

Supporting materials

Table S1 Two LC gradient programs of PPCPs #1–#10 and PPCPs #11–#27

LC gradient program	Time (min)	A (%)	B (%)
PPCPs #1–#10 ^{a)}	0	80	20
	1	50	50
	3	50	50
	9	0	100
	14	0	100
	14.1	80	20
	25	80	20
	PPCPs #11–#27 ^{b)}	0	97
7		85	15
9		85	15
13		70	30
18		58	42
20		97	3
28		97	3

Notes: a) A is water containing 10 mmol/L acetic ammonia; B is MeOH; b) A is water containing 0.01% formic acid; B is ACN

Table S2 Matrix effect (ME%) of 27 targeted PPCPs spiked in drinking water, river, the effluent and influent of wastewater

No.	PPCPs	Drinking water (%)	River (%)	Effluent (%)	Influent (%)
#1	PPN	4	-2	1	2
#2	CBZ	11	12	17	5
#3	DEET	9	14	14	1
#4	CF	4	15	18	2
#5	DF	9	10	-13	-17
#6	IM	-1	-5	-20	-20
#7	MA	6	3	-18	-22
#8	BF	5	6	10	9
#9	CA	12	12	14	-13
#10	CP	5	1	6	8
#11	TCN	3	-3	2	10
#12	ATP	16	-7	-6	-
#13	EM	2	6	14	-21
#14	RXM	-3	5	-3	-8
#15	PCG	14	12	1	2
#16	SD	14	20	20	16
#17	ST	13	12	10	12
#18	SIX	19	20	19	15
#19	SMP	8	8	19	3
#20	SQX	4	9	12	0
#21	SMT	-18	-14	-21	-14
#22	SDM	5	11	9	13
#23	SMX	-4	-1	-6	-15
#24	SMZ	17	12	19	10
#25	SM	1	1	-3	-18
#26	CDM	12	12	-12	20
#27	LCM	9	20	-17	-12

Table S3 The MDLs and MQLs of 27 PPCPs (ng/L)

No.	PPCPs	1	2	3	4	5	6	7	RSD	MDL	MQL
#1	PPN	2.44	2.46	2.54	2.35	2.47	2.37	2.42	0.06	0.20	0.64
#2	CBZ	2.33	2.30	2.54	2.30	2.50	2.28	2.39	0.10	0.33	1.04
#3	DEET	2.59	2.55	2.68	2.55	2.64	2.68	2.66	0.06	0.18	0.58
#4	CF	2.32	2.28	2.30	2.24	2.28	2.37	2.33	0.04	0.13	0.41
#5	DF	2.55	2.60	2.58	2.48	2.64	2.56	2.60	0.05	0.16	0.51
#6	IM	2.24	2.29	2.27	2.25	2.35	2.20	2.28	0.05	0.15	0.47
#7	MA	2.62	2.58	2.62	2.44	2.37	2.62	2.50	0.10	0.32	1.01
#8	BF	2.45	2.47	2.57	2.52	2.40	2.45	2.43	0.06	0.18	0.58
#9	CA	2.63	2.55	2.66	2.55	2.68	2.64	2.66	0.05	0.17	0.53
#10	CP	2.28	2.41	2.40	2.22	2.30	2.24	2.27	0.07	0.23	0.75
#11	TCN	18.6	17.8	18.3	16.2	17.4	17.8	17.6	0.77	2.41	7.67
#12	ATP	2.63	2.50	2.78	2.43	2.65	2.68	2.67	0.12	0.37	1.17
#13	EM	2.07	2.10	1.65	1.70	1.73	1.75	1.74	0.18	0.58	1.84
#14	RXM	2.60	2.50	2.50	2.47	2.50	2.58	2.54	0.05	0.15	0.48
#15	PCG	2.98	3.08	3.18	2.74	2.73	2.85	2.79	0.18	0.55	1.76
#16	SD	2.53	2.93	2.58	2.70	2.38	2.50	2.44	0.19	0.58	1.85
#17	ST	2.88	2.63	2.60	2.85	2.88	2.73	2.81	0.12	0.37	1.17
#18	SIX	3.05	3.03	3.15	2.98	3.03	3.10	3.07	0.05	0.17	0.55
#19	SMP	3.33	3.45	3.35	3.13	3.33	3.33	3.33	0.10	0.30	0.95
#20	SQX	2.63	2.75	2.80	2.68	2.73	2.74	2.74	0.05	0.17	0.54
#21	SMT	2.53	2.48	2.49	2.53	2.66	2.46	2.56	0.07	0.21	0.67
#22	SDM	2.65	2.50	2.53	2.58	2.63	2.65	2.64	0.06	0.19	0.62
#23	SMX	3.08	3.22	2.97	3.16	3.08	2.95	3.02	0.10	0.31	0.98
#24	SMZ	3.13	2.92	2.93	2.90	3.10	3.05	3.08	0.10	0.30	0.95
#25	SM	2.72	2.95	2.80	2.70	2.69	2.80	2.75	0.09	0.28	0.90
#26	CDM	2.73	2.55	2.38	2.53	2.85	2.53	2.69	0.16	0.49	1.57
#27	LCM	3.08	3.13	3.03	2.60	2.89	3.28	3.09	0.22	0.68	2.16

Table S4 The recovery (%) of 27 PPCPs spiked in ultrapure water over 70 days

No.	PPCPs	0 d	3 d	7 d	14 d	21 d	27 d	36 d	40 d	49 d	56 d	63 d	70 d
#1	PPN	105	109	110	111	111	108	104	104	87	90	88	88
#2	CBZ	113	106	109	100	105	100	111	114	121	117	118	117
#3	DEET	114	117	111	113	114	109	111	113	117	117	120	123
#4	CF	111	111	111	110	114	105	107	116	113	110	110	111
#5	DF	115	117	112	108	112	100	109	106	105	103	104	104
#6	IM	110	115	109	107	113	108	110	114	111	107	109	108
#7	MA	100	107	109	109	103	98	102	110	106	110	101	109
#8	BF	106	109	109	104	106	102	104	107	110	105	109	110
#9	CA	114	117	116	113	118	114	117	118	115	116	116	114
#10	CP	107	109	113	110	112	105	106	106	110	110	110	108
#11	TCN	106	103	106	105	104	105	105	105	106	102	106	103
#12	ATP	110	114	110	110	109	103	103	105	111	112	115	114
#13	EM	106	110	108	112	110	112	110	106	113	110	109	108
#14	RXM	89	93	91	90	89	94	90	90	84	85	88	86
#15	PCG	109	115	106	109	110	127	128	131	127	135	132	133
#16	SD	109	109	107	102	104	109	102	104	108	109	105	100
#17	ST	113	115	112	116	118	111	117	111	112	108	112	106
#18	SIX	107	107	107	107	111	116	118	117	115	117	113	117
#19	SMP	112	111	111	111	112	106	103	93	93	97	90	90
#20	SQX	112	107	110	101	105	101	104	97	97	102	94	92
#21	SMT	81	81	80	82	82	79	79	83	87	82	83	80
#22	SDM	108	106	110	109	111	109	105	100	106	103	107	101
#23	SMX	126	120	122	119	121	119	130	132	131	133	133	120
#24	SMZ	119	117	115	121	115	118	117	121	123	117	114	115
#25	SM	109	104	108	105	104	105	103	103	100	107	100	101
#26	CDM	106	107	109	105	108	110	109	104	109	103	103	104
#27	LCM	119	121	121	122	123	125	127	120	124	119	120	119

Table S5 The recovery (%) of 27 PPCPs spiked in drinking water over 70 days

No.	PPCPs	0 d	3 d	7 d	14 d	21 d	27 d	36 d	40 d	49 d	56 d	63 d	70 d
#1	PPN	104	109	109	105	108	108	103	103	90	92	89	91
#2	CBZ	113	105	109	105	106	103	114	117	126	122	127	125
#3	DEET	109	109	108	109	109	105	108	110	113	111	112	114
#4	CF	104	109	111	105	112	106	114	117	112	104	109	106
#5	DF	113	112	113	108	110	99	106	111	106	105	98	100
#6	IM	100	101	106	99	107	99	106	111	109	103	99	101
#7	MA	110	113	110	116	113	108	116	114	115	115	115	108
#8	BF	105	110	113	106	112	108	105	110	112	114	115	111
#9	CA	112	115	118	112	120	112	113	120	121	117	117	121
#10	CP	105	108	109	111	112	101	102	105	112	114	113	110
#11	TCN	107	108	105	111	110	104	108	106	103	104	99	104
#12	ATP	116	118	123	120	122	123	117	121	119	124	116	117
#13	EM	102	109	109	106	110	113	112	107	110	109	113	108
#14	RXM	99	93	94	100	94	97	90	87	91	87	92	86
#15	PCG	114	111	110	108	112	127	121	114	136	124	138	129
#16	SD	117	118	116	115	114	118	112	118	117	115	118	118
#17	ST	113	110	115	116	114	112	102	101	94	94	92	94
#18	SIX	119	123	121	119	121	125	124	127	124	126	128	127
#19	SMP	108	112	111	107	110	98	99	94	91	91	92	95
#20	SQX	104	104	107	103	106	102	96	94	95	97	89	92
#21	SMT	73	76	76	72	76	74	86	85	82	80	79	77
#22	SDM	105	102	110	105	105	113	101	102	106	102	110	101
#23	SMX	110	109	114	110	108	114	120	122	123	127	130	129
#24	SMZ	119	114	113	121	115	116	118	115	114	118	121	117
#25	SM	101	106	101	100	99	98	101	92	96	98	97	95
#26	CDM	112	110	114	112	108	101	107	108	101	105	102	102
#27	LCM	109	115	116	117	114	116	113	112	108	111	107	114

Table S6 The recovery (%) of 27 PPCPs spiked in surface water over 70 days

No.	PPCPs	0 d	3 d	7 d	14 d	21 d	27 d	36 d	40 d	49 d	56 d	63 d	70 d
#1	PPN	98	109	108	105	105	101	102	103	87	90	85	88
#2	CBZ	112	106	112	109	114	110	116	119	125	123	127	123
#3	DEET	114	112	111	110	111	109	111	113	114	114	111	113
#4	CF	98	100	98	97	98	94	96	97	100	94	97	97
#5	DF	111	115	110	111	111	106	107	112	107	104	105	104
#6	IM	99	100	102	97	104	96	104	106	99	103	98	100
#7	MA	110	106	108	114	110	107	114	116	109	115	109	110
#8	BF	106	109	110	106	110	105	108	105	109	111	109	107
#9	CA	112	117	118	115	117	111	113	118	120	117	114	117
#10	CP	101	102	109	108	110	101	102	106	110	110	106	106
#11	TCN	102	109	100	106	108	113	109	111	111	103	104	110
#12	ATP	134	127	128	135	131	126	126	127	132	129	127	128
#13	EM	106	109	108	110	109	107	110	116	114	114	118	120
#14	RXM	105	106	105	108	111	108	92	91	89	95	87	92
#15	PCG	112	107	114	104	107	117	116	121	116	124	126	127
#16	SD	120	120	122	122	126	127	123	128	126	122	127	120
#17	ST	112	112	107	106	112	106	108	104	98	89	89	87
#18	SIX	120	120	124	121	118	119	126	131	130	128	131	130
#19	SMP	108	112	116	112	113	100	98	99	101	93	87	90
#20	SQX	109	106	110	108	110	100	95	93	97	100	90	95
#21	SMT	79	76	78	75	72	73	76	76	80	76	72	75
#22	SDM	111	115	111	110	113	111	110	112	117	112	119	114
#23	SMX	110	111	107	112	118	117	125	131	129	131	130	130
#24	SMZ	120	118	126	120	115	116	118	114	126	124	124	126
#25	SM	101	98	99	98	100	101	98	98	96	103	96	94
#26	CDM	112	113	117	111	110	109	108	110	108	109	108	111
#27	LCM	120	122	123	125	124	119	117	125	117	125	122	118

Table S7 The recovery (%) of 27 PPCPs spiked in wastewater effluent over 70 days

No.	PPCPs	0 d	3 d	7 d	14 d	21 d	27 d	36 d	40 d	49 d	56 d	63 d	70 d
#1	PPN	101	106	105	102	106	101	103	100	86	92	87	91
#2	CBZ	122	117	114	118	115	113	121	118	124	116	126	115
#3	DEET	125	125	122	123	128	124	128	126	126	123	124	126
#4	CF	98	104	101	97	97	94	95	99	101	95	97	100
#5	DF	126	127	129	127	133	117	127	134	126	126	124	122
#6	IM	98	100	96	100	108	95	113	106	111	106	100	110
#7	MA	104	103	100	98	97	94	107	104	102	103	102	101
#8	BF	110	112	116	109	110	106	108	109	112	115	113	110
#9	CA	116	113	116	117	118	113	115	120	123	115	113	118
#10	CP	121	126	128	128	127	119	123	125	127	124	128	123
#11	TCN	107	105	103	102	106	102	105	107	104	94	96	92
#12	ATP	122	123	123	125	122	123	121	120	125	124	125	127
#13	EM	122	121	118	123	123	128	125	124	135	132	133	138
#14	RXM	126	127	121	128	123	117	116	109	112	111	108	112
#15	PCG	101	99	98	96	99	133	130	133	131	132	130	126
#16	SD	120	120	117	115	116	114	120	116	121	116	112	120
#17	ST	110	106	111	104	102	99	95	100	97	97	89	91
#18	SIX	119	120	124	127	127	127	130	139	140	140	138	140
#19	SMP	119	125	121	122	125	104	105	106	106	95	96	90
#20	SQX	112	112	110	108	107	105	94	98	96	98	92	95
#21	SMT	79	76	81	78	81	76	74	78	74	78	77	79
#22	SDM	109	112	109	106	114	111	111	105	111	109	108	114
#23	SMX	117	118	125	123	123	119	132	132	135	138	138	136
#24	SMZ	119	124	129	125	122	122	125	124	128	125	127	128
#25	SM	97	100	95	101	96	103	105	86	90	87	84	84
#26	CDM	108	111	112	112	110	104	108	106	107	106	110	105
#27	LCM	106	105	104	107	104	103	107	103	105	102	102	104