.46	0.31	0.74	0.53
DIL	0.00	0.00	0.00	0.25	0.35	0.40	0.67	0.00	0.32
CRO	1.00	0.55	0.74	0.38	0.54	0.65	0.66	0.38	0.54
CBZ	0.94	0.30	0.57	0.39	0.43	0.57	0.62	0.55	0.61
GLI	1.00	0.49	0.71	0.55	0.38	0.62	0.56	0.44	0.51
GLY	0.60	0.41	0.49	0.16	0.05	0.08	0.83	1.00	1.00
TOL	0.00	0.00	0.00	0.55	0.53	0.76	0.60	0.00	0.27
DEET	1.00	1.00	1.00	0.39	0.52	0.63	0.57	0.76	0.70
BF	0.94	0.32	0.58	0.27	0.18	0.26	0.91	0.78	0.92
GF	1.00	0.52	0.72	0.37	0.51	0.62	1.00	0.63	0.89
ACE	0.20	0.84	0.57	0.44	0.63	0.76	0.29	0.68	0.49
DCF	1.00	0.80	0.89	0.30	0.25	0.34	0.96	0.72	0.91
NAP	0.40	0.84	0.65	0.45	0.43	0.60	0.74	0.88	0.87
CF	0.94	0.52	0.70	0.41	0.60	0.73	0.20	0.82	0.52
ATE	0.20	0.72	0.50	0.38	0.48	0.60	0.24	0.57	0.39
MTP	0.94	0.44	0.65	0.39	0.37	0.50	0.52	0.59	0.58

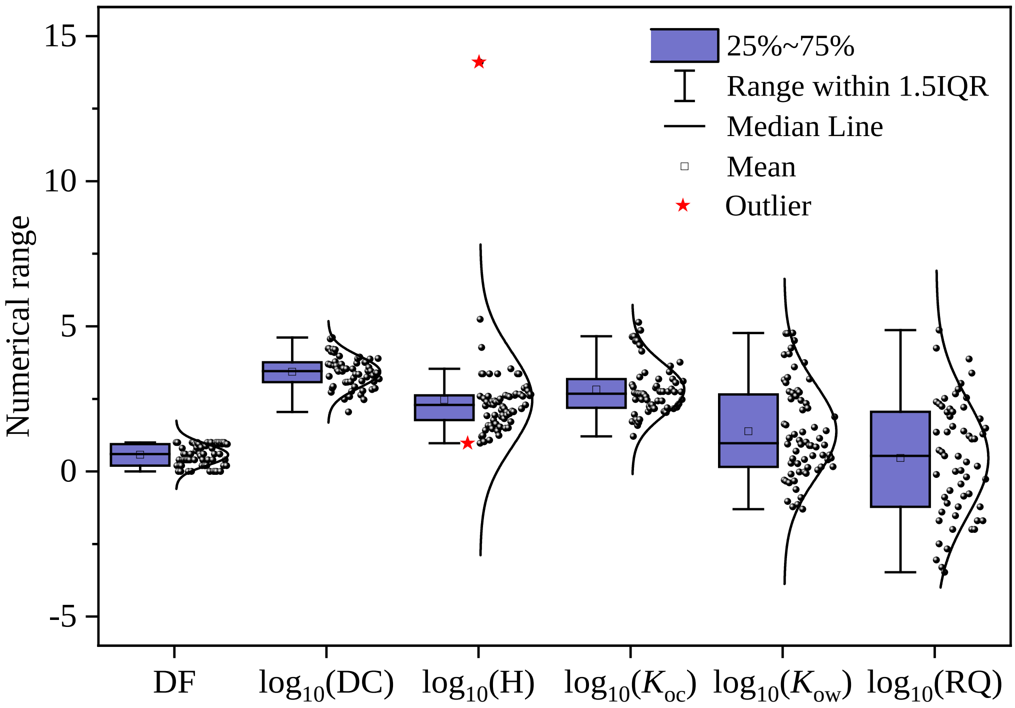

Fig. S1 Distribution of data for each index: detection frequency (DF), detection concentration (DC), persistence (H: half-life), transportability (K_{oc}), bioaccumulation (K_{ow}) and eco-toxicity (represented by RQ).

S3 Principal Component Analysis (PCA) for ranking

PCA is a common statistical method for reducing the number of variables by transforming them into principal components (PC). The selection of principal components depends on their eigenvalues (λ). Based on the Kaiser criterion (Kaiser, 1960; Jardim et al., 2021), when eigenvalues are above 1.0, the generated components explain a relevant amount of information contained in the original data; inversely, components with eigenvalues below 1.0 will be discarded.

In the beginning, when ranking scores are assigned, each criterion (occurrence, exposure potential, and ecological effect) needed to be pre-treated to convert individual values of multiple indexes into synthesis scores. The pre-treatments were conducted by PCA (Fig. S2). The first eigenvalues (λ1) of PC1 for the three criteria were above 1 (1.35, 1.18, and 1.06 respectively), and their second eigenvalues (λ2) were less than 1, indicating that the PPCP scores for the three criteria in PC1 reflected relevant information contained in the original data. The normalized PC1 scores of each criterion for 68 PPCPs are listed in Table S7.

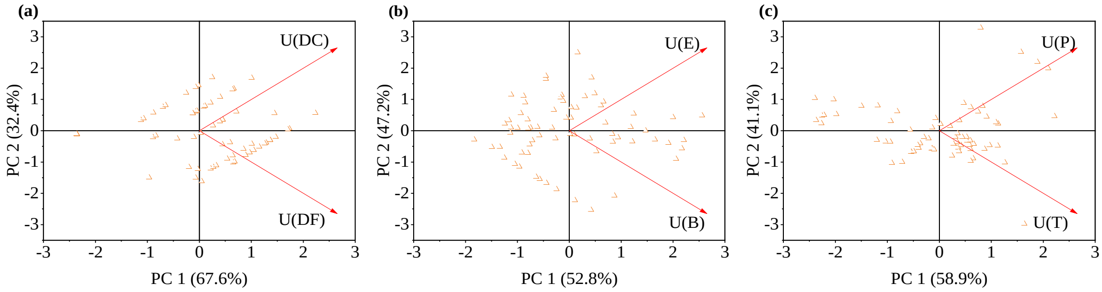

Fig. S2 PCA results of (a) occurrence, (b) exposure potential and (c) ecological effects of PPCPs.

PCA was implemented to acquire the ranking list of 68 PPCPs using data on occurrence, exposure potential and ecological effect, and the overall scores for ranking were calculated through weighted arithmetic mean by the eigenvalues and PC scores (Sharma, 2008; Thomaz and Giraldi, 2010). The first two eigenvalues were above 1 (1.47 and 1.05, respectively) and the first two components accounted for 84.1% of the cumulative variance, while the third eigenvalue was less than 1 (the value of $\lambda 3$ was 0.48); this indicated that PC1 and PC2 together played a major role in the total variance. PC1 scores and PC2 scores were used to calculate overall scores of 68 PPCPs (Table S8).

Table S8 Overall PCA scores and overall scores of PPCPs for three criteria.

PPCPs	PC1 (49.0%)	PC2 (35.1%)	Overall score	PPCPs	PC1 (49.0%)	PC2 (35.1%)	Overall score
ATM	2.91	−0.93	3.29	CTC	−0.32	−0.78	0.17
CTM	1.47	−1.97	1.11	DMC	0.29	0.32	1.57
ETM	2.52	−0.84	2.97	DTC	0.29	0.26	1.53
LEM	−1.56	−0.79	−1.07	OTC	−0.87	−0.42	−0.12
RTM	1.13	−2.08	0.69	TC	0.28	−0.30	1.11
TYL	0.38	−2.01	−0.01	CP	−0.82	0.26	0.42
FQ	−2.52	−0.02	−1.48	FF	−1.45	−0.07	−0.45
OA	−0.47	−0.59	0.16	LIN	0.44	1.59	2.63
CLX	0.22	2.26	2.89	TIA	1.23	−2.14	0.74
CPX	0.15	0.28	1.40	TP	−0.64	0.14	0.51
DAX	−0.52	−0.10	0.46	SAL	−2.08	−0.87	−1.64
DIX	−0.09	−0.50	0.61	CIM	−0.17	1.16	1.72
EFX	0.52	−0.12	1.49	ABZ	0.93	1.34	2.94
LFX	−0.49	−0.74	0.04	FBZ	0.72	1.32	2.72
MAX	−0.72	−0.33	0.10	THP	−1.76	1.47	0.35
NFX	−0.08	0.14	1.07	TCS	−0.15	−2.38	−0.80
OFX	−2.66	−0.80	−2.18	WAR	0.34	1.34	2.35
PFX	−0.81	−0.27	0.05	FLU	−0.60	−1.99	−0.97
SFX	1.01	−0.77	1.51	SP	1.13	0.63	2.63
SPX	0.01	−0.33	0.83	DIL	−1.14	−1.72	−1.32
SC	−2.32	−0.70	−1.76	CRO	0.59	1.00	2.36
SD	0.17	1.06	1.99	CBZ	0.62	0.29	1.88
SDM	−0.44	0.48	0.96	GLI	0.49	0.83	2.13
SF	−0.39	0.64	1.12	GLY	2.60	−1.50	2.58
SG	−1.33	0.86	0.34	TOL	−1.96	−0.58	−1.32
SIM	−0.89	1.10	0.95	DEET	1.67	1.62	3.88
SIX	−1.09	−0.35	−0.29	BF	2.19	−0.66	2.77
SMR	−0.94	0.14	0.22	GF	1.71	0.83	3.35
SMT	−0.25	0.65	1.26	ACE	−0.14	0.91	1.56
SMX	−0.38	0.54	1.06	DCF	2.63	0.38	3.96
SMZ	−0.15	0.87	1.52	NAP	1.54	0.60	3.03
SPZ	−0.23	0.44	1.14	CF	0.29	1.15	2.16
SQX	−0.18	−0.33	0.64	ATE	−0.26	0.21	0.94
STZ	−0.43	0.56	1.02	MTP	0.81	0.30	2.08

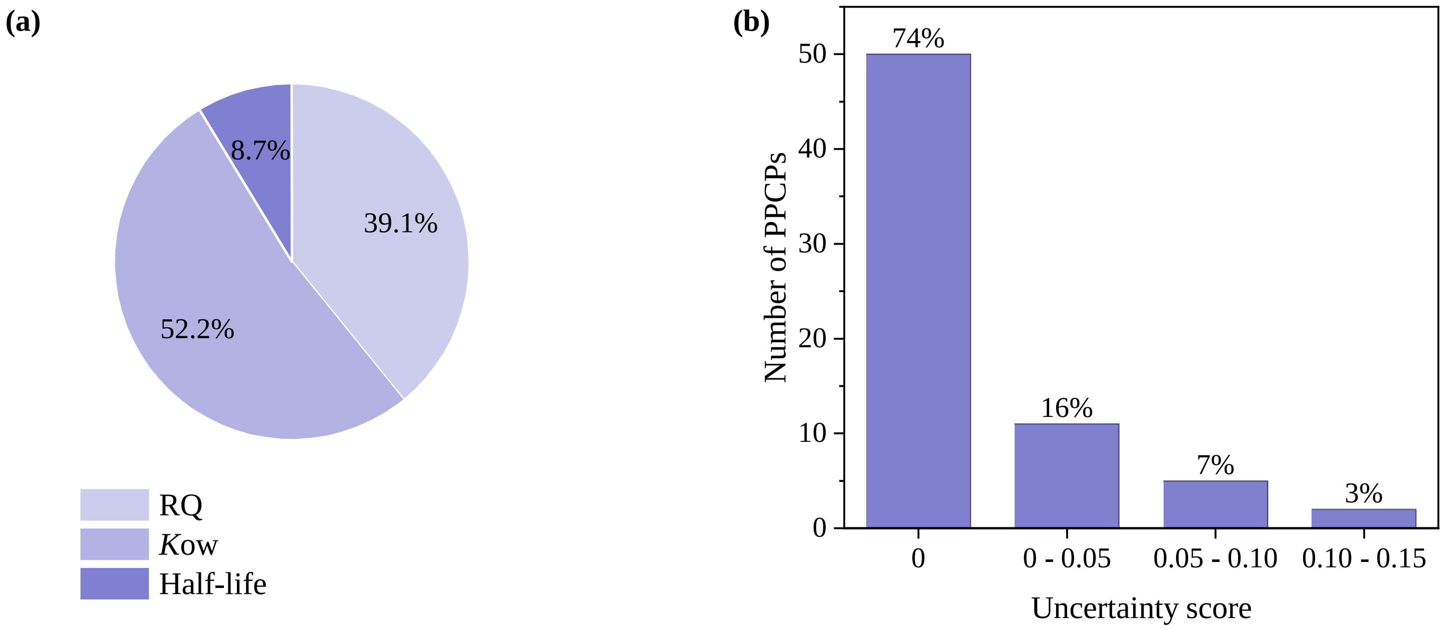

Fig. S3 Contribution of each criterion to total uncertainty of the ranking list (a) and distribution of uncertainty for target PPCPs (b).

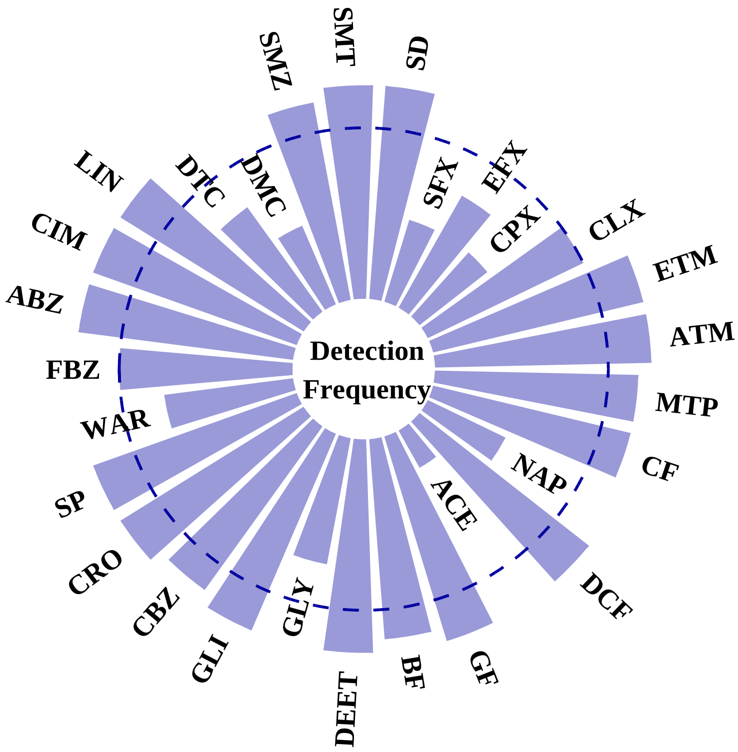

Fig. S4 Detection frequency of PPCPs in landfill leachates (the blue dash line represents a detection frequency of 80%).

Table S9 The concentrations (median) of 20 PPCPs in untreated and treated municipal wastewater, and livestock wastewater.

PPCPs	Concentration (ng/L)		
	Untreated municipal wastewater	Treated municipal wastewater	Livestock wastewater
ATM	95.3	82.9	3.57×10^3
ETM	21.0	23.0	253
CLX	13.2	3.50	33.4×10^3
SD	9.40	1.21	9.31×10^3
SMT	< MQL [a)]	< MQL	3.32×10^3
SMZ	19.3	5.27	28.8×10^3
LIN	223	46.45	32.8×10^3
CIM	< MQL	< MQL	717
ABZ	< MQL	< MQL	664
FBZ	< MQL	< MQL	2.85×10^3
SP	0.41	0.64	< MQL
CRO	10.0	10.6	< MQL
CBZ	1.34	5.18	< MQL
GLI	57.2	22.5	< MQL
DEET	4.99×10^3	< MQL	511
BF	28.9	11.4	< MQL
GF	< MQL	< MQL	< MQL
DCF	138	62.7	13.2×10^3
CF	5.30×10^3	29.49	751
MTP	83.5	123	< MQL

Notes: a) < MQL: the concentration is below the method quantification limits.

Table S10 Significant analysis of i-PPCP candidates among four pollution sources.

i-PPCP candidates	*p* value[a)]	Significance level
ATM	0.018	Significant
ETM	0.002	Significant
CIM	0.001	Significant
ABZ	0.000	Significant
SP	0.000	Significant
CRO	0.000	Significant
CBZ	0.001	Significant
GLI	0.000	Significant
DEET	0.000	Significant
BF	0.010	Significant
GF	0.000	Significant
MTP	0.007	Significant

Notes: a) $p > 0.05$, not significant; $p < 0.05$, significant.

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