Supplementary materials

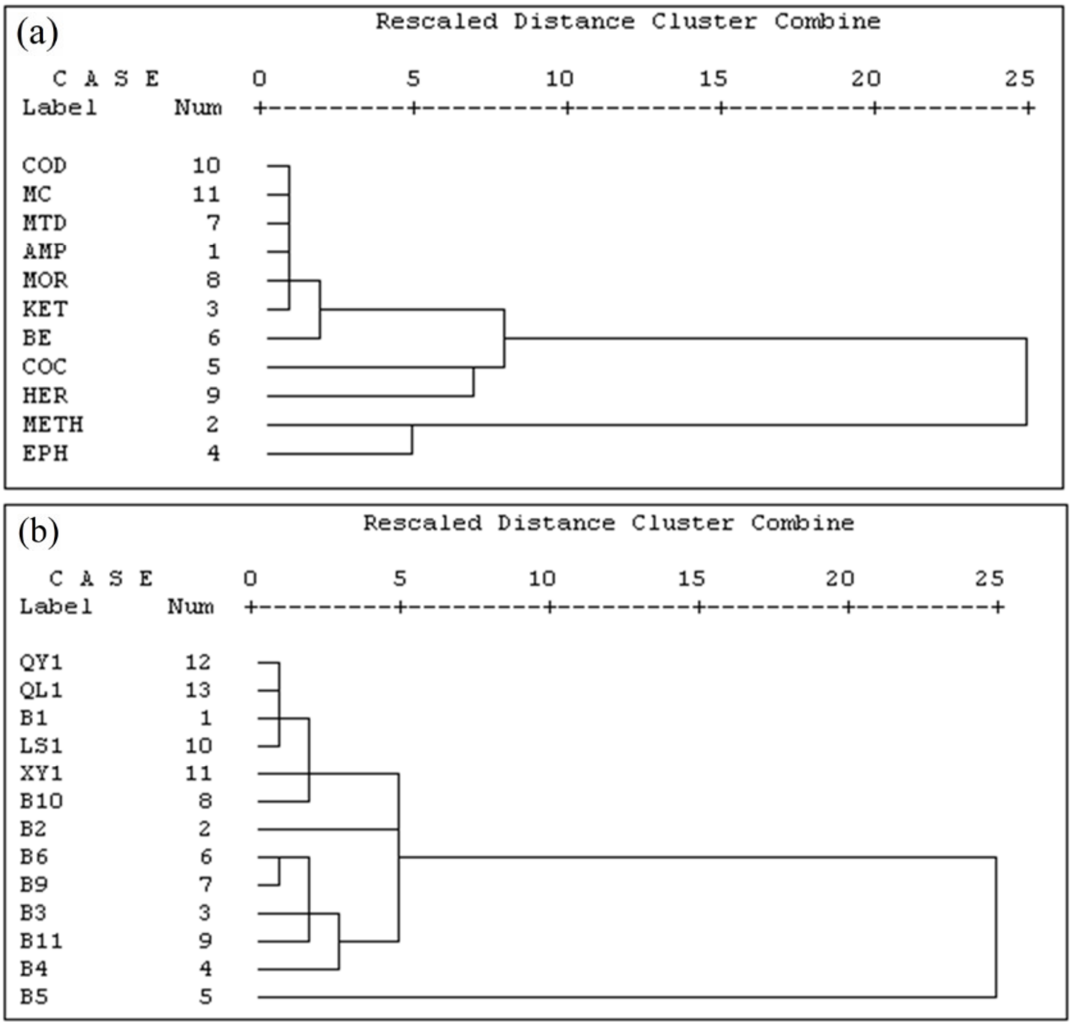
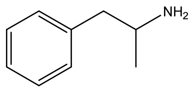
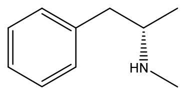
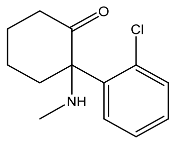
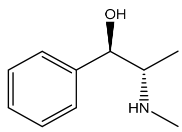
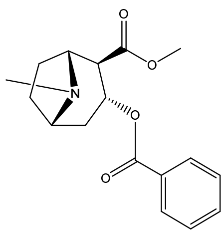
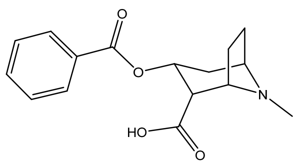
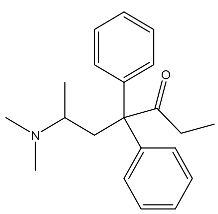
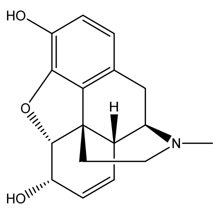


Fig. S1 Hierarchical cluster analysis of abused drugs in surface water

Table S1 Summary of different extraction procedures published to determine abused drugs in solid matrices

Matrix	Extraction method	Determination	Compounds	Recovery (%)	LOD	References
Sewage sludge	SLE	LC-MS	Amphetamine	90	2 μg/kg	Kaleta et al., 2006
Particulate matter of sewage	SPE(Oasis HLB)	LC-MS/MS	Amphetamine and cocainics	–	0.01–0.16 ng/g	Metcalfe et al., 2010
Particulate matter and soil	PLE-SPE(Oasis HLB)	LC-MS/MS	Opioids	4–145	0.01–1.31 ng/g	Baker and Kasprzyk-Hordern, 2011
Sewage sludge	PLE Al_2O_3	LC-ESI-MS/MS	Cocainics, amphetamines, opioids, benzodiazepines, LSD, cannabinoids	5–135	0.5–6.4 ng/L	Mastroianni et al., 2013
Particulate matter and sludge	PLE-SPE(Oasis MCX)	LC-MS/MS	Amphetamines, cannabinoids, morphine derivatives	3–101	0.1–3.1 ng/g	Senta et al., 2013
Sewage sludge	PLE Cl_2CH_2	LC–MS/MS	Nicotine, opioids, alkaloids	44–95	0.5–10 μg/kg	Arbeláez et al., 2014
Sewage sludge	MeOH-Milli-Q water	LC-MS/MS	Illicit drugs	17–126	0.6–19.9 ng/g	Gago-Ferrero et al., 2015

Table S2 Physico-chemical properties of abused drugs in this study

Compound	Structure	Empirical formula	MW (g/mol)	pKa	CAS Number
AMP		$C_9H_{13}N$	135.21	10.1	300-62-9
METH		$C_{10}H_{15}N$	149.23	9.9	4846-07-5
KET		$C_{13}H_{16}ClNO$	237.73	7.5	6740-88-1
EPH		$C_{10}H_{15}NO$	165.23	10.3	299-42-3
COC		$C_{17}H_{21}NO_4$	303.36	8.61	50-36-2
BE		$C_{16}H_{19}NO_4$	289.33	10.1	519-09-5
MTD		$C_{21}H_{27}NO$	309.45	8.94	76-99-3
MOR		$C_{17}H_{19}NO_3$	285.34	8.21	57-27-2

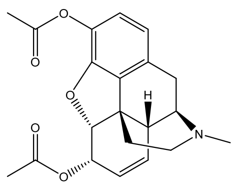
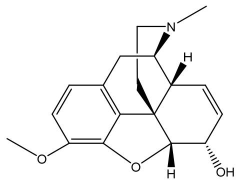
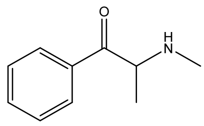
HER		$C_{21}H_{23}NO_5$	369.41	7.95	561-27-3
COD		$C_{18}H_{21}NO_3$	299.37	8.21	76-57-3
MC		$C_{10}H_{13}NO$	163.22	8.02	5650-44-2

Table S3 Sampling information and chemical analyses of sediments

Sampling location	Geographic location	pH of sediment samples	f_{oc} of sediment samples (%)
B2	39°51′2”N 116°45′24”E	7.07	4.05
B3	39°48′56”N 116°46′36”E	7.31	4.22
LS1	39°47′43”N 116°46′37”E	8.36	5.27
B4	39°46′3”N 116°52′34”E	7.52	2.35
B5	39°44′47”N 116°56′4”E	7.36	4.17
B6	39°42′47”N 116°56′36”E	7.90	3.02
XY1	39°42′29”N 116°54′59”E	8.12	5.37
QY1	39°41′6”N 116°55′22”E	8.42	3.94
B7	39°40′43”N 116°56′36”E	7.8	2.25
QL1	39°41′9”N 116°57′4”E	8.91	5.89
B8	39°35′57”N 116°59′32”E	8.11	2.93
B9	39°31′47”N 117°0′31”E	7.06	3.36
B10	36°26′37”N 117°3′3”E	7.87	2.87
B11	39°21′37”N 117°3′23”E	7.79	3.37

Table S4 Analyte ions monitored for LC-MS/MS, and conditions of collision voltage and declustering potential

Analytes	Precursor ion (m/z)	Product ion 1 (Quantifier)	CV(eV)[a)]	Product ion 2 (Qualifier)	CV(eV)	DP(V)[b)]
AMP	136.1	91.0	23	119.1	13	30
AMP-d8	144.1	97.1	24	–	–	40
METH	150.1	91.0	16	119.2	26.0	30
METH-d8	158.1	93.1	20	–	–	40
KET	238.2	207.1	40	125.1	20	50
KET-d4	242.2	129.1	42	–	–	60
EPH	166.0	148.1	17	133.2	28	30
EPH-d8	174.0	125.0	20	–	–	40
COC	304.1	296.0	16	274.2	20	35
COC-d3	307.2	235.1	20	–	–	40
BE	290.1	105.1	40	253.1	15	108
BE-d3	293.2	171.2	27	–	–	95
MTD	310.2	276.3	20	249.2	18	40
MTD-d5	315.2	195.2	15	–	–	50
MOR	286.1	201.3	40	235.1	26	90
MOR-d3	289.2	181.1	51	–	–	95
HER	370.1	301.1	26	269.1	24	30
HER-d9	379.2	256.2	30	–	–	40
COD	300.1	215.1	35	220.3	16	90
COD-d6	306.2	165.2	55	–	–	100
MC	164.1	98.0	24	124.1	28	30
MC-d8	172.1	95.1	40	–	–	50

Notes: a) Collision voltage; b) Declustering potential

Table S5 Recoveries (%) of abused drugs from different matrix

Analytes	Tap water		Surface water		Sediment	
	Mean	RSD	Mean	RSD	Mean	RSD
AMP	90.12	1.64	78.68	4.96	71.97	8.68
METH	82.80	2.80	76.85	3.73	81.06	12.20
KET	83.17	0.81	71.79	3.06	70.28	6.46
EPH	89.47	1.48	73.84	4.25	91.35	11.24
COC	77.36	3.64	78.62	4.55	69.36	4.89
BE	86.23	2.83	81.23	3.16	101.37	7.35
MTD	93.56	3.54	92.15	5.06	78.18	4.18
MOR	76.98	2.72	75.44	4.53	75.34	6.48
HER	84.26	0.99	80.83	2.34	88.69	5.39
COD	79.60	4.23	75.39	4.11	85.72	10.08
MC	78.78	2.60	72.84	3.38	68.41	7.86

Table S6 Recoveries (%) of abused drugs at different spiking concentrations

Analytes	Surface water				Sediment			
	10 ng/L		100 ng/L		10 ng/g		100 ng/g	
	Mean	RSD	Mean	RSD	Mean	RSD	Mean	RSD
AMP	79.52	7.32	77.65	8.41	72.18	2.56	74.74	4.99
METH	75.58	4.60	75.46	5.63	82.15	3.56	82.34	5.25
KET	70.49	5.02	72.35	8.65	71.23	2.45	71.23	4.84
EPH	74.55	0.86	75.37	3.56	90.32	5.65	90.36	5.23
COC	79.73	2.48	78.16	5.66	68.33	6.32	67.86	3.25
BE	82.75	10.25	84.40	7.65	102.24	5.69	99.37	4.43
MTD	91.06	7.52	91.88	3.91	76.18	2.34	75.93	5.96
MOR	72.09	8.20	76.79	6.33	77.64	2.45	74.73	6.15
HER	81.66	6.25	82.71	4.36	85.83	1.96	86.24	4.67
COD	74.12	2.36	76.94	3.23	84.29	4.87	86.33	2.35
MC	73.97	2.42	74.03	4.55	67.74	6.74	69.16	5.12

Table S7 Occurrence of abused drugs in surface waters in different areas in the world

References	Study area	Drugs of abuse and Concentration (ng/L)										
		AMP	METH	KET	EPH	COC	BE	MTD	MOR	HER	COD	MC
Bartelt-Hunt et al., 2009	Nebraska, America	< LOQ	< LOQ-350.1	< LOQ	< LOQ	–	–	–	–	–	–	–
Zuccato et al., 2008	River Olona, Italy	< 0.65	1.7	–	18	44	183	8.6	38	–	51	–
	River Lambro, Italy	< 0.65	2.1	–	9.9	15	50	3.4	3.5	–	12	–
	River Po, Italy	< 0.65	< 0.41	–	0.6–1.9	0.3–0.8	2.2–5.1	0.2–0.8	< 0.55	–	1.0–2.7	–
	River Arno, Italy	< 0.65	< 0.41	–	1.6–6.6	0.3–2.9	8.1–37.2	–	1.3–4.7	–	4.7–8.8	–
	River Thames, UK	< 0.65	< 0.41	–	–	< 0.3–6	4–17.8	–	< 0.65–46.7	–	–	–
Mendoza et al., 2014	Rivers Jarama and Manzanares, Spain	Nd-14	7.7-54.8	–	30.6–288.0	44.2–103.0	20.8–823.0	–	21.6–148.0	nd	–	2.2–16.6
Boleda et al., 2009	Catalonia, Spain	–	–	–	2.0–16.0	–	–	0.8–4.4	< LOD–7.0	nd	2.0–39.5	–
Berset et al., 2010	Switzerland	< LOQ-1.2	–	–	–	< LOQ–3.7	< LOQ–11	< LOQ–4.6	< LOQ–14	–	< LOQ–18	nd
Li et al., 2016	Pearl River, China	0.5–1.4	17.4–58.2	9.9–21.7	–	nd	< LOQ–0.6	–	–	–	0.4–2.1	–

	Yangtze River, China	nd	1.3–2.8	1.8–3.7	–	0.2–0.7	0.8–1.4	–	–	–	< LOQ–0.1	–
Zhang et al., 2017	Beijing, China	1.5–11.2	2.7–99.5	1.0–16.3	1.2–75.1	–	–	–	–	–	–	–
Lin et al., 2010; Lin et al., 2014	Taiwan, China	–	< LOQ–405	< LOQ–108	–	–	–	0.2–4.3	< LOQ–341	–	< LOQ–57	–
This study	Beiyunhe River	nd–11.3	2.6–92.2	1.5–12.3	5.6–70.4	nd–10.7	nd–14.6	nd–6.3	nd–6.1	nd	nd–5.6	nd

Notes: nd, not detected; –, no data

Table S8 The Pearson correlations of abused drugs in surface water

Analytes	AMP	METH	KET	EPH	COC	BE	MTD	MOR	HER	COD
AMP	1									
METH	**0.904****	1								
KET	–0.077	–0.207	1							
EPH	**0.661***	**0.832****	–0.433	1						
COC	–0.086	–0.010	0.347	0.071	1					
BE	–0.391	–0.035	–0.145	0.205	0.337	1				
MTD	–0.070	–0.144	–0.073	0.173	–0.053	0.024	1			
MOR	–0.045	–0.043	–0.192	0.004	–0.238	–0.350	–0.244	1		
HER	0.388	**0.626***	–0.215	**0.635***	0.087	0.484	–0.317	–0.248	1	
COD	0.162	0.123	–0.291	0.023	0.101	–0.047	0.034	–0.035	–0.188	1

Notes: **, Correlation is significant at the 0.01 level (2-tailed); ***,** Correlation is significant at the 0.05 level (2-tailed)

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