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Supplementary Information for

Social, demographic and economic correlates of chemical and food consumption measured by wastewater-based epidemiology

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Supplementary Information Text 1

Amphetamine and methamphetamine use in Australia.

In Australia, there is limited prescription use of amphetamine and no therapeutic use of methamphetamine. According to the Australian Pharmaceutical Benefits Scheme, 12,754 boxes of 100x5mg amphetamine tablets were dispensed in August 2016 (time of sampling) (1). This equates to per capita consumption of 0.009mg/day/1000 people, and per capita excretion would be even lower than this value. Our average amphetamine values were 0.301 mg/day/1000 people (range: 115-558), and therefore we consider that the majority of amphetamine detected comes from illicit use. Furthermore, discussions in the Australian National Wastewater Drug Monitoring Report suggests that the majority of amphetamine loads in wastewater derives from methamphetamine metabolism rather than amphetamine consumption (2).

Supplementary Information Text 2

Tobacco biomarker outlier. A closer look at the dataset showed the unusually high tobacco marker loads from on particular catchment, catchment 10, masked a strong trend in the remainder of the dataset. Catchment 10 is located in the capital city of the Northern Territory (NT), the state/territory with the highest prevalence of smoking in Australia (3).Previous WBE reports have found tobacco biomarker loads from the NT to be around twofold greater than the national average throughout 2016 (4). Therefore, we consider that the tobacco biomarker loads from catchment 10 to be valid but atypical (i.e. a potential outlier) in the context of accepted trends with IRSAD. Indeed, exclusion of catchment 10 produced significant negative correlations between IRSAD and nicotine (RP = -0.504) (*SI Appendix* Figure S5). Our results highlight catchment 10 as having far higher nicotine consumption than the other catchments studied.

Table S1. Chemicals featured in the present study.

Name	Category	Biomarker for	CAS	Manufacturer	Method
Hydroxycotinine	Licit drug	Tobacco	34834-67-8	Cerilliant	B
Cotinine	Licit drug	Tobacco	486-56-6	Cerilliant	B
Nicotine	Licit drug	Tobacco	54-11-5	Cerilliant	A
Paraxanthine	Licit drug	Caffeine	611-59-6	Cerilliant	B
Caffeine	Licit drug	Caffeine	58-08-2	Cerilliant	B
Ethyl sulfate	Licit drug	Ethanol (alcohol)	540-82-9	Lipomed	A
Amphetamine	Illicit drug	Meth/amphetamine	300-62-9	Cerilliant	A
Methamphetamine	Illicit drug	Meth/amphetamine	7632-10-2	Cerilliant	A
Methadone	Opioid	Methadone	76-99-3	Cerilliant	A
EDDP	Opioid	Methadone	76-99-3	Cerilliant	A
Codeine	Opioid	Codeine	76-57-3	Cerilliant	A
Morphine	Opioid	Morphine	57-27-2	Cerilliant	A
Oxycodone	Opioid	Oxycodone	76-42-6	Cerilliant	A
Noroxycodone	Opioid	Oxycodone	52446-25-0	Cerilliant	B
Tramadol	Opioid	Tramadol	36282-47-0	Cerilliant	B
Desvenlafaxine	Antidepressant	Venlafaxine	93413-62-8	Cerilliant	B
Venlafaxine	Antidepressant	Venlafaxine	99300-78-4	Cerilliant	B
Citalopram	Antidepressant	Citalopram	59729-32-7	Cerilliant	B
Mirtazapine	Antidepressant	Mirtazapine	85650-52-8	Cerilliant	B
Amitriptyline	Antidepressant	Amitriptyline	549-18-8	Cerilliant	B
Carbamazepine	Anticonvulsant	Carbamazepine	298-46-4	Cerilliant	A
Gabapentin	Anticonvulsant	Gabapentin	60142-96-3	Cerilliant	B
Pregabalin	Anticonvulsant	Pregabalin	148553-50-8	Sigma Aldrich	B
Ibuprofen	Antiinflammatory	Ibuprofen	15687-27-1	Cerilliant	A
Naproxen	Antiinflammatory	Naproxen	22204-53-1	Cerilliant	B
Fexofenadine	Antihistamine	Fexofenadine	153439-40-8	Cayman Chemical	B
Cetirizine	Antihistamine	Cetirizine	83881-52-1	Cerilliant	B
Atenolol	Beta blocker	Atenolol	29122-68-7	Cerilliant	A
Hydrochlorothiazide	Antidiuretic	Hydrochlorothiazide	58-93-5	Cerilliant	A
Cephalexin	Antibiotic	Cephalexin	15686-71-2	Sigma Aldrich	B
Sulfamethoxazole	Antibiotic	Sulfamethoxazole	723-46-6	Toronto Research Chemicals	B
Trimethoprim	Antibiotic	Trimethoprim	738-70-5	Dr Ehrenstorfer	B
Fluconazole	Antifungal	Fluconazole	86386-73-4	TRC	B
Acesulfame	Sweetener	Acesulfame	55589-62-3	Dr Ehrenstorfer	B
Saccharin	Sweetener	Saccharin	81-07-2	Sigma Aldrich	B
Sucralose	Sweetener	Sucralose	56038-13-2	Sigma Aldrich	B
2PY	Vitamin	Vitamin B6	701-44-0	Cayman Chemical	B
4PY	Vitamin	Vitamin B6	769-49-3	Toronto Research Chemicals	B
αCEHC	Vitamin	Vitamin E	4071-32-6	Cayman Chemical	B
4-Pyridoxic acid	Vitamin	Vitamin B3	82-82-6	Sigma Aldrich	B
Proline betaine	Food	Citrus	471-87-4	Cayman Chemical	B
Enterodiol	Food	Fiber	80226-002	Sigma Aldrich	B
Enterolactone	Food	Fiber	78473-71-9	Sigma Aldrich	B
Hydroxycotinine D3	Internal standard	-	159956-78-2	Cerilliant	B
Cotinine D3	Internal standard	-	110952-70-0	Cerilliant	B
Codeine D3	Internal standard	-	70420-71-2	Cerilliant	A/B
Norfentanyl D5	Internal standard	-	1435933-84-8	Cerilliant	B
Caffeine 13C3	Internal standard	-	78072-66-9	Cerilliant	B
Venlafaxine D6	Internal standard	-	1062606-12-5	Cerilliant	B
Citalopram D6	Internal standard	-	1190003-26-9	Cerilliant	B
Carbamazepine D10	Internal standard	-	132183-78-9	Cerilliant	B
Gabapentin D10	Internal standard	-	1024922-02-8	Cerilliant	B
Pregabalin D4	Internal standard	-	1276197-54-6	Toronto Research Chemicals	B
Ibuprofen D3	Internal standard	-	121662-14-4	Cerilliant	B
Fexofenadine D6	Internal standard	-	548783-71-7	Cayman Chemical	B
Cetirizine D4	Internal standard	-	1219803-84-5	CDN Isotopes	B
Atenolol D7	Internal standard	-	1202864-50-3	Toronto Research Chemicals	B
Sulfamethoxazole D4	Internal standard	-	1020719-86-1	Toronto Research Chemicals	B
Acesulfame D4	Internal standard	-	55589-62-3	Toronto Research Chemicals	B
Saccharin D4	Internal standard	-	1189466-17-8	Toronto Research Chemicals	B
Sucralose D6	Internal standard	-	1459161-55-7	Toronto Research Chemicals	B
Nicotine D4	Internal standard	-	350818-69-8	Cerilliant	A
Ampehtamine D6	Internal standard	-	73758-26-6	Cerilliant	A
Methamphetamine D9	Internal standard	-	169565-19-9	Cerilliant	A
Methadone D3	Internal standard	-	60263-63-0	Cerilliant	A
Morphine D3	Internal standard	-	67293-88-3	Cerilliant	A
Hydrochlorthiazide 13CD2	Internal standard	-	1190006-03-1	Toronto Research Chemicals	A

Method B was performed on an AB Sciex 6500+. Method A was performed on an AB Sciex 5500+. Details are available in the materials and methods section.
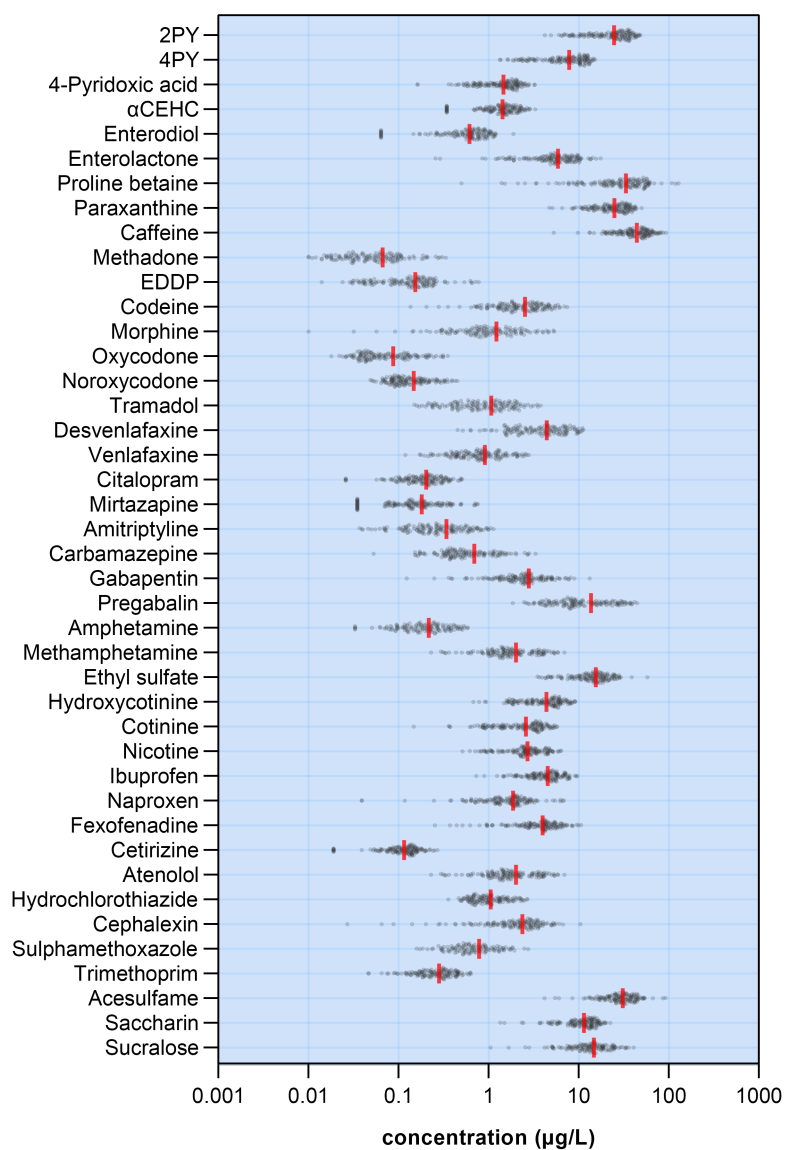
Fig. S1. Concentrations of biomarkers in wastewater analyzed in the present study. Mean concentration for each biomarker is indicated by a red line. 2PY: N-methyl-2-pyridone-5-carboxamide, 4PY: N-methyl-4-pyridone-3-carboxamide, αCEHC: α-carboxyethyl hydrochroman, EDDP: 2-ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine.
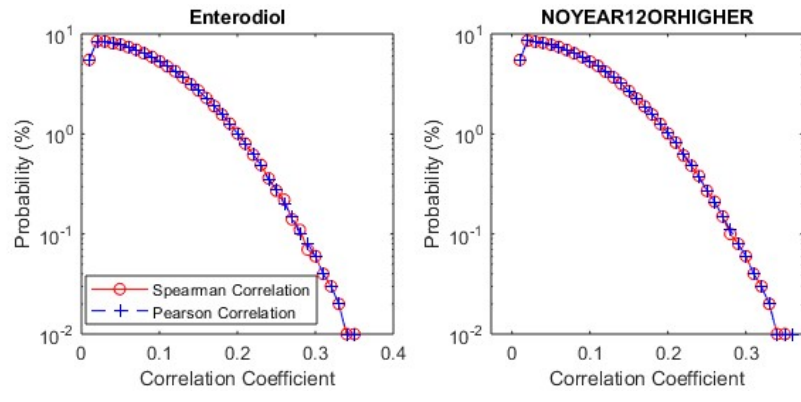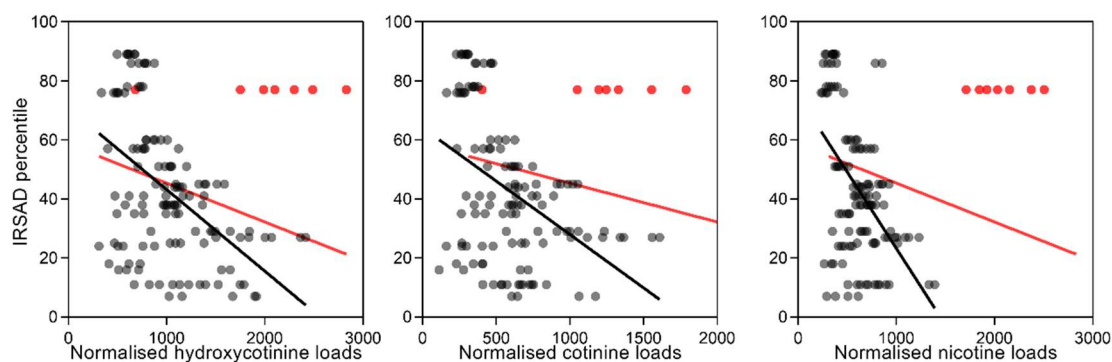
Fig. S2. Probability of false positive detection as determined using the confusion matrix (i.e. bootstrapping) method.

Fig. S3. Pearson correlations between catchment median age, IRSAD and per capita biomarker loads. Cells are shaded on a gradient of blue (-1) to red (1).

Fig. S4. Spearman correlations between catchment median age, IRSAD and per capita biomarker loads. Cells are shaded on a gradient of blue (-1) to red (1).

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Fig. S5. Tobacco biomarker associations with index of relative socioeconomic advantage and disadvantage (IRSAD) before (red) and after (black) catchment 10 is removed from the dataset. Measurements from catchment 10 and regressions from including catchment 10 are highlighted in red. Excluding catchment 10 from the dataset resulted in R-value changes from -0.261 to -0.488 for hydroxycotinine, -0.233 to -0.435 for cotinine and -0.032 to -0.504 for nicotine. Loads are mg/24h/1,000 capita.

Fig. S6. Pearson correlations between biomarkers and SEIFA descriptors. SEIFA descriptor definitions are provided in Table 1. Cells are shaded on a gradient of blue (-1) to red (1).

Fig. S7. Spearman correlations between biomarkers and SEIFA descriptors. SEIFA descriptor definitions are provided in Table 1. Cells are shaded on a gradient of blue (-1) to red (1).

Table S2. LC-MS/MS parameters of chemicals measured using method B.

Chemical	RT	Parent	DP	Quantifier	CE	CXP	Qualifier	CE	CXP	IS	Polarity
2PY	1.34	143.1	95	108	29	17	110	28	12	Pregabalin D4	Positive
4PY	2.22	153.1	40	136	18	16	92	29	11	Pregabalin D4	Positive
4-pyridoxic acid	1.42	182.1	-25	138	-19	-17	108	-28	-9	Acesulfame D4	Negative
αCEHC	7.14	277	-96	233	-21	-13	163	-30	-15	Sucralose D6	Negative
Enterodiol	6.37	301	-100	253	-32	-13	271	-32	-17	Ibuprofen D3	Negative
Enterolactone	6.91	297	-100	253	-28	-16	189	-30	-14	Ibuprofen D3	Negative
Proline betaine	0.74	144.1	80	58	33	16	84	30	9	Hydroxycotinine D3	Positive
Paraxanthine	4.97	502.1	22	484.1	32	28	466.1	38	24	Caffeine 13C3	Positive
Caffeine	5.73	389.1	45	201.1	25	11	165.1	85	17	Caffeine 13C3	Positive
Noroxycodone	4.96	305.1	70	287.1	22	16	230.1	38	12	Codeine D3	Positive
Tramadol	5.81	264.2	40	58	42	8	42	123	5	Caffeine 13C3	Positive
Desvenlafaxine	5.39	264.1	40	107.1	46	12	133.1	33	15	Caffeine 13C3	Positive
Venlafaxine	6.23	278.2	40	58	48	9	121	38	14	Venlafaxine D6	Positive
Citalopram	6.55	325.3	70	109	36	14	262.2	26	24	Citalopram D6	Positive
Mirtazapine	6.36	266	70	195	34	24	72	24	10	Citalopram D6	Positive
Amitriptyline	7.08	278.1	65	191.1	32	10	117	29	14	Cetirizine D4	Positive
Carbamazepine	7.09	237.2	86	194	29	14	193	45	12	Carbamazepine D10	Positive
Gabapentin	4.44	172.1	45	154	19	14	137	23	14	Gabapentin D10	Positive
Pregabalin	3.21	160.2	38	142.1	15	15	55	30	14	Pregabalin D4	Positive
Hydroxycotinine	2.16	141	44	95	20	12	68	36	16	Hydroxycotinine D3	Positive
Cotinine	4.5	315.1	47	176.1	23	20	130.1	31	16	Cotinine D3	Positive
Ibuprofen	7.48	205.1	-32	161	-10	-15	159	-9	-15	Ibuprofen D3	Negative
Naproxen	7.34	136.1	53	60	29	19	77.1	17	12	Cetirizine D4	Positive
Fexofenadine	7.14	502.1	22	484.1	32	28	466	38	24	Fexofenadine D6	Positive
Cetirizine	7.34	389.1	45	201.1	25	11	165.1	85	17	Cetirizine D4	Positive
Cephalexin	5.5	348.3	24	158.1	20	11	174.1	25	13	Sulfamethoxazole D4	Positive
Sulfamethoxazole	5.84	254.2	100	156	37	12	92	20	15	Sulfamethoxazole D4	Positive
Trimethoprim	5.25	292.4	90	231.2	30	15	261.2	25	12	Codeine D3	Positive
Fluconazole	5.95	307.3	48	220.1	22	21	238.1	21	15	SMTZ D4	Positive
Acesulfame	1.19	162	-25	82	-18	-9	78	-43	-9	Acesulfame D4	Negative
Saccharin	3.27	182	-125	42	-59	-19	106	-25	-12	Saccharin D4	Negative
Sucralose	4.78	394.8	-32	35	-64	-15	359	-15	-13	Sucralose D6	Negative
Hydroxycotinine D3	2.11	196.1	84	80	35	13	134.1	26	20	-	Positive
Pregabalin D4	3.12	164.2	56	146.2	15	16	85.1	21	10	-	Positive
Gabapentin D10	4.38	182	45	164	19	14	147	23	14	-	Positive
Cotinine D3	4.48	180.1	100	80	34	10	101	30	10	-	Positive
Codeine D3	5.08	303.3	96	152	89	15	115	103	14	-	Positive
Caffeine 13C3	5.73	198.3	60	140.1	24	17	112.1	33	14	-	Positive
Sulfamethoxazole D4	5.83	258.2	100	160	35	12	96	30	15	-	Positive
Venlafaxine D6	6.21	284.2	40	64	48	9	121	38	14	-	Positive
Citalopram D6	6.54	331.2	80	262.1	28	15	247.1	42	13	-	Positive
Carbamazepine D10	7.06	247.2	65	204.2	28	18	202.1	49	17	-	Positive
Fexofenadine D6	7.13	508.2	140	472.2	38	15	490.2	31	15	-	Positive
Cetirizine D4	7.33	393.1	51	201.1	25	11	165.1	82	18	-	Positive
Ibuprofen D3	7.48	208.1	-30	164	-10	-15	161	-9	-13	-	Negative
Acesulfame D4	1.16	166	-25	86	-20	-9	78	-43	-9	-	Negative
Saccharin D4	3.15	186	-75	42	-60	-18	106	-27	-10	-	Negative
Sucralose D6	4.77	400.8	-120	35	-58	-15	265	-16	-12	-	Negative

RT: retention time (mins), DP: declustering potential (V), CE: collision energy (V), CXP: collision exit potential (V), IS: internal standard.

Table S3. Validation of method B for limit of detection (LOD), limit of quantitation (LOQ), linearity, range and relative matrix effect (RME).

	LOD (ppb)	LOQ (ppb)	Linearity (R^2)	Range (ppb)	RME (%)
2PY	0.01	0.04	0.9968	0.05-50	-22.5
4PY	0.02	0.05	0.9967	0.05-50	-13.3
αCEHC	0.21	0.68	0.9995	0.5-50	-10.3
4-Pyridoxic acid	0.02	0.06	0.9970	0.2-150	8.3
Enterodiol	0.01	0.04	0.9985	0.05-50	0.5
Enterolactone	0.01	0.03	0.9984	0.05-50	-0.5
Proline betaine	0.03	0.09	0.9973	0.2-150	-18.6
Paraxanthine	0.02	0.07	0.9999	0.05-150	-20.1
Caffeine	0.01	0.03	0.9997	0.05-150	-40.9
Noroxycodone	0.01	0.03	0.9987	0.05-50	-6.9
Tramadol	0.02	0.06	0.9995	0.05-50	-16.5
Desvenlafaxine	0.03	0.09	0.9985	0.05-50	-17.1
Venlafaxine	0.03	0.10	0.9999	0.05-50	-10.3
Citalopram	0.02	0.05	0.9960	0.05-50	-10.7
Mirtazapine	0.02	0.07	0.9997	0.05-50	-15.8
Amitriptyline	0.03	0.09	0.9953	0.05-50	-12.3
Carbamazepine	0.01	0.04	0.9999	0.05-50	-10.2
Gabapentin	0.01	0.03	0.9992	0.05-50	-16.5
Pregabalin	0.27	0.82	0.9998	2-150	-14.8
Hydroxycotinine	0.01	0.04	0.9988	0.05-50	37.6
Cotinine	0.01	0.30	0.9996	0.05-50	-13.1
Ibuprofen	0.04	0.13	0.9997	0.2-50	0.3
Naproxen	0.02	0.08	0.9993	0.05-50	-10.6
Fexofenadine	0.04	0.12	0.9983	0.05-50	-11.9
Cetirizine	0.01	0.04	0.9991	0.05-50	-22.5
Cephalexin	0.03	0.10	0.9995	0.05-50	-9.8
Sulfamethoxazole	0.02	0.07	0.9997	0.05-50	-10.9
Trimethoprim	0.02	0.07	0.9990	0.05-50	-7.4
Fluconazole	0.01	0.03	0.9988	0.05-50	-4.4
Acesulfame	0.01	0.04	1.0000	0.05-150	-3.8
Saccharin	0.04	0.13	0.9999	0.05-150	-1.5
Sucralose	0.02	0.07	0.9973	0.2-150	-2.7

LOD and LOQ were calculated as 3.3 and 10 times (respectively) of the standard deviation of seven repeat injections of the lowest detectable standard. RME was calculated as the ratio of the slope of calibration curves made in pooled wastewater (pH2) and MilliQ water (pH2) when no internal standard is used. Positive RME indicates matrix enhancement, and negative RME indicates matrix suppression. 2PY: N-methyl-2-pyridone-5-carboxamide, 4PY: N-methyl-4-pyridone-3-carboxamide, αCEHC: α-carboxyethyl hydrochroman.

Table S4. Validation of method B for instrumental precision and accuracy in pH2 MillQ water.

	Precision (% RSD)						Accuracy (%)					
	Intraday			Interday			Intraday			Interday		
	0.2 µg/L	2 µg/L	20 µg/L	0.2 µg/L	2 µg/L	20 µg/L	0.2 µg/L	2 µg/L	20 µg/L	0.2 µg/L	2 µg/L	20 µg/L
2PY	2.0	0.4	0.7	1.7	0.9	0.7	3.6	-4.0	-3.6	6.8	-1.3	0.3
4PY	3.0	1.0	0.7	4.3	0.9	1.1	-4.1	-4.1	-0.7	-5.3	-3.7	-0.1
αCEHC	1.5	0.8	0.9	2.4	1.2	1.1	-5.9	-6.6	-5.2	-5.8	-3.1	2.0
4-Pyridoxic acid	2.7	1.0	0.5	2.0	1.0	0.4	-1.5	-6.3	-2.6	-2.9	-3.1	-0.5
Enterodiol	2.8	1.6	1.1	3.4	1.2	1.1	6.3	0.5	2.9	5.9	-1.4	1.7
Enterolactone	0.7	1.5	1.2	1.6	0.7	1.4	3.4	0.1	-6.7	5.5	3.0	-3.7
Proline betaine	2.1	1.7	0.7	4.1	0.5	1.0	0.3	3.3	-3.4	1.2	3.3	-2.0
Paraxanthine	2.0	1.6	0.7	1.7	0.9	1.5	-5.9	-4.6	-0.8	-5.4	-3.7	-0.1
Caffeine	2.1	1.3	0.9	1.9	0.8	0.9	-8.9	-8.8	-4.7	-7.2	-7.8	-2.6
Noroxycodone	3.4	0.7	1.1	4.5	1.1	1.1	-8.4	-9.0	-5.0	-5.7	-7.0	-0.5
Tramadol	5.2	2.9	3.6	4.6	3.1	-2.3	-8.6	-9.7	-1.7	-6.3	-8.9	-2.1
Desvenlafaxine	2.0	1.8	3.0	3.9	2.2	2.1	-4.0	0.8	2.2	-1.2	-0.5	0.6
Venlafaxine	3.8	1.9	1.7	3.6	1.3	3.3	-0.2	0.5	2.2	-0.4	-2.9	-2.8
Citalopram	ND	4.5	1.4	ND	2.6	2.5	ND	-7.7	1.6	ND	-3.9	0.5
Mirtazapine	5.8	1.6	0.8	4.6	1.2	0.8	-1.8	-3.6	1.1	2.4	-2.3	0.4
Amitriptyline	4.4	2.1	1.4	3.6	2.4	1.6	-5.3	-6.4	0.2	-6.0	-7.2	-3.0
Carbamazepine	3.7	1.3	2.5	3.9	2.3	1.3	-6.5	-5.1	2.9	-7.6	-7.4	1.7
Gabapentin	2.5	1.4	0.9	4.2	0.9	0.7	-4.1	-7.7	-0.4	-5.4	-7.2	-2.1
Pregabalin	5.4	4.3	1.2	5.7	4.1	2.0	-3.3	-0.5	4.4	-0.5	-0.4	0.9
Hydroxycotinine	3.5	1.4	1.0	1.2	2.9	1.6	-2.7	-3.9	1.7	-6.2	-5.8	-2.9
Cotinine	3.5	1.5	0.6	2.1	1.4	0.9	-3.3	-1.9	0.9	-3.8	-2.8	0.3
Ibuprofen	1.6	2.5	1.0	1.7	1.8	2.1	-4.4	-0.4	5.5	2.2	-1.9	0.6
Naproxen	1.7	1.1	0.7	1.4	1.2	0.8	-2.2	-2.6	-0.2	-3.3	-2.1	-0.3
Fexofenadine	1.8	0.9	0.5	3.2	0.9	0.6	-3.3	-0.9	1.2	-0.5	-0.9	1.1
Cetirizine	3.6	2.8	1.0	7.9	-2.8	1.2	1.4	-0.9	3.1	6.4	-1.9	1.0
Cephalexin	2.0	1.4	1.8	3.2	-1.5	-1.7	5.8	8.9	6.1	7.5	5.1	8.5
Sulfamethoxazole	2.5	2.2	1.6	2.4	1.8	1.9	6.8	9.7	5.3	6.8	7.4	3.3
Trimethoprim	ND	4.6	1.2	ND	3.1	2.4	ND	6.2	2.3	ND	5.7	4.5
Fluconazole	3.2	1.8	0.7	7.5	-1.0	0.7	-4.3	-2.1	4.7	0.0	5.7	-0.5
Acesulfame	4.7	1.3	0.5	3.5	1.4	1.2	-4.1	-12.3	-7.5	-0.7	-5.1	1.8
Saccharin	2.1	0.7	0.9	4.2	2.0	1.4	5.0	7.6	2.0	6.4	6.7	4.9
Sucralose	1.5	0.7	1.2	0.0	1.6	1.0	6.4	3.8	3.1	6.7	5.6	4.3

Precision was calculated as the standard deviation divided by the average of seven repeat injections at 0.2, 2 and 20 µg/L. Accuracy was determined using the deviation of a measured value from its spiked value, using seven repeat injections at 0.2, 2 and 20 µg/L. Interday samples were analyzed on a different batch a week after intraday samples. ND: not detected. 2PY: N-methyl-2-pyridone-5-carboxamide, 4PY: N-methyl-4-pyridone-3-carboxamide, αCEHC: α-carboxyethyl hydrochroman.

Table S5. Validation of method B for instrumental precision and accuracy in pH2 pooled wastewater.

	Precision (% RSD)						Accuracy (%)					
	Intraday			Interday			Intraday			Interday		
	0.2 µg/L	2 µg/L	20 µg/L	0.2 µg/L	2 µg/L	20 µg/L	0.2 µg/L	2 µg/L	20 µg/L	0.2 µg/L	2 µg/L	20 µg/L
Hydroxycotinine	3.6	2.8	3.4	4.1	3.4	1.4	3.8	7.1	3.4	4.7	5.3	-2.2
Cotinine	2.3	1.9	2.7	4.6	2.4	1.2	5.5	4.1	2.7	5.2	7.1	2.4
Paraxanthine	ND	3.3	1.1	ND	2.7	2.4	ND	3.1	1.1	ND	7.0	0.1
Caffeine	4.2	1.4	1.3	3.1	3.1	1.0	3.8	2.6	1.3	2.5	2.6	0.3
Noroxycodone	3.6	1.2	1.0	1.8	1.4	0.6	7.2	5.9	1.0	7.1	0.2	-3.2
Tramadol	6.9	2.4	2.0	4.1	0.8	1.9	6.2	4.4	2.0	5.8	7.4	4.2
Desvenlafaxine	7.3	3.6	1.7	8.3	3.7	0.6	3.0	5.3	1.7	7.0	0.2	-2.5
Venlafaxine	2.4	2.8	1.5	6.6	3.3	1.6	7.4	7.6	1.5	7.0	4.3	2.0
Citalopram	5.7	6.8	1.2	5.8	2.8	0.8	5.8	6.2	1.2	8.9	4.2	-0.3
Mirtazapine	2.6	1.4	1.8	2.1	0.9	3.1	-1.5	5.6	1.8	-1.8	5.8	9.0
Amitriptyline	2.3	0.7	1.0	4.6	2.4	1.7	5.5	9.6	1.0	6.9	5.7	-0.9
Carbamazepine	3.6	1.4	1.1	3.5	1.3	0.5	4.5	3.9	1.1	9.0	8.8	3.1
Gabapentin	3.1	1.3	1.0	3.1	1.2	1.5	0.6	1.3	1.0	3.9	0.1	0.8
Pregabalin	0.6	1.0	1.0	2.2	0.7	0.5	-0.2	-8.8	1.0	-0.7	-4.0	1.7
Ibuprofen	3.2	1.2	1.3	2.5	0.6	1.1	-4.9	-3.6	1.3	-3.6	-5.5	-1.0
Naproxen	5.1	3.4	1.8	5.9	3.2	2.3	-5.2	-8.4	1.8	-0.5	-2.0	5.2
Fexofenadine	3.6	2.8	1.9	4.2	1.9	3.8	0.8	4.2	1.9	-3.8	3.2	0.9
Cetirizine	7.4	2.0	1.5	3.2	1.6	1.7	4.1	11.1	1.5	6.5	6.7	0.2
Cephalexin	9.2	3.7	2.5	6.5	3.1	1.1	2.7	1.3	2.5	7.7	0.9	0.0
Sulfamethoxazole	2.7	1.8	0.8	3.2	1.4	0.5	0.3	-10.6	0.8	-0.5	4.1	-0.6
Trimethoprim	1.9	1.2	0.8	2.8	1.7	1.1	8.9	3.1	0.8	6.6	2.5	-0.7
Fluconazole	6.7	2.6	1.3	3.2	2.8	1.0	-1.0	2.8	1.3	7.2	2.2	0.4
Acesulfame	10.8	2.7	2.1	5.8	1.2	1.7	3.9	5.5	2.1	7.7	-1.8	-3.4
Saccharin	9.2	1.7	1.5	6.1	3.9	2.2	-1.1	-7.3	1.5	2.3	-7.4	1.4
Sucralose	2.0	0.9	1.6	2.0	1.3	0.7	-8.7	-9.3	1.6	-4.3	-8.5	2.3
2PY	5.3	4.9	1.5	5.1	3.2	3.0	-2.6	-1.2	1.5	-0.3	-2.1	3.2
4PY	6.5	1.3	0.6	4.2	0.9	1.1	1.4	-1.4	0.6	5.8	0.2	-0.5
αCEHC	3.6	2.2	1.1	2.8	1.2	1.4	2.0	13.7	1.1	-1.4	6.3	-3.2
4-Pyridoxic acid	2.2	3.9	1.9	3.5	1.5	2.1	-1.7	-5.0	1.9	1.2	-2.6	0.6
Proline betaine	1.9	3.0	0.9	4.5	0.8	0.8	5.3	4.8	0.9	8.6	3.7	1.6
Enterodiol	4.2	1.2	0.5	3.4	0.8	0.5	3.1	5.5	0.5	5.9	3.7	0.8
Enterolactone	3.1	1.7	1.6	4.6	3.8	1.5	7.1	6.5	1.6	-1.4	2.9	0.7

Precision was calculated as the standard deviation divided by the average of seven repeat injections at 0.2, 2 and 20 µg/L. Accuracy was determined using the deviation of a measured value from its spiked value, using seven repeat injections at 0.2, 2 and 20 µg/L. Interday samples were analyzed on a different batch a week after intraday samples. ND: not detected. 2PY: N-methyl-2-pyridone-5-carboxamide, 4PY: N-methyl-4-pyridone-3-carboxamide, αCEHC: α-carboxyethyl hydrochroman.

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