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Multi-residue analysis of 90 emerging contaminants in liquid and solid environmental matrices by ultra-high-performance liquid chromatography tandem mass spectrometry. [Dataset].

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Supplementary material

Multi-residue analysis of 90 emerging contaminants in liquid and solid environmental matrices by ultra-performance liquid chromatography tandem mass spectrometry

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The supplementary material contains one figure and five tables. These detail results of MAE method development (Figure S1), chemical information of ECs studied (Table S1), intra- and inter-day precision (Table S2), intra- and inter-day accuracy (Table S3), absolute and corrected recoveries for environmental matrices (Table S4) and matrix suppression in environmental extracts (Table S5).

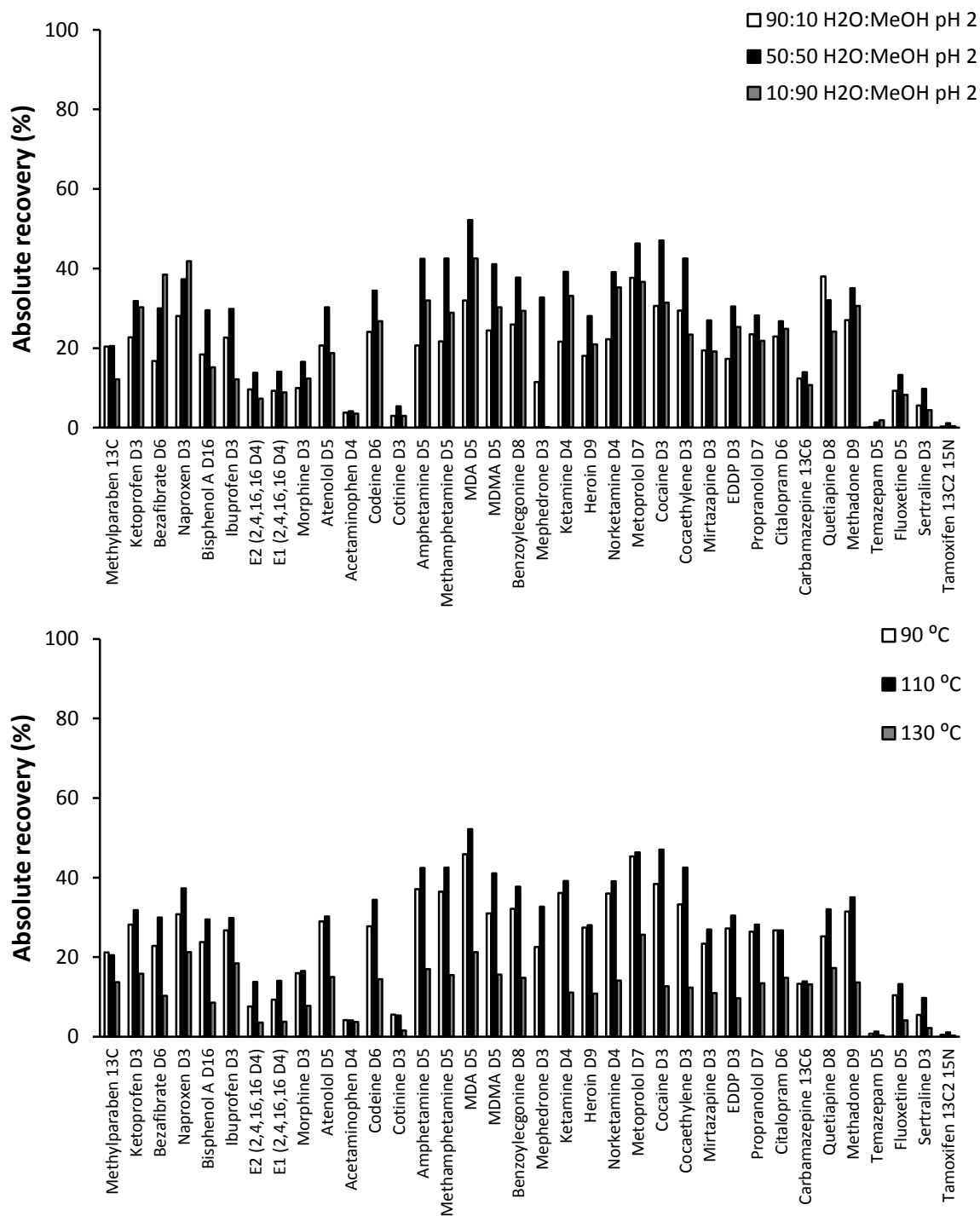


Figure S1. Impact of solvent composition whilst at constant temperature (110 °C) and extraction temperature whilst using the same solvent composition (50:50 H₂O:MeOH pH 2) for the extraction of deuterated ECs from digested sludge using MAE

Table S1. General and chemical information of ECs included within the analytical method (ordered by chemical class)

EC Class	Chemical	CAS No.	Molecular Formula	Molecular Weight (g mol ⁻¹)	Prescription 2012 (kg)	Water Solubility (mg L ⁻¹) ⁱ	Log Kow ⁱⁱ	Log Koc ⁱⁱⁱ	Log Dow ^{iv}	Henry's Law Constant (atm m ³ mol ⁻¹) ^v	Vapour Pressure (Torr) ^{vi}	pKa (Most acidic) ^{vii}	pKa (Most basic) ^{viii}
UV filters	Benzophenone-1	131-56-6	C ₁₃ H ₁₀ O ₃	214.22	-	413.4	2.96	2.65E-11	2.90	2.65E-11	2.84E-07	7.72±0.35	-
	Benzophenone-2	131-55-5	C ₁₃ H ₁₀ O ₅	246.22	-	398.5	2.78	3.61E-16	2.35	3.61E-16	6.69E-12	6.98±0.35	-
	Benzophenone-3	131-57-7	C ₁₄ H ₁₂ O ₃	228.25	-	68.6	3.52	1.50E-08	3.06	1.50E-08	5.26E-06	7.56±0.35	-
	Benzophenone-4	4065-45-6	C ₁₄ H ₁₂ O ₆ S	308.31	-	2.03E+04	0.37	7.03E-15	-0.53	7.06E-15	-	-0.70±0.50	-
Parabens	Methylparaben	99-76-3	C ₈ H ₈ O ₃	152.15	-	5.98E+03	2.00	2.23E-09	1.63	3.61E-09	5.55E-03	8.31±0.13	-
	Ethylparaben	120-47-8	C ₉ H ₁₀ O ₃	166.18	-	1.89E+03	2.49	3.01E-09	1.99	4.79E-09	7.59E-04	8.31±0.13	-
	Propylparaben	94-13-3	C ₁₀ H ₁₂ O ₃	180.21	-	529.3	2.98	4.25E-09	2.51	4.25E-12	9.30E-04	8.23±0.15	-
	Butylparaben	94-26-8	C ₁₁ H ₁₄ O ₃	194.23	-	159.0	3.47	6.00E-009	2.96	6.00E-09	3.56E-04	8.22±0.15	-
Plasticizer	Bisphenol-A	80-05-7	C ₁₅ H ₁₆ O ₂	228.29	-	172.7	3.64	9.16E-12	4.04	9.16E-12	5.34E-07	10.29±0.10	-
Steroid estrogens	E1	53-16-7	C ₁₈ H ₂₂ O ₂	270.37	-	146.8	3.43	3.80E-10	4.31	3.80E-10	1.54E-08	10.25±0.40	-
	E2	50-28-2	C ₁₈ H ₂₄ O ₂	272.39	84	82.0	3.94	1.41E-12	3.74	1.41E-12	9.82E-09	10.27±0.60	-
	EE2	57-63-6	C ₂₀ H ₂₄ O ₂	296.41	12	116.4	4.12	7.94E-12	3.90	7.94E-12	3.74E-09	10.24±0.60	-
Antibacterials/ antibiotics	Sulfasalazine	599-79-1	C ₁₈ H ₁₄ N ₄ O ₅ S	398.40	54,039	2.4	3.81	2.19E-18	-1.76	2.19E-18	5.95E-20	2.70±0.10	0.90±0.10
	Clarithromycin	81103-11-9	C ₃₈ H ₆₉ NO ₁₃	747.97	16,508	0.3	3.18	1.73E-29	2.31	1.73E-29	5.06E-30	13.08±0.70	8.16±0.70
	Azithromycin	83905-01-5	C ₃₈ H ₇₂ N ₂ O ₁₂	749.00	1,965	6.20E-02	3.24	5.30E-29	-2.48	5.30E-29	2.51E-31	13.28±0.70	8.59±0.70
	Trimethoprim	738-70-5	C ₁₄ H ₁₈ N ₄ O ₃	290.32	10,998	2.33E+03	0.73	2.39E-14	1.13	2.39E-14	3.74E-11	-	7.04±0.10
	Sulfamethoxazole	723-46-6	C ₁₀ H ₁₁ N ₃ O ₅ S	253.28	-	3.94E+03	0.48	9.56E-13	-0.03	9.56E-13	1.87E-09	5.81±0.50	1.39±0.10
	Triclosan	3380-34-5	C ₁₂ H ₇ Cl ₃ O ₂	289.55	-	4.6	4.66	2.13E-08	4.76	2.13E-08	3.26E-05	7.80±0.35	-
Hypertension	Valsartan	137862-53-4	C ₂₄ H ₂₉ N ₅ O ₃	435.53	6,484	1.4	3.65	1.82E-18	1.15	1.82E-18	1.06E-19	3.56±0.10	0.60±0.10

	Irbesartan	138402-11-6	C ₂₅ H ₂₈ N ₆ O	428.53	8,353	-	-	-	4.97	-	1.05E-16	4.16±0.10	2.60±0.20
	Lisinopril	76547-98-3	C ₂₁ H ₃₁ N ₃ O ₅	405.50	4,799	8.6	-0.94	1.89E-22	-3.23	1.89E-22	1.14E-18	2.18±0.10	10.50±0.10
NSAIDS	Ketoprofen	22071-15-4	C ₁₆ H ₁₄ O ₃	254.29	243	120.4	3.00	2.12E-11	0.08	2.12E-11	3.32E-08	4.23±0.10	-
	Ibuprofen	15687-27-1	C ₁₃ H ₁₈ O ₂	206.29	108,435	41.1	3.79	1.52E-07	1.25	1.52E-07	1.39E-04	4.41±0.10	-
	Naproxen	22204-53-1	C ₁₄ H ₁₄ O ₃	230.27	126,258	144.9	3.10	3.39E-10	-0.54	3.39E-10	3.01E-07	4.84±0.30	-
	Diclofenac	15307-86-5	C ₁₄ H ₁₁ Cl ₂ NO ₂	296.15	10,652	4.5	4.02	4.73E-12	0.73	4.73E-12	1.59E-07	4.18±0.10	-2.26±0.50
	Acetaminophen	103-90-2	C ₈ H ₉ NO ₂	151.17	>2,000,000	3.04E+04	0.27	6.42E-13	0.90	6.42E-13	1.43E-06	9.86±0.13	1.72±0.50
Lipid regulators	Bezafibrate	41859-67-0	C ₁₉ H ₂₀ ClNO ₄	361.83	7,966	1.2	4.25	2.12E-15	0.46	2.12E-15	6.29E-14	3.29±0.10	-2.06±0.70
	Atorvastatin	134523-00-5	C ₃₃ H ₃₅ FN ₂ O ₅	558.66	13,937	1.12E-03	6.36	2.41E-23	1.86	2.41E-23	6.84E-22	4.29±0.10	0.38±0.50
Antihistamines	Fexofenadine	83799-24-0	C ₃₂ H ₃₉ NO ₄	501.67	8,715	2.36E-02	2.81	1.19E-18	2.93	1.19E-18	2.08E-20	4.43±0.10	9.42±0.10
	Cetirizine	83881-51-0	C ₂₁ H ₂₅ ClN ₃ O ₃	388.90	1,612	1.1	-0.61	4.19E-17	0.69	4.19E-17	1.39E-12	3.46±0.10	6.71±0.10
Diabetes	Metformin	657-24-9	C ₄ H ₁₁ N ₅	129.17	-	1.00E+06	-2.64	7.64E-16	-6.45	7.64E-16	1.33	-	12.27±0.10
	Glicazide	21187-98-4	C ₁₅ H ₂₁ N ₃ O ₅ S	323.41	35,194	138.4	2.12	7.95E-13	0.79	7.95E-13	-	6.07±0.10	3.89±0.20
Cough suppressant	Pholcodine	509-67-1	C ₂₃ H ₃₀ N ₂ O ₄	398.51	600	1.01E+04	0.59	3.42E-19	-0.48	3.42E-19	3.44E-14	13.40±0.20	8.22±0.40
Beta-blocker	Atenolol	29122-68-7	C ₁₄ H ₂₂ N ₂ O ₃	266.34	20,725	685.2	-0.03	1.37E-18	-1.71	1.37E-18	3.82E-11	13.88±0.20	9.43±0.10
	Metoprolol	51384-51-1	C ₁₅ H ₂₅ NO ₃	267.37	2,311	4.77E+03	1.69	1.40E-13	-0.38	1.40E-13	4.52E-07	13.89±0.20	9.43±0.10
	Propranolol	525-66-6	C ₁₆ H ₂₁ NO ₂	259.35	9,076	228.0	2.60	7.98E-13	0.45	7.98E-13	2.48E-08	13.84±0.20	9.50±0.30
H ₂ receptor agonists	Ranitidine	66357-35-5	C ₁₃ H ₂₂ N ₄ O ₃ S	314.41	35,665	2.47E+04	0.29	3.42E-15	-1.56	3.42E-15	7.66E-08	-	8.35±0.28
	Cimetidine	51481-61-9	C ₁₀ H ₁₆ N ₆ S	252.34	3,195	1.05E+04	0.57	9.55E-16	-0.30	9.55E-16	3.13E-09	14.13±0.10	7.07±0.61
X-ray contrast media	Iopromide	73334-07-3	C ₁₈ H ₂₄ I ₃ N ₃ O ₈	791.12	-	23.8	-2.49	1.00E-028	-0.44	1.00E-28	5.00E-30	10.62±0.70	-2.60±0.70
Drug precursor and metabolite	Ephedrine/	299-42-3	C ₁₀ H ₁₅ NO	165.24	622	7.15E+04	0.68	8.65E-11	-1.13	8.65E-11	8.65E-03	13.96±0.20	9.38±0.10

	pseudoephedrine												
Anti-cancer	Norephedrine	492-39-7	C ₉ H ₁₃ NO	151.21	-	1.49E+05	0.22	3.94E-11	-1.40	3.94E-11	1.10E-03	12.07±0.45	8.47±0.10
	Azathioprine	446-86-6	C ₉ H ₇ N ₇ O ₂ S	277.26	2,768	272.3	-0.09	2.64E-15	1.21	2.64E-15	5.94E-11	-	7.47±0.20
	Methotrexate	59-05-2	C ₂₀ H ₂₂ N ₈ O ₅	454.45	126	2.60E+03	-1.28	1.54E-31	-7.06	1.54E-31	-	3.47±0.10	5.56±0.10
	Ifosfamide	3778-73-2	C ₇ H ₁₃ Cl ₂ N ₂ O ₂ P	261.09	-	3.78E+03	0.97	1.36E-11	0.10	1.36E-11	1.15E-04	-	1.44±0.20
Anaesthetic and metabolite	Tamoxifen	10540-29-1	C ₂₆ H ₂₉ NO	371.53	453	0.2	6.30	4.49E-10	5.07	4.49E-10	1.85E-09	-	8.69±0.28
	Ketamine	6740-88-1	C ₁₃ H ₁₆ ClNO	237.73	64	3.87E+03	3.12	1.38E-08	3.18	1.38E-08	1.76E-05	-	6.46±0.20
	Norketamine	35211-10-0	C ₁₅ H ₁₁ ClN ₂ O	233.70	-	-	-	-	2.71	1.78E-10	1.26E-05	-	6.25±0.20
Anti-depressants and metabolites	Venlafaxine	93413-69-5	C ₁₇ H ₂₇ N ₁ O ₂	277.41	16,211	266.7	3.28	2.87E-11	1.32	2.87E-11	4.92E-07	14.84±0.20	9.26±0.28
	Desmethylvenlafaxine	93413-62-8	C ₁₆ H ₂₅ NO ₂	263.38	-	-	-	-	1.17	-	3.03E-07	10.04±0.26	9.33±0.28
	Fluoxetine	54910-89-3	C ₁₇ H ₁₈ F ₃ NO	309.33	5,319	60.3	4.65	8.90E-08	1.92	8.90E-08	1.88E-06	-	10.05±0.10
	Norfluoxetine	83891-03-6	C ₁₆ H ₁₆ F ₃ NO	295.30	-	-	-	-	1.54	-	5.21E-06	-	9.05±0.13
	Sertraline	79617-96-2	C ₁₇ H ₁₇ Cl ₂ N	306.24	11,429	3.5	5.29	5.10E-08	3.11	5.10E-08	3.85E-07	-	9.47±0.40
	Mirtazapine	85650-52-8	C ₁₇ H ₁₉ N ₃	265.35	3,239	-	-	-	3.15	-	1.11E-07	-	8.10±0.20
	Citalopram	59729-33-8	C ₂₀ H ₂₁ FN ₂ O	324.40	8,878	31.1	3.74	2.69E-11	1.50	2.69E-11	1.53E-07	-	9.57±0.28
	Desmethylcitalopram	62498-67-3	C ₁₉ H ₁₉ FN ₂ O	310.37	-	-	-	-	0.14	-	1.40E-07	-	10.50±0.10
Anti-epileptic and metabolites	Carbamazepine	298-46-4	C ₁₅ H ₁₂ N ₂ O	236.28	44,498	17.7	2.25	1.08E-10	2.77	1.08E-10	5.78E-07	13.94±0.20	-0.49±0.20
	Carbamazepine10,11-epoxide	36507-30-9	C ₁₅ H ₁₂ N ₂ O ₂	252.27	-	-	-	-	1.97	-	2.69E-06	13.91±0.20	-0.50±0.20
	10,11-Dihydro-10-hydroxycarbamazepine	29331-92-8	C ₁₅ H ₁₄ N ₂ O ₂	254.28	-	-	-	-	1.73	-	3.33E-08	13.75±0.20	-0.53±0.40
Calcium channel blocker	Diltiazem	42399-41-7	C ₂₂ H ₂₆ N ₂ O ₄ S	414.52	21,922	12.3	2.79	8.61E-17	1.97	8.61E-17	4.27E-14	-	8.94±0.28

Hypnotic	Temazepam	846-50-4	C ₁₆ H ₁₅ ClN ₂ O ₂	300.75	833	163.9	2.15	1.13E-08	2.79	1.13E-08	6.33E-13	11.66±0.40	1.58±0.50
Anti-psychotic	Quetiapine	111974-69-7	C ₂₁ H ₂₅ N ₃ O ₂ S	384.52	9,155	0.6	3.17	7.45E-18	2.67	7.45E-18	3.22E-13	14.41±0.10	6.74±0.10
Veterinary	Tylosin	1401-69-0	C ₄₆ H ₇₇ NO ₁₇	916.12	-	0.5	1.05	5.77E-38	2.14	5.77E-38	0	13.06±0.70	7.39±0.70
Human indicators and metabolites	Creatinine	60-27-5	C ₄ H ₇ N ₃ O	113.12	-	1.66E+05	-1.21	2.42E-12	-1.07	2.42E-12	0.313	-	6.89±0.20
	Nicotine	54-11-5	C ₁₀ H ₁₄ N ₂	162.24	442	1.00E+06	1.00	3.00E-09	-2.34	3.00E-09	0.0303	-	8.00±0.50
	Caffeine	58-08-2	C ₈ H ₁₀ N ₄ O ₂	194.19	-	2.63E+03	0.16	3.58E-11	-0.55	3.58E-11	3.72E-07	-	0.52±0.70
	Cotinine	486-56-6	C ₁₀ H ₁₂ N ₂ O	176.22	-	9.99E+05	0.34	3.33E-12	0.21	3.33E-12	4.21E-04	-	4.72±0.12
	1,7 dimethylxantine	611-59-6	C ₇ H ₈ N ₄ O ₂	180.17	4	4.14E+03	-0.39	1.75E-12	0.24	1.75E-12	-	8.50±0.50	0.21±0.70
Analgesics and metabolites	Morphine	57-27-2	C ₁₇ H ₁₉ NO ₃	285.35	5,684	2.64E+04	0.72	1.33E-16	-0.37	1.33E-16	7.06E-10	9.48±0.40	8.25±0.40
	Dihydromorphine	509-60-4	C ₁₇ H ₂₁ NO ₃	287.36	-	2.38E+04	0.93	1.51E-16	-0.26	1.51E-16	7.65E-10	9.56±0.40	8.44±0.40
	Normorphine	466-97-7	C ₁₆ H ₁₇ NO ₃	271.32	-	2.56E+05	0.50	6.07E-17	-2.05	6.07E-17	2.99E-10	9.17±0.40	9.54±0.40
	Methadone	76-99-3	C ₂₁ H ₂₇ NO	309.46	1,687	48.5	4.17	4.97E-10	3.39	4.97E-10	2.20E-07	-	9.50±0.50
	EDDP	30223-73-5	C ₂₀ H ₂₃ N	277.40	-	-	-	-	2.50	-	2.06E-06	-	7.71±0.60
	Codeine	76-57-3	C ₁₈ H ₂₁ NO ₃	299.37	34,626	1.22E+04	1.28	7.58E-14	-0.23	7.58E-14	2.47E-09	13.40±0.20	8.23±0.40
	Norcodeine	467-15-2	C ₁₇ H ₁₉ NO ₃	285.35	-	3.92E+04	1.07	3.45E-14	-2.28	3.45E-14	1.51E-09	13.34±0.20	9.28±0.40
	Dihydrocodeine	125-28-0	C ₁₈ H ₂₃ NO ₃	301.39	9,720	6.53E+03	1.49	8.61E-14	-0.11	8.61E-14	2.48E-09	14.22±0.20	8.43±0.40
	Tramadol	27203-92-5	C ₁₆ H ₂₅ NO ₂	263.38	41,445	1.15E+03	3.01	1.54E-11	0.72	1.54E-11	1.02E-06	14.47±0.40	9.61±0.28
	N-desmethyltramadol	75377-45-6	C ₁₅ H ₂₃ NO ₂	249.35	-	-	-	-	-0.27	-	9.16E-06	14.46±0.40	10.56±0.10
O-desmethyltramadol	185453-02-5	C ₁₅ H ₂₃ NO ₂	249.35	-	-	-	-	0.38	-	3.14E-07	10.00±0.10	9.61±0.28	
Stimulants and metabolites	Amphetamine	300-62-9	C ₉ H ₁₃ N	135.21	-	2.80E+04	1.76	1.08E-06	-1.23	1.08E-06	0.307	-	9.94±0.10
	Methamphetamine	537-46-2	C ₁₀ H ₁₅ N	149.24	-	1.33E+04	2.22	2.37E-06	-1.01	2.37E-06	0.147	-	10.38±0.10

	MDMA	42542-10-9	C ₁₁ H ₁₅ NO ₂	193.25	-	7.03E+03	2.28	2.75E-09	-1.38	2.75E-09	3.17E-03	-	10.32±0.10
	MDA	101-77-9	C ₁₃ H ₁₄ N ₂	198.27	-	1.96E+03	2.18	1.58E-11	-1.61	1.58E-11	1.52E-06	-	5.32±0.25
	Cocaine	50-36-2	C ₁₇ H ₂₁ NO ₄	303.36	-	1.30E+03	2.17	4.24E-11	0.92	4.24E-11	1.87E-06	-	8.97±0.60
	Benzoylcegonine	519-09-5	C ₁₆ H ₁₉ NO ₄	289.33	-	1.61E+03	-1.32	1.03E-13	-0.60	1.03E-13	1.32E-08	3.35±0.40	10.83±0.40
	Anhydroecgonine methylester	43021-26-7	C ₁₀ H ₁₅ NO ₂	181.23	-	-	-	-	0.21	-	0.0219	-	7.97±0.40
	Cocaethylene	529-38-4	C ₁₈ H ₂₃ NO ₄	317.38	-	-	-	-	1.35	-	6.80E-07	-	9.04±0.60
	Mephedrone	1189805-46-6	C ₁₁ H ₁₅ NO	177.24	-	-	-	-	1.47	-	3.84E-03	-	7.41±0.10
	MDPV	687603-66-3	C ₁₆ H ₂₁ NO ₃	275.34	-	-	-	-	2.77	-	4.09E-07	-	8.41±0.20
Opioid and metabolite	Heroin	561-27-3	C ₂₁ H ₂₃ NO ₅	369.42	-	2.15E+03	1.80	6.15E-13	-0.06	6.15E-13	7.38E-10	-	7.93±0.40
	6-acetylmorphine	2784-73-8	C ₁₉ H ₂₁ NO ₄	327.37	-	-	-	-	-0.22	-	1.83E-09	9.41±0.40	8.03±0.40

ⁱAs calculated by EPI Suite [1] at 25°C

ⁱⁱAs calculated by EPI Suite [1] (KOWWIN v1.68 estimate)

ⁱⁱⁱAs calculated by EPI Suite [1] based on Log Kow

^{iv}As calculated by Marvin Beans [2] at pH 7.5

^vAs calculated by EPI Suite [1] based on Bond SAR method

^{vi}As stated on Scifinder calculated using Advanced Chemistry Development (ACD/Labs) Software v11.02 (©1994-2015 ACD/Labs) [3]

^{vii}As stated on Scifinder calculated using Advanced Chemistry Development (ACD/Labs) Software v11.02 (©1994-2015 ACD/Labs) at 25°C [3]

Table S2. Method detail including chromatographic retention time and mass spectrometry parameters used in the determination of ECs (ordered by retention time)

Chemical	No.	t_R (min)	Precursor ion (m/z)	Product ion 1 (m/z)	CV (V)	CE (eV)	Product ion 2 (m/z)	CV (V)	CE (eV)	Ion ratio ^a	Corresponding labelled internal standard
<i>Chemicals determined in ESI- mode</i>											
4-benzophenone	1	6.94	307.0	227.1	44	24	211.1	42	35	1.37 ±0.05	Methylparaben 13C
Sulfasalazine	2	7.06	396.8	197.0	45	25	239.9	45	25	8.87 ±0.65	Naproxen D3
Methylparaben	3	7.50	150.8	91.8	34	20	135.8	20	14	2.36 ±0.05	Methylparaben 13C
Valsartan	4	7.64	434.0	350.1	35	20	179.1	35	25	1.07 ±0.02	Naproxen D3
Ketoprofen	5	7.74	253.0	209.0	15	7	-	-	-	-	Ketoprofen D3
Bezafibrate	6	7.87	360.1	274.0	30	19	154.0	30	28	3.10 ±0.07	Bezafibrate D6
2-benzophenone	7	7.89	244.9	134.9	32	13	108.9	32	20	1.42 ±0.03	Bisphenol A D16
Naproxen	8	8.11	229.0	185.0	20	7	170.0	20	13	1.22 ±0.05	Naproxen D3
Ethylparaben	9	8.32	164.9	91.9	20	20	136.6	26	14	1.69 ±0.04	Naproxen D3
Fexofenadine	10	8.38	500.1	456.1	33	14	378.1	33	19	1.48 ±0.05	Naproxen D3
Irbesartan	11	8.61	427.1	193.0	50	28	121.0	50	65	17.3 ±0.52	Bisphenol A D16
Bisphenol A	12	8.96	227.3	212.1	40	22	132.7	40	25	1.60 ±0.08	Bisphenol A D16
Diclofenac	13	9.04	293.8	249.9	22	13	-	-	-	-	Naproxen D3
Propylparaben	14	9.19	179.0	91.8	34	25	136.0	20	16	3.12 ±0.10	Bisphenol A D16
Atorvastatin	15	9.26	557.1	397.1	50	30	278.1	50	45	1.02 ±0.03	Naproxen D3
1-benzophenone	16	9.60	213.0	134.8	36	20	90.8	34	25	1.22 ±0.02	Ibuprofen D3
E2	17	9.74	271.1	183.0	60	40	144.9	60	45	1.04 ±0.05	E2 (2,4,16,16 D4)
Ibuprofen	18	9.77	204.9	161.5	26	6	-	-	-	-	Ibuprofen D3
EE2	19	9.80	295.2	144.9	60	40	158.8	60	40	1.94 ±0.18	E2 (2,4,16,16 D4)
E1	20	9.82	269.0	145.0	55	40	158.0	55	40	8.85 ±0.27	E1 (2,4,16,16 D4)
Butylparaben	21	10.12	193.1	91.8	34	25	136.0	40	16	2.07 ±0.05	E1 (2,4,16,16 D4)
Triclosan	22	12.30	288.8	34.8	18	10	36.8	18	10	1.82 ±0.06	E1 (2,4,16,16 D4)
Methylparaben 13C	-	7.50	156.9	97.9	30	20	-	-	-	-	-
Ketoprofen D3	-	7.74	256.0	212.0	15	7	-	-	-	-	-
Bezafibrate D6	-	7.85	366.0	274.0	30	19	-	-	-	-	-
Naproxen D3	-	8.06	232.0	188.0	15	8	-	-	-	-	-
Bisphenol A D16	-	8.87	241.1	223.1	40	20	-	-	-	-	-
Ibuprofen D3	-	9.77	208.0	164.0	20	6	-	-	-	-	-
E2 (2,4,16,16 D4)	-	9.72	275.1	147.0	60	40	-	-	-	-	-
E1 (2,4,16,16 D4)	-	9.81	273.1	147.0	55	40	-	-	-	-	-
<i>Chemicals determined in ESI+ mode</i>											
Creatinine	23	2.73	114.0	44.0	30	15	86.1	31	11	4.22 ±0.10	Metformin D6
Metformin	24	2.84	130.0	60.0	30	15	71.0	30	20	1.89 ±0.02	Metformin D6
Dihydromorphine	25	3.30	288.2	185.0	28	42	213.0	28	32	2.82 ±0.14	Morphine D3
Nicotine	26	3.34	163.1	130.0	37	20	117.0	37	24	1.37 ±0.02	Atenolol D7

Normorphine	27	3.41	272.1	165.0	45	43	152.1	45	49	1.16 ±0.05	Morphine D3
Anhydroecgonine methylester	28	3.45	182.1	118.0	39	23	122.1	37	20	1.23 ±0.03	Atenolol D7
Morphine	29	3.46	286.2	165.1	53	38	152.1	53	56	0.98 ±0.04	Morphine D3
Pholcodine	30	3.70	399.2	381.2	55	25	100.1	55	37	3.00 ±0.43	Atenolol D7
Atenolol	31	4.32	267.3	145.1	38	30	190.1	38	16	1.61 ±0.07	Atenolol D7
Ranitidine	32	4.62	315.9	176.0	26	17	123.9	26	24	8.44 ±0.50	Atenolol D7
Iopromide	33	4.89	792.0	573.0	46	25	558.9	46	32	1.45 ±0.06	Acetaminophen D4
Acetaminophen	34	5.11	151.9	110.0	26	16	92.9	26	24	5.54 ±0.13	Acetaminophen D4
Cimetidine	35	5.32	252.9	159.4	22	16	211.2	22	10	9.02 ±0.40	Acetaminophen D4
Dihydrocodeine	36	5.47	302.1	199.1	53	33	128.1	53	60	1.91 ±0.05	Codeine D6
Codeine	37	6.05	300.2	215.1	49	25	152.1	49	57	1.17 ±0.04	Codeine D6
Norephedrine	38	6.34	152.2	134.1	23	10	117.1	23	16	2.99 ±0.06	1S,2R-(+) Ephedrine D3
Norcodeine	39	6.45	286.1	165.1	46	40	268.2	46	20	1.11 ±0.04	Codeine D6
1,7 dimethylxanthine	40	6.78	181.0	124.1	54	21	-	-	-	-	Cotinine D3
Lisinopril	41	7.14	406.2	84.0	38	27	246.1	38	22	9.42 ±0.30	Amphetamine D5
Ephedrine/pseudoephedrine	42	7.22	166.1	148.1	23	12	133.1	23	21	6.58 ±0.12	1S,2R-(+) Ephedrine D3
Cotinine	43	7.22	177.1	80.0	34	21	98.1	34	22	2.91 ±0.05	Cotinine D3
6-acetylmorphine	44	7.65	328.1	165.1	52	39	211.1	52	26	1.46 ±0.04	Cotinine D3
Azathioprine	45	7.75	278.0	142.0	28	13	85.0	28	20	5.49 ±0.17	Cotinine D3
Methotrexate	46	7.89	455.1	308.1	40	20	175.1	40	35	1.93 ±0.50	Amphetamine D5
Caffeine	47	8.29	195.1	138.0	38	15	110.0	38	23	2.56 ±0.05	Cotinine D3
O-desmethyltramadol	48	8.29	250.2	58.0	30	18	232.1	30	10	181 ±6.40	Cotinine D3
Amphetamine	49	8.39	136.2	91.1	18	16	119.1	18	8	1.20 ±0.04	Amphetamine D5
Trimethoprim	50	8.43	291.2	230.2	26	26	123.1	26	36	1.07 ±0.03	Methamphetamine D5
Methamphetamine	51	8.51	150.2	91.1	24	19	119.1	24	10	1.73 ±0.03	Methamphetamine D5
MDA	52	8.59	180.0	163.1	21	11	105.1	21	22	2.73 ±0.06	MDA D5
MDMA	53	8.62	194.1	163.1	24	13	105.1	24	24	2.34 ±0.03	MDMA D5
Sulfamethoxazole	54	9.56	254.1	92.2	36	30	156.1	36	20	1.44 ±0.03	Benzoyllecgonine D8
Benzoyllecgonine	55	9.68	290.2	168.1	38	19	105.1	38	30	1.95 ±0.03	Benzoyllecgonine D8
Mephedrone	56	9.79	178.1	160.1	10	12	145.0	10	22	1.55 ±0.06	Mephedrone D3
Ketamine	57	10.59	238.1	125.0	31	27	220.1	31	15	2.93 ±0.04	Ketamine D4
Desmethylvenlafaxine	58	10.79	264.0	107.1	25	24	246.3	25	20	2.00 ±0.04	Metoprolol D7
Heroin	59	10.85	370.2	165.1	51	50	268.1	51	29	1.41 ±0.02	Heroin D9
Tramadol	60	10.97	264.0	58.0	28	45	120.7	28	46	270 ±21.4	Metoprolol D7
Norketamine	61	11.08	224.0	207.1	23	12	125.0	23	27	1.00 ±0.02	Norketamine D4
Metoprolol	62	11.17	268.3	116.1	42	20	121.1	42	22	2.36 ±0.04	Metoprolol D7
Cocaine	63	11.32	304.2	182.1	40	20	82.1	40	31	2.75 ±0.09	Cocaine D3
N-desmethyltramadol	64	11.88	250.1	44.0	25	12	232.1	25	8	38.6 ±0.06	Cocaine D3
MDPV	65	12.11	276.1	126.1	40	28	135.0	40	25	1.48 ±0.04	Cocaethylene D3

Ifosfamide	66	12.69	261.0	92.0	40	28	154.0	40	22	1.89 ±0.03	Metoprolol D7
Cocaethylene	67	12.91	318.2	196.2	38	20	82.1	38	30	1.90 ±0.05	Cocaethylene D3
Carbamazepine 10,11-epoxide	68	13.47	253.1	180.1	39	25	210.1	39	12	1.96 ±0.04	Carbamazepine 13C6
10,11-Dihydro-10-hydroxycarbamazepine	69	13.49	255.1	194.1	20	20	179.1	20	40	9.75 ±0.29	Carbamazepine 13C6
Mirtazapine	70	13.52	266.1	195.0	44	26	72.0	44	18	1.05 ±0.03	Mirtazapine D3
Azithromycin	71	13.95	749.5	116.1	60	54	83.1	60	60	0.95 ±0.02	EDDP D3
Venlafaxine	72	14.14	278.2	58.1	27	40	260.1	27	12	1.78 ±0.02	Metoprolol D7
EDDP	73	14.80	278.2	234.1	50	29	249.1	50	24	2.40 ±0.05	EDDP D3
Citalopram	74	15.06	325.1	262.1	46	18	109.9	46	26	21.8 ±3.45	Citalopram D6
Propranolol	75	15.14	260.2	183.1	42	18	116.1	42	16	1.88 ±0.09	Propranolol D7
Desmethylcitalopram	76	15.17	311.4	109.0	46	27	262.0	46	18	3.58 ±0.11	Citalopram D6
Carbamazepine	77	16.15	237.0	194.1	40	20	179.1	40	38	10.6 ±0.15	Carbamazepine 13C6
Diltiazem	78	16.72	415.0	178.0	40	25	310.1	40	25	23.4 ±1.30	Carbamazepine 13C6
Tylosin	79	17.25	916.5	174.2	80	45	101.0	80	56	1.88 ±0.07	Methadone D9
Methadone	80	17.59	310.2	265.1	31	15	105.1	31	28	1.50 ±0.05	Methadone D9
Gliclazide	81	17.80	324.1	127.0	41	20	110.0	41	20	0.98 ±0.04	Quetiapine D8
Quetiapine	82	17.87	384.1	253.1	50	21	221.1	50	40	1.97 ±0.04	Quetiapine D8
Temazepam	83	18.16	301.1	255.1	37	21	283.1	37	14	2.21 ±0.05	Temazepam D5
Fluoxetine	84	18.35	310.2	44.1	34	10	148.1	34	10	14.9 ±0.54	Fluoxetine D5
Norfluoxetine	85	18.42	296.1	134.1	18	6	-	-	-	-	Fluoxetine D5
Cetirizine	86	18.68	389.1	201.0	32	21	166.0	32	40	2.51 ±0.05	Temazepam D5
Clarithromycin	87	18.87	748.5	158.1	40	31	590.4	40	20	3.71 ±0.03	Methadone D9
Sertraline	88	19.22	306.0	159.0	23	27	275.0	23	10	1.26 ±0.02	Sertraline D3
3-benzophenone	89	21.23	229.0	151.0	35	18	105.0	35	20	1.58 ±0.04	Methadone D9
Tamoxifen	90	22.39	372.2	72.0	50	25	129.0	50	28	30.6 ±0.91	Tamoxifen 13C2 15N
Metformin D6	-	2.69	136.1	77.0	30	19	-	-	-	-	-
Morphine D3	-	3.43	289.1	152.1	53	56	-	-	-	-	-
Atenolol D5	-	4.26	274.3	145.1	44	30	-	-	-	-	-
Acetaminophen D4	-	5.22	156.0	114.0	26	16	-	-	-	-	-
Codeine D6	-	5.84	306.2	218.1	52	28	-	-	-	-	-
Cotinine D3	-	7.21	180.1	80.0	44	24	-	-	-	-	-
1S,2R-(+) Ephedrine D3	-	7.21	169.2	151.0	23	18	-	-	-	-	-
Amphetamine D5	-	8.42	141.1	92.8	20	14	-	-	-	-	-
Methamphetamine D5	-	8.56	155.1	91.8	28	18	-	-	-	-	-
MDA D5	-	8.66	185.1	168.1	21	11	-	-	-	-	-
MDMA D5	-	8.69	199.1	165.1	26	13	-	-	-	-	-
Benzoyllecgonine D8	-	9.68	298.2	171.1	38	19	-	-	-	-	-
Mephedrone D3	-	9.86	181.1	148.0	30	22	-	-	-	-	-
Ketamine D4	-	10.59	242.1	129.1	31	27	-	-	-	-	-

Heroin D9	-	10.84	379.2	165.8	51	50	-	-	-	-	-
Norketamine D4	-	11.05	228.1	128.9	32	28	-	-	-	-	-
Metoprolol D7	-	11.23	275.4	123.1	44	20	-	-	-	-	-
Cocaine D3	-	11.40	307.2	185.1	40	20	-	-	-	-	-
Cocaethylene D3	-	12.98	321.2	199.1	40	22	-	-	-	-	-
Mirtazapine D3	-	13.40	269.0	194.9	35	25	-	-	-	-	-
EDDP D3	-	14.91	281.2	234.1	50	29	-	-	-	-	-
Propranolol D7	-	15.12	267.0	188.8	40	18	-	-	-	-	-
Citalopram D6	-	15.16	331.0	109.0	46	28	-	-	-	-	-
Carbamazepine 13C6	-	16.22	243.1	200.1	40	20	-	-	-	-	-
Quetiapine D8	-	17.56	392.1	258.1	50	23	-	-	-	-	-
Methadone D9	-	17.60	319.3	268.2	31	15	-	-	-	-	-
Temazepam D5	-	18.12	306.7	260.1	37	21	-	-	-	-	-
Fluoxetine D5	-	18.32	315.3	153.2	26	8	-	-	-	-	-
Sertraline D3	-	19.23	309.1	159.0	23	27	-	-	-	-	-
Tamoxifen 13C2 15N	-	22.36	375.1	75.0	50	25	-	-	-	-	-

Key: CV, cone voltage; CE, collision energy; ESI, electrospray ionisation

^aMRM ratio: Product ion 1/Product ion 2 ratio average over the entire calibration range

Table S3. Intra- and inter-day precision for target ECs at 10, 100 and 500 ng mL⁻¹ (ordered by retention time)

Chemical	Intra-day precision (%)			Inter-day precision (%)		
	10 ng mL ⁻¹	100 ng mL ⁻¹	500 ng mL ⁻¹	10 ng mL ⁻¹	100 ng mL ⁻¹	500 ng mL ⁻¹
<i>Chemicals determined in ESI - mode</i>						
4-benzophenone	2.5	2.7	1.8	7.0	3.3	1.1
Sulfasalazine	4.0	4.3	3.3	3.4	1.4	2.4
Methylparaben	0.7	0.4	2.1	5.2	11.5	1.4
Valsartan	1.6	0.8	3.4	2.7	3.2	4.8
2-benzophenone	1.3	1.2	0.8	4.1	6.1	2.6
Bezafibrate	4.2	2.0	0.7	4.3	1.4	2.7
Ketoprofen	3.6	0.5	2.4	3.9	3.5	0.5
Naproxen	1.7	1.0	1.8	3.0	3.6	0.9
Ethylparaben	4.6	1.2	2.2	2.2	4.1	0.1
Fexofenadine	1.6	3.4	1.3	4.4	13.6	1.3
Irbesartan	4.2	2.9	0.8	6.1	3.8	2.2
Diclofenac	8.6	9.9	5.3	5.5	5.0	2.9
Bisphenol A	2.9	2.6	1.8	0.9	2.6	0.3
Propylparaben	2.3	12.2	-	2.8	9.3	-
Atorvastatin	4.7	2.5	0.6	1.6	7.9	1.1
1-benzophenone	4.9	1.1	0.9	2.4	6.4	1.0
EE2	2.1	3.9	1.8	7.0	1.3	1.5
Ibuprofen	3.8	0.9	2.6	3.7	1.3	1.8
E2	3.5	4.5	1.1	2.3	5.2	0.4
E1	2.0	1.6	1.7	3.5	1.8	1.0
Butylparaben	5.1	9.2	0.8	3.7	6.2	1.1
Triclosan	10.0	16.1	2.0	2.9	13.7	2.8
<i>Chemicals determined in ESI + mode</i>						
Creatinine	2.5	1.9	3.9	1.1	0.9	2.3
Metformin	1.7	1.2	0.9	2.6	1.1	0.8
Dihydromorphine	0.4	2.5	5.3	3.8	2.5	6.8
Nicotine	2.6	4.1	0.4	1.1	2.1	0.5
Normorphine	3.6	1.1	1.9	2.2	1.5	0.9
Anhydroecgonine methylester	1.2	2.3	3.8	1.6	2.5	2.8
Morphine	3.9	0.1	3.4	6.4	0.2	2.1
Pholcodine	0.4	6.4	3.0	0.5	6.1	7.3
Atenolol	4.5	2.0	0.5	3.9	1.5	0.9
Ranitidine	3.5	10.9	14.6	3.9	0.5	3.1
Iopromide	14.7	10.3	11.2	7.0	5.2	2.6
Acetaminophen	4.3	0.9	2.7	1.6	1.6	1.6
Cimetidine	3.0	13.8	10.1	5.2	2.6	4.7
Dihydrocodeine	0.8	1.7	3.7	2.7	0.5	1.4
Codeine	3.5	4.3	4.1	3.8	1.0	1.1
Norephedrine	7.2	4.8	3.3	5.6	4.1	3.2
Norcodeine	6.7	4.2	3.4	3.5	2.4	2.4
1,7 dimethylxanthine	6.8	9.0	13.9	13.0	2.9	2.1
Lisinopril	13.0	1.4	-	0.9	3.4	-
Ephedrine/pseudoephedrine	2.5	4.1	3.5	4.5	3.6	4.1
Cotinine	1.5	1.2	1.8	0.8	2.2	1.6
6-acetylmorphine	3.5	3.4	8.3	1.1	9.6	7.5
Azathioprine	14.6	11.0	16.2	14.8	5.8	2.3
Methotrexate	0.8	5.0	6.5	11.9	7.5	6.8
Caffeine	1.9	5.4	0.9	2.0	1.8	1.3
O-desmethyltramadol	3.1	6.7	-	2.0	4.6	-
Amphetamine	1.3	1.3	2.2	0.8	2.1	1.5
Trimethoprim	1.6	1.8	3.2	1.4	3.5	4.1
Methamphetamine	1.2	0.3	2.4	1.6	0.2	1.3
MDA	0.6	0.4	1.1	1.4	1.1	0.7
MDMA	3.3	0.5	1.2	0.6	1.2	2.1
Sulfamethoxazole	0.7	2.2	4.3	2.0	3.0	5.6
Benzoyllecgonine	0.7	1.1	0.9	1.4	3.3	2.5
Mephedrone	4.9	3.0	0.9	1.8	0.9	2.8
Ketamine	0.4	1.8	1.6	2.7	1.7	1.1
Desmethylvenlafaxine	2.4	2.4	1.4	4.0	2.3	2.0
Heroin	2.5	1.3	1.7	2.7	2.2	0.8
Tramadol	1.2	2.6	1.9	1.7	1.7	1.5

Norketamine	4.8	3.7	0.9	2.9	1.9	0.6
Metoprolol	0.9	3.2	1.8	2.0	1.2	0.6
Cocaine	1.1	1.1	2.2	2.2	2.7	1.7
N-desmethyltramadol	3.2	1.2	2.2	3.4	3.0	1.1
MDPV	0.3	0.6	1.1	4.2	2.3	0.2
Ifosfamide	4.0	3.3	0.7	2.9	3.1	1.3
Cocaethylene	2.0	1.2	1.8	5.9	0.8	1.6
Carbamazepine10,11-epoxide	2.0	2.4	2.0	0.9	0.1	3.7
10,11-Dihydro-10-hydroxycarbamazepine	5.1	3.8	7.9	3.7	2.0	2.8
Mirtazapine	2.2	3.0	2.9	3.9	4.2	2.1
Azithromycin	1.3	3.5	1.4	3.6	4.5	3.2
Venlafaxine	1.4	1.3	2.4	3.9	2.0	1.6
EDDP	1.3	1.2	1.0	1.4	0.5	1.8
Citalopram	1.7	4.9	1.2	0.5	0.8	0.8
Propranolol	0.4	0.7	1.9	2.1	1.5	2.5
Desmethylcitalopram	1.7	4.4	3.0	0.1	2.9	2.4
Carbamazepine	2.4	1.1	1.3	2.6	1.7	1.6
Diltiazem	3.2	2.2	1.4	0.4	1.5	4.9
Tylosin	5.8	2.8	3.3	2.9	2.2	1.6
Methadone	1.7	1.2	-	0.7	2.3	-
Gliclazide	2.5	5.0	0.8	0.8	4.4	1.1
Quetiapine	1.0	1.0	1.7	1.8	1.1	1.4
Temazepam	1.1	1.4	2.4	1.7	1.0	0.4
Fluoxetine	2.2	1.3	1.9	1.5	2.1	1.4
Norfluoxetine	4.1	2.9	2.3	2.5	1.6	0.4
Cetirizine	0.8	0.4	2.6	2.0	0.9	0.8
Clarithromycin	4.0	2.0	1.2	5.1	1.5	1.3
Sertraline	0.7	1.7	2.7	3.0	1.0	0.9
3-benzophenone	4.3	4.6	-	2.5	3.8	-
Tamoxifen	2.2	0.7	4.3	4.5	1.8	5.6

Table S4. Intra- and inter-day accuracy for target ECs at 10, 100 and 500 ng mL⁻¹ (ordered by retention time)

Chemical	Intra-day accuracy (%)			Inter-day accuracy (%)		
	10 ng mL ⁻¹	100 ng mL ⁻¹	500 ng mL ⁻¹	10 ng mL ⁻¹	100 ng mL ⁻¹	500 ng mL ⁻¹
<i>Chemicals determined in ESI- mode</i>						
4-benzophenone	115.0	89.0	105.0	117.0	92.3	105.8
Sulfasalazine	115.4	101.3	98.8	112.3	100.4	101.3
Methylparaben	90.7	94.0	95.3	94.4	101.0	96.9
Valsartan	157.4	95.6	94.5	157.0	98.7	100.0
2-benzophenone	90.4	110.0	98.2	90.8	106.4	95.6
Bezafibrate	91.4	99.5	102.3	92.6	100.3	100.8
Ketoprofen	99.6	99.1	101.1	101.4	96.2	100.5
Naproxen	90.2	102.5	100.3	91.9	101.8	101.4
Ethylparaben	117.3	121.6	98.0	120.2	120.9	98.0
Fexofenadine	98.4	111.4	109.0	101.5	103.9	108.4
Irbesartan	83.3	108.7	98.8	85.1	108.6	101.3
Diclofenac	78.0	95.5	95.3	80.4	97.9	97.2
Bisphenol A	107.0	106.1	97.7	107.0	108.7	98.0
Propylparaben	97.1	100.4	-	99.8	102.9	-
Atorvastatin	101.9	89.6	102.6	100.9	98.2	103.8
1-benzophenone	103.6	119.0	97.9	106.3	116.2	97.6
EE2	86.1	95.2	102.5	84.3	94.3	101.1
Ibuprofen	81.8	97.8	101.7	83.1	98.4	101.0
E2	93.7	96.9	99.2	95.7	93.7	99.5
E1	96.2	96.7	97.9	99.1	97.7	98.9
Butylparaben	93.6	99.2	98.4	97.2	103.9	99.7
Triclosan	69.4	66.3	73.2	69.8	72.4	72.1
<i>Chemicals determined in ESI+ mode</i>						
Creatinine	93.3	109.7	97.5	93.3	110.8	97.2
Metformin	88.7	101.5	100.7	86.2	101.6	101.2
Dihydromorphine	115.1	104.0	106.3	110.6	102.0	105.3
Nicotine	103.2	89.6	102.3	102.2	90.0	102.6
Normorphine	98.6	102.3	98.5	101.1	102.7	99.1
Anhydroecgonine methylester	107.1	88.5	100.4	109.1	90.8	103.5
Morphine	87.7	106.3	98.5	94.6	106.3	96.5
Pholcodine	80.0	100.4	117.3	78.7	105.7	114.1
Atenolol	86.9	100.6	102.8	83.3	99.9	102.8
Ranitidine	95.7	95.4	101.3	100.2	95.0	105.0
Iopromide	100.1	103.8	112.2	94.0	100.6	109.0
Acetaminophen	98.1	99.3	99.5	96.4	98.0	97.7
Cimetidine	99.0	96.0	102.9	105.3	98.2	108.8
Dihydrocodeine	87.4	102.8	93.4	84.8	103.4	94.4
Codeine	91.4	99.0	94.8	87.6	98.2	94.6
Norephedrine	97.6	89.5	98.6	101.2	92.3	95.4
Norcodeine	106.3	95.1	94.2	105.7	94.7	95.2
1,7 dimethylxanthine	90.0	98.4	96.3	84.2	99.9	98.7
Lisinopril	103.0	87.3	-	103.6	90.7	-
Ephedrine/pseudoephedrine	99.5	95.1	97.4	92.3	95.7	94.1
Cotinine	95.1	100.9	100.3	94.4	99.6	101.3
6-acetylmorphine	105.0	83.0	112.3	104.7	75.0	106.3
Azathioprine	100.1	99.6	92.6	93.9	106.3	92.2
Methotrexate	119.7	110.1	106.8	108.1	103.6	112.3
Caffeine	115.2	89.5	96.5	113.2	90.1	95.4
O-desmethyltramadol	94.2	102.8	-	92.6	97.9	-
Amphetamine	100.8	101.6	99.8	100.3	102.9	99.2
Trimethoprim	104.6	94.2	99.6	104.5	96.8	89.3
Methamphetamine	100.4	101.5	101.3	99.0	101.7	102.3
MDA	100.0	100.8	99.3	98.4	99.6	97.3
MDMA	103.2	97.9	98.3	102.5	96.7	98.3
Sulfamethoxazole	106.1	93.6	88.3	104.3	91.6	89.3
Benzoylcegonine	105.2	103.2	101.4	104.3	101.6	104.4
Mephedrone	75.9	89.9	91.4	77.3	89.6	94.4
Ketamine	77.3	105.3	98.2	75.6	103.6	98.5
Desmethylvenlafaxine	105.9	102.2	98.9	101.4	101.3	101.3
Heroin	100.4	98.8	98.6	98.3	97.0	99.4
Tramadol	99.0	99.0	97.3	100.6	100.6	99.0

Norketamine	82.2	98.1	101.8	80.3	99.4	102.4
Metoprolol	90.9	96.7	100.7	91.3	98.1	101.1
Cocaine	98.2	100.4	98.4	96.7	98.1	96.8
N-desmethyltramadol	94.7	93.9	94.7	91.1	92.8	93.6
MDPV	108.7	96.5	99.1	105.8	94.1	99.0
Ifosfamide	96.4	92.5	96.9	94.5	90.6	95.6
Cocaethylene	88.3	101.2	94.5	88.2	101.8	95.2
Carbamazepine10,11-epoxide	94.0	80.5	95.1	94.8	80.4	91.3
10,11-Dihydro-10-hydroxycarbamazepine	94.8	98.6	88.1	94.6	96.5	85.4
Mirtazapine	94.0	101.6	97.3	90.3	99.0	95.0
Azithromycin	114.7	80.9	100.0	110.2	77.0	97.7
Venlafaxine	72.9	96.7	101.7	74.6	96.2	102.7
EDDP	91.2	102.6	95.5	92.6	102.1	94.5
Citalopram	102.0	101.3	102.1	101.6	100.5	101.7
Propranolol	125.4	98.4	94.8	122.5	96.8	97.0
Desmethylcitalopram	112.2	99.4	98.7	122.1	99.1	97.8
Carbamazepine	86.3	94.5	97.2	84.1	94.8	96.1
Diltiazem	94.0	94.6	92.1	93.8	93.4	91.0
Tylosin	108.2	92.7	99.8	104.9	92.2	101.3
Methadone	101.1	99.3	-	100.4	97.1	-
Gliclazide	87.3	97.2	101.5	86.7	92.5	100.3
Quetiapine	85.1	102.5	101.5	83.4	101.3	101.3
Temazepam	93.8	98.7	101.1	92.3	98.0	100.6
Fluoxetine	92.3	103.0	99.6	91.1	101.1	98.1
Norfluoxetine	106.3	104.8	98.1	107.0	103.3	97.8
Cetirizine	103.8	99.2	99.4	101.8	99.2	100.4
Clarithromycin	102.6	99.3	103.6	97.5	99.9	102.0
Sertraline	84.3	101.9	100.9	84.0	100.8	101.1
3-benzophenone	84.4	89.2	-	83.4	86.3	-
Tamoxifen	93.0	105.2	92.3	88.8	106.1	93.2

Table S5. Absolute and corrected recoveries of ECs in crude wastewater, final effluent, river water and digested sludge (ordered by retention time)

Chemical	Crude wastewater ^a		Final effluent ^a		River water ^b		Digested sludge ^c	
	Abs. rec. (%)	Corr. rec. (%)	Abs. rec. (%)	Corr. rec. (%)	Abs. rec. (%)	Corr. rec. (%)	Abs. rec. (%)	Corr. rec. (%)
<i>Chemicals determined in ESI - mode</i>								
4-benzophenone	38.9	101.9	52.7	122.8	72.8	92.6	7.6	47.0
Sulfasalazine	21.8	62.7	28.4	58.7	31.8	64.2	-	-
Methylparaben	39.9	99.8	59.4	100.8	70.2	96.3	18.1	110.3
Valsartan	46.9	101.1	53.1	79.9	60.6	76.0	-	-
2-benzophenone	26.7	45.4	29.0	40.3	31.0	44.6	11.1	105.5
Bezafibrate	46.3	91.4	78.3	92.9	73.7	94.2	16.4	112.5
Ketoprofen	45.6	107.2	67.8	109.2	72.9	92.0	23.1	119.4
Naproxen	15.7	82.7	84.5	98.0	80.5	91.0	16.4	107.9
Ethylparaben	68.5	87.5	73.0	83.5	70.1	77.5	19.5	118.7
Fexofenadine	50.7	107.3	71.0	83.8	67.6	74.9	-	-
Irbesartan	40.3	97.6	53.6	107.4	56.2	112.3	-	-
Diclofenac	46.5	103.9	71.8	116.0	70.5	120.0	4.2	40.8
Bisphenol A	37.4	112.2	56.8	100.7	60.5	108.7	11.9	95.7
Propylparaben	55.6	112.6	75.1	125.3	69.8	117.4	16.0	153.6
Atorvastatin	58.6	94.0	59.9	91.9	35.5	54.7	-	-
1-benzophenone	49.5	75.6	80.2	89.2	81.3	99.9	8.1	69.7
EE2	51.9	87.9	64.9	84.6	48.3	86.3	-	-
Ibuprofen	57.9	78.9	126.2	110.8	85.6	115.5	14.9	105.5
E2	51.5	106.6	67.5	87.9	52.9	79.3	6.4	113.6
E1	50.6	99.1	64.3	92.7	63.2	97.2	5.9	106.6
Butylparaben	47.9	102.4	82.3	118.3	76.8	115.4	11.2	179.6
Triclosan	69.3	117.5	75.1	100.8	58.3	86.5	-	-
<i>Chemicals determined in ESI + mode</i>								
Creatinine	22.8	46.9	24.8	42.9	31.0	59.6	-	-
Metformin	36.7	78.7	53.0	96.0	55.2	93.3	-	-
Dihydromorphine	19.9	95.7	31.4	96.2	45.4	92.8	11.0	74.3
Nicotine	98.5	77.3	55.7	83.9	45.3	54.9	45.6	165.4
Normorphine	30.3	109.5	38.6	106.5	42.8	87.3	17.4	109.9
Anhydroecgonine methylester	33.9	91.3	50.2	109.5	53.6	79.5	-	-
Morphine	34.2	93.9	47.8	109.8	57.1	112.5	15.8	114.0
Pholcodine	13.7	42.0	43.1	102.0	76.9	119.6	22.8	87.8
Atenolol	42.8	88.6	54.6	109.7	76.0	115.1	30.8	121.0
Ranitidine	70.1	97.8	46.4	106.8	65.0	88.6	21.5	82.1

Iopromide	47.2	138.5	82.1	123.7	97.0	143.0	-	-
Acetaminophen	77.8	77.8	44.8	116.4	44.4	140.5	3.9	57.7
Cimetidine	20.6	123.7	33.4	106.2	32.7	95.3	-	-
Dihydrocodeine	34.7	85.7	54.8	118.6	66.4	98.5	27.8	101.0
Codeine	39.0	94.8	68.4	102.8	67.5	93.1	30.2	105.3
Norephedrine	26.9	85.4	28.9	100.9	28.4	78.2	27.0	92.6
Norcodeine	35.5	95.7	36.4	87.5	52.5	90.6	24.0	87.8
1,7 dimethylxanthine	89.3	79.6	26.6	110.6	47.5	75.5	-	-
Lisinopril	28.6	102.3	21.9	88.5	21.4	93.7	37.7	127.8
Ephedrine/pseudoephedrine	23.0	92.8	18.7	88.6	25.4	67.8	28.2	97.9
Cotinine	37.4	85.2	47.3	101.5	72.0	105.9	4.1	112.1
6-acetylmorphine	33.9	103.6	40.0	85.4	52.9	72.6	-	-
Azathioprine	72.0	109.5	81.5	83.8	88.9	66.4	-	-
Methotrexate	39.1	98.8	30.7	114.1	22.6	95.7	16.9	59.3
Caffeine	82.9	96.6	89.8	131.7	137.0	122.8	-	-
O-desmethyltramadol	31.8	87.3	36.0	93.9	58.6	108.1	-	-
Amphetamine	24.5	91.7	27.4	107.8	22.5	98.7	34.1	118.3
Trimethoprim	41.4	109.6	59.8	123.7	59.2	118.0	44.9	138.5
Methamphetamine	31.9	102.1	42.5	97.1	47.7	97.6	33.8	104.4
MDA	30.7	99.4	30.3	99.1	28.7	99.6	-	-
MDMA	29.4	118.5	37.0	112.9	50.0	100.9	28.1	105.6
Sulfamethoxazole	42.1	102.8	64.0	111.0	78.9	108.4	24.4	74.4
Benzoylcegonine	46.5	106.3	55.1	116.4	74.2	126.2	35.7	117.3
Mephedrone	18.2	94.8	22.8	103.7	22.8	97.3	15.9	99.4
Ketamine	41.7	111.6	53.8	115.6	68.2	107.7	29.0	105.3
Desmethylvenlafaxine	35.9	101.5	45.9	100.0	62.5	107.4	33.9	96.9
Heroin	23.9	105.3	29.1	103.0	54.1	100.9	17.9	91.7
Tramadol	33.3	69.5	47.0	88.3	60.9	104.8	30.7	87.7
Norketamine	42.2	98.9	53.9	108.6	65.7	103.2	30.3	109.7
Metoprolol	36.2	97.4	53.1	104.3	71.8	107.8	36.6	99.7
Cocaine	21.7	97.4	44.9	105.2	71.4	106.9	32.8	104.7
N-desmethyltramadol	17.9	81.3	33.4	98.8	42.2	69.1	24.7	83.4
MDPV	20.8	136.8	85.5	87.9	112.2	78.9	24.6	79.7
Ifosfamide	33.4	89.2	41.9	80.2	62.9	90.8	-	-
Cocaethylene	7.6	109.9	48.1	107.4	71.3	105.9	30.0	98.9
Carbamazepine 10,11-epoxide	56.7	143.7	55.0	126.9	94.8	136.1	-	-
10,11-Dihydro-10-hydroxycarbamazepine	50.3	152.2	59.5	120.6	74.1	125.1	11.5	100.1
Mirtazapine	25.8	84.7	39.8	97.0	57.5	99.1	18.5	98.2
Azithromycin	42.8	100.1	23.6	87.5	22.8	107.6	-	-

Venlafaxine	23.8	70.2	36.3	89.5	58.8	96.8	11.3	61.9
EDDP	44.1	111.6	33.9	113.6	23.8	105.2	25.5	103.8
Citalopram	40.3	119.9	35.5	124.1	41.1	115.0	30.4	112.7
Propranolol	38.7	105.0	36.1	102.7	45.4	107.2	20.9	91.5
Desmethylcitalopram	32.5	93.1	27.5	110.9	36.2	89.5	20.8	82.2
Carbamazepine	37.4	88.3	55.5	102.5	68.2	101.7	10.8	94.5
Diltiazem	36.3	118.1	30.1	82.3	43.7	82.9	-	-
Tylosin	34.3	98.3	50.3	110.0	43.8	100.4	-	-
Methadone	49.6	109.0	47.9	111.7	46.5	119.2	29.2	102.8
Gliclazide	46.4	80.1	61.8	108.4	32.9	69.5	-	-
Quetiapine	37.8	72.6	46.8	95.1	51.6	87.2	19.1	81.9
Temazepam	54.5	107.3	72.5	113.9	66.3	115.3	6.1	92.3
Fluoxetine	19.8	110.7	7.1	111.1	4.4	112.3	9.4	121.2
Norfluoxetine	23.6	94.8	7.9	91.7	3.0	74.4	7.4	95.1
Cetirizine	48.6	77.3	78.8	114.3	47.9	77.3	-	-
Clarithromycin	33.2	80.9	40.1	97.2	31.0	77.6	-	-
Sertraline	13.4	91.5	8.3	105.0	3.1	108.0	5.8	101.9
3-benzophenone	27.0	58.5	51.9	89.4	33.0	74.4	-	-
Tamoxifen	9.5	85.2	8.7	98.4	0.2	112.8	0.3	112.7

^aRecoveries determined at spike concentrations of 100 and 1,000 ng L⁻¹ (10 and 100 µg L⁻¹ where SPE was not performed)

^bRecoveries determined at spike concentrations of 50 and 500 ng L⁻¹ (10 and 100 µg L⁻¹ where SPE was not performed)

^cRecoveries determined at spike concentrations of 50 and 100 ng g⁻¹

Table S6. Matrix suppression on EC signal strength in crude wastewater, final effluent and river water extracts (ordered by retention time)

Chemical	Matrix suppression			
	Crude wastewater (%)	Final effluent (%)	River water (%)	Digested sludge (%)
<i>Chemicals determined in ESI - mode</i>				
4-benzophenone	42.5	23.0	-1.2	48.0
Sulfasalazine	-53.4	-81.7	-105.8	-
Methylparaben	60.2	49.1	41.9	30.6
Valsartan	-77.4	-105.4	-139.2	-
2-benzophenone	55.5	49.2	43.8	35.1
Bezafibrate	0.7	-19.6	-24.5	67.8
Ketoprofen	36.3	9.9	8.5	70.3
Naproxen	29.8	-18.7	-13.2	88.6
Ethylparaben	37.0	29.8	27.8	38.7
Fexofenadine	27.1	11.2	10.3	-
Irbesartan	-14.3	-25.3	-23.8	-
Diclofenac	-104.5	-141.7	-127.3	59.2
Bisphenol A	29.4	12.4	15.0	42.8
Propylparaben	37.3	21.6	21.7	41.8
Atorvastatin	-152.8	-160.3	-155.7	-
1-benzophenone	30.6	2.0	0.6	41.5
EE2	13.2	-24.4	-6.1	-
Ibuprofen	-15.6	-24.3	-13.6	80.0
E2	31.8	8.0	8.3	39.4
E1	28.6	5.0	4.5	38.9
Butylparaben	35.9	11.0	8.0	43.1
Triclosan	-99.0	-100.9	-62.3	-
<i>Chemicals determined in ESI + mode</i>				
Creatinine	77.2	75.2	69.0	-
Metformin	63.3	47.0	44.8	-
Dihydromorphine	67.5	49.9	32.9	27.5
Nicotine	47.0	5.0	1.2	53.0
Normorphine	60.3	46.8	27.7	34.1
Anhydroecgonine methylester	48.4	28.0	12.5	-
Morphine	69.0	47.3	30.1	30.5
Pholcodine	90.0	45.5	11.4	38.6
Atenolol	59.7	48.0	22.3	44.2
Ranitidine	56.8	35.0	18.2	46.6
Iopromide	39.1	26.1	11.8	-
Acetaminophen	22.2	50.6	27.8	81.3
Cimetidine	61.9	48.4	23.4	-
Dihydrocodeine	58.0	49.7	21.7	45.9
Codeine	59.8	53.7	25.9	45.9
Norephedrine	41.3	38.4	18.2	42.7
Norcodeine	53.5	49.1	33.1	42.7
1,7 dimethylxanthine	10.7	44.9	28.1	-
Lisinopril	23.1	8.6	-12.3	71.7
Ephedrine/pseudoephedrine	67.7	59.8	36.5	43.2
Cotinine	67.3	55.6	33.0	42.1
6-acetylmorphine	66.9	65.1	46.0	-
Azathioprine	51.1	45.0	32.8	-
Methotrexate	51.1	52.3	43.2	64.6
Caffeine	17.1	53.4	22.2	-
O-desmethyltramadol	62.5	59.2	34.6	-
Amphetamine	50.2	36.5	23.6	57.1
Trimethoprim	49.1	51.0	38.2	64.0
Methamphetamine	67.0	44.1	23.0	41.2
MDA	50.5	44.9	29.7	-
MDMA	69.2	58.8	36.3	39.9

Sulfamethoxazole	47.6	38.1	28.4	56.5
Benzoyllecgonine	61.6	52.0	21.9	52.4
Mephedrone	64.6	44.6	24.6	50.4
Ketamine	51.5	42.7	25.8	49.2
Desmethylvenlafaxine	65.1	59.1	29.9	50.5
Heroin	61.4	45.4	25.0	48.7
Tramadol	65.1	54.5	31.8	46.4
Norketamine	45.4	34.6	21.6	48.7
Metoprolol	65.7	49.5	27.6	42.9
Cocaine	73.4	49.8	32.7	40.1
N-desmethyltramadol	80.4	55.6	30.2	36.8
MDPV	85.6	42.1	22.7	35.4
Ifosfamide	55.9	46.7	26.1	-
Cocaethylene	64.3	51.8	31.6	38.5
Carbamazepine10,11-epoxide	41.3	32.2	18.3	-
10,11-Dihydro-10-hydroxycarbamazepine	37.3	33.2	20.3	51.1
Mirtazapine	65.2	50.2	26.0	34.5
Azithromycin	56.8	78.6	55.1	-
Venlafaxine	71.5	56.5	27.5	31.3
EDDP	55.4	45.1	23.4	38.9
Citalopram	63.7	70.1	52.0	35.8
Propranolol	56.7	59.0	31.2	42.8
Desmethylcitalopram	54.5	65.6	40.6	43.8
Carbamazepine	61.4	46.6	61.4	32.4
Diltiazem	61.4	53.6	37.9	-
Tylosin	64.9	43.4	31.4	-
Methadone	45.2	48.4	32.0	40.8
Gliclazide	38.2	23.6	19.0	-
Quetiapine	51.7	50.9	35.0	43.5
Temazepam	36.0	22.3	14.4	50.2
Fluoxetine	53.9	84.9	75.1	30.3
Norfluoxetine	54.8	86.6	79.5	35.5
Cetirizine	30.5	18.0	16.9	-
Clarithromycin	54.0	54.1	52.0	-
Sertraline	57.1	88.4	88.1	37.3
3-benzophenone	20.7	7.7	-5.1	-
Tamoxifen	30.3	14.6	93.2	39.5

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