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Supplementary Information for

Comparing non-targeted chemical persistence assessed using an unspiked OECD 309 test to field measurements

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Text S1. HRMS data post-processing workflow parameters in CompoundDiscoverer

Step I – Peak Picking

- RT range: 0.2 – 10 min
- m/z range: 80 – 1000 Da
- S/N threshold: 5
- Minimum scan number: 5
- Minimum intensity: 5000

Step II – Retention Time Alignment

- Alignment model: adaptive curve
- Maximum shift: 0.5 min
- Mass tolerance: 5 ppm

Step III – Compound Detection

- Considered elements: C50, H100, Br5, Cl6, F10, I5, N10, O15, P5, S5
- Isotope grouping:
  mass tolerance: 5 ppm
  intensity tolerance: 40%
  minimum isotopes: 2
- Considered adducts:
  Positive mode: $[M+ACN+H]^{1+}$, $[M+H]^{1+}$, $[M+K]^{1+}$, $[M+Na]^{1+}$
  Negative mode: $[2M+FA-H]^{1-}$; $[2M-H]^{1-}$; $[M-2H+K]^{1-}$; $[M-H]^{1-}$; $[M-H-H_2O]^{1-}$
- Adduct grouping:
  Mass tolerance: 5 ppm
  intensity tolerance: 30%

Step IV – Background Subtraction

- Maximum sample/blank ratio: 3
- Mass tolerance: 5 ppm

Step V – Database (mzCloud) Searching

- Compound classes: all
- Match ion activation type: true
- Match ion activation energy: match tolerance
- Ion activation energy tolerance: 30
- Apply intensity threshold: true
- Identity search: HighChem HighRes
- Similarity search: none
- Mass tolerance: 5 ppm
- Match score threshold: 75

Text S2. Model assumptions for estimating half-life in the field

Equation 1 in the paper is based on a simple mass balance model of the lake. The following assumptions were made:

- The volume of the lake was constant
- The only sources of contaminant to the lake were the Sundet WWTP and inflowing water from the lake Södra Bergundasjön
- The only sinks of contaminant in the lake were outflow via the stream and degradation
- The lake was well-mixed
- The contaminant concentration in the lake was equal to the contaminant concentration in the water in the outflowing stream
- The amount of chemical stored in the bottom sediment was negligible
- The contaminant concentration in the weekly grab samples of inflowing water and outflowing water equaled the average concentration during the previous 7 days
- Chemical degradation was first order
- The rate constant for chemical degradation was constant
- The rate constant could be approximated by dividing the rate of loss of contaminant (mol d^{-1}) by the average inventory of chemical in the lake during the study (this approximation is exact when the inventory is constant over time).

Steady state was not assumed. The change in chemical inventory during the study period was considered in the mass balance calculation (Equation 1 in the paper).

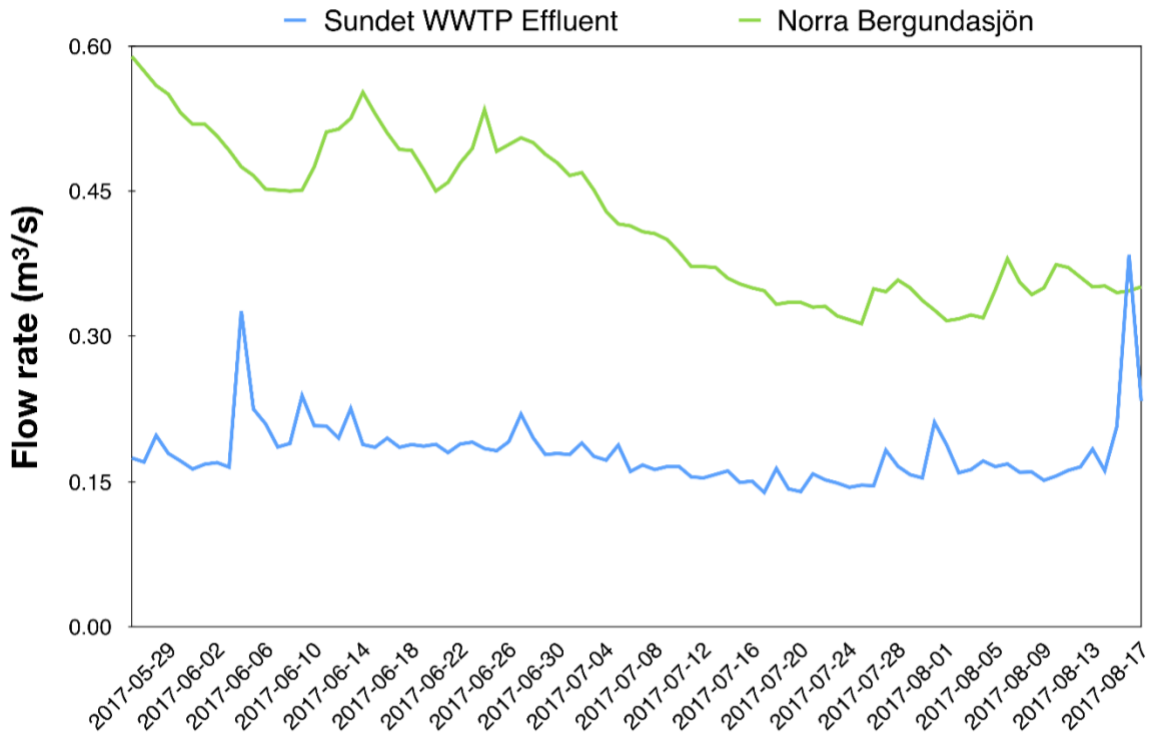

Figure S2. Discharge rate (m^3/s) of Sundet WWTP effluent and flow rate (m^3/s) of Norra Bergundasjön during the sampling period. The data were provided by Andreas Hedrén from Växjö Municipality.

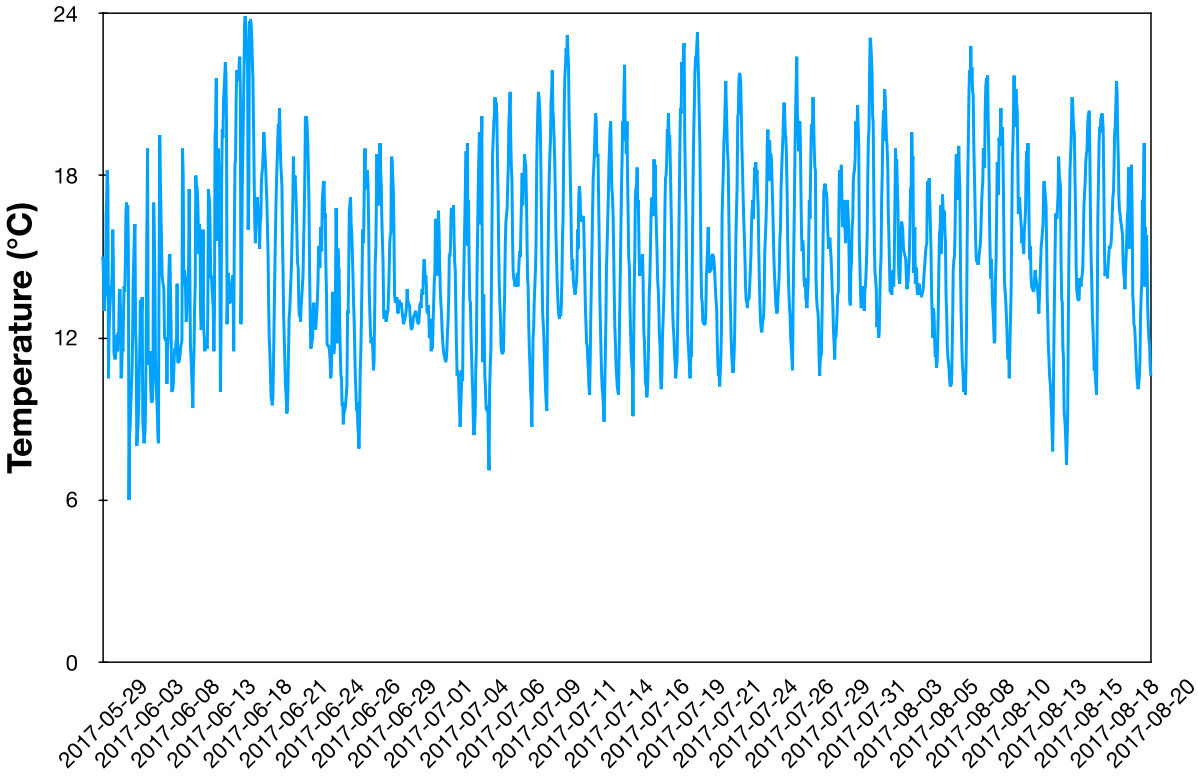

Figure S3. Air temperature (°C) at the Växjö meteorological station during the sampling period. The data were obtained from the Swedish Meteorological and Hydrological Institute.

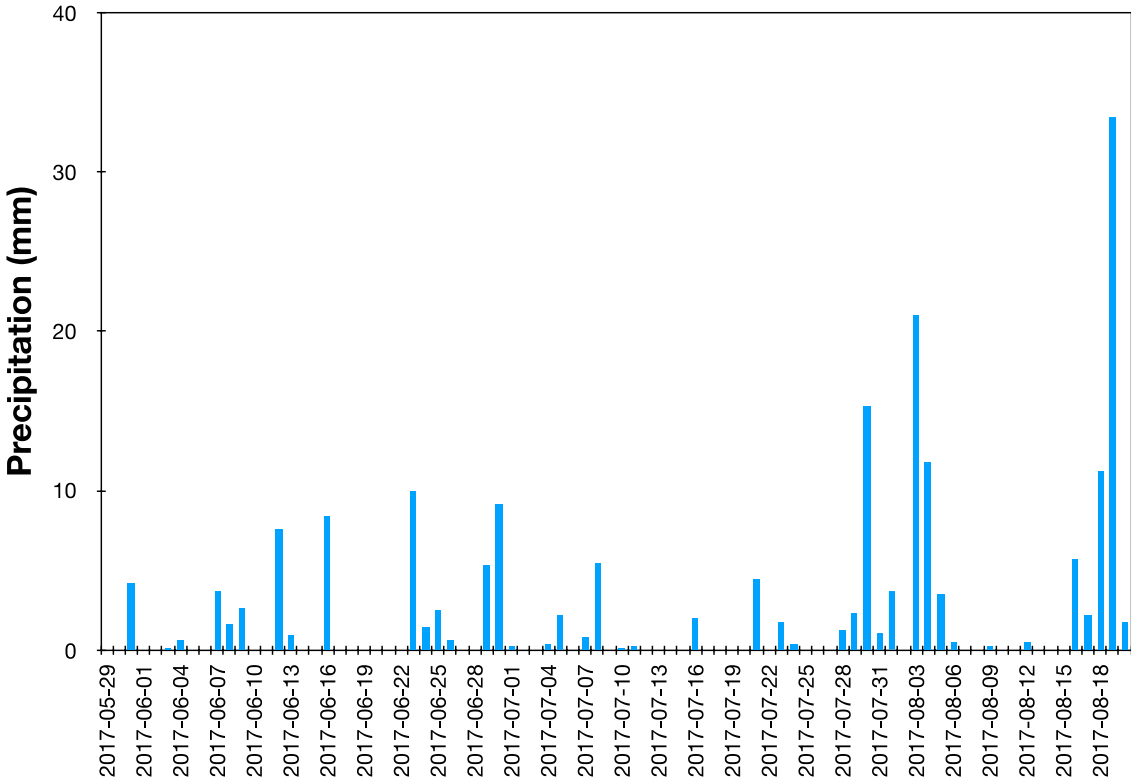

Figure S4. Precipitation (mm) in the study area during the sampling period. The data were obtained from the Swedish Meteorological and Hydrological Institute.

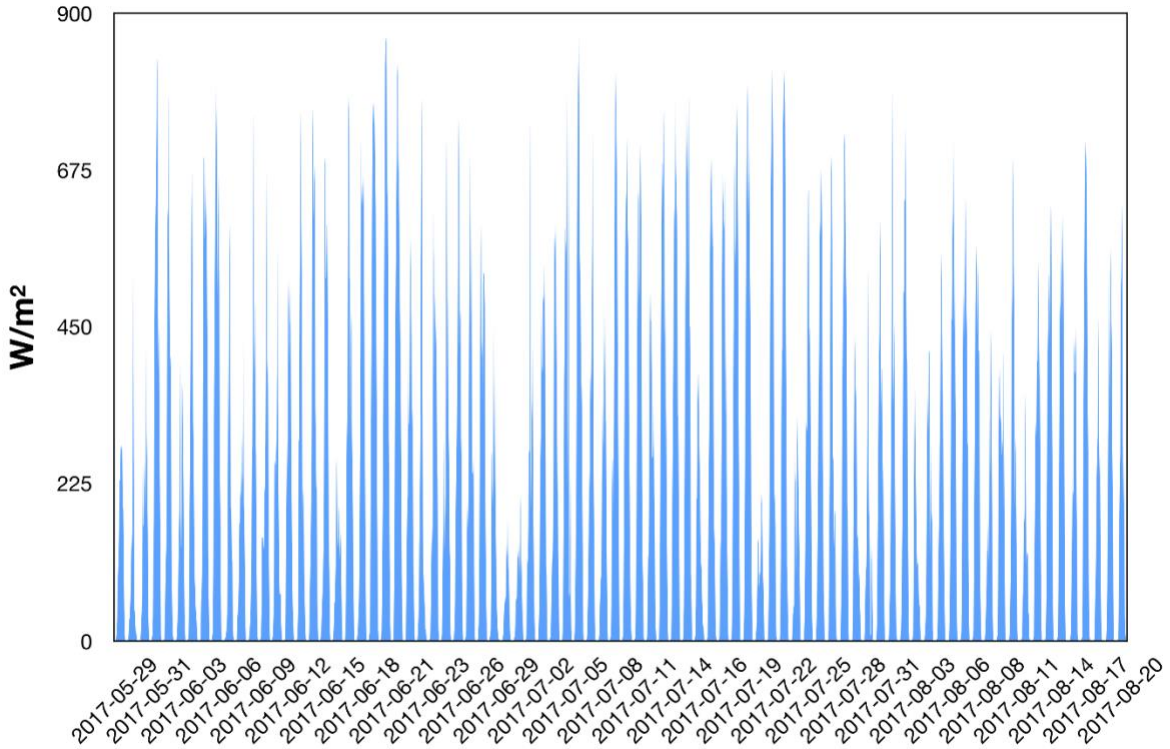

Figure S5. Global irradiation (W/m^2) at the Växjö meteorological station during the sampling period. The data were obtained from the Swedish Meteorological and Hydrological Institute.

Table S1. Matrix effect of the isotopic-labeled chemicals during the sampling period, presented as peak area (outflow)/peak area (effluent).

isotopic-labeled standard	sampling week number											
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
metformin-d6	1.3	1.3	1.3	1.2	1.1	1.1	1.3	1.3	1.2	1.2	1.3	1.3
sotalol-d6	1.5	1.4	1.4	1.4	1.3	1.3	1.5	1.4	1.3	1.4	1.5	1.4
acetaminophen-d4	1.4	1.4	1.3	1.3	1.2	1.2	1.4	1.3	1.2	1.2	1.2	1.2
atenolol-d7	1.4	1.3	1.3	1.4	1.2	1.2	1.4	1.3	1.3	1.3	1.4	1.4
ranitidine-d6	1.3	1.2	1.2	1.2	1.2	1.1	1.3	1.2	1.1	1.1	1.2	1.1
gabapentin-d6	1.7	1.6	1.6	1.6	1.5	1.5	1.8	1.7	1.5	1.6	1.8	1.7
metoprolol acid-d5	1.4	1.4	1.3	1.4	1.3	1.3	1.5	1.3	1.3	1.4	1.6	1.5
caffeine-d9	1.6	1.5	1.4	1.4	1.4	1.5	1.6	1.5	1.4	1.3	1.4	1.4
methotrexate-d3	1.6	1.4	1.5	1.5	1.3	1.3	1.6	1.6	1.3	1.6	1.6	1.6
1H-benzotriazole-d4	1.9	1.7	1.7	1.6	1.7	1.8	1.8	2.0	1.7	1.7	1.8	1.7
fluconazole-d4	1.7	1.5	1.5	1.6	1.4	1.4	1.7	1.5	1.5	1.6	1.7	1.6
metoprolol-d7	1.4	1.2	1.3	1.2	1.1	1.1	1.4	1.3	1.2	1.3	1.3	1.3
tramadol-d6	1.4	1.3	1.3	1.2	1.2	1.1	1.4	1.3	1.2	1.2	1.4	1.3
sulfamethoxazole-d4	1.6	1.4	1.4	1.4	1.3	1.2	1.5	1.4	1.4	1.4	1.5	1.3
venlafaxine-d6	1.4	1.2	1.2	1.2	1.1	1.2	1.3	1.3	1.3	1.3	1.4	1.3
carbamazepine-d8	1.3	1.3	1.3	1.2	1.2	1.2	1.4	1.3	1.3	1.4	1.5	1.4
proranolol-d7	1.3	1.2	1.2	1.2	1.1	1.1	1.2	1.2	1.2	1.2	1.3	1.2
anastrozole-d12	1.4	1.4	1.4	1.3	1.3	1.4	1.6	1.4	1.4	1.6	1.6	1.4
oxazepam-d5	1.9	1.7	1.7	1.6	1.6	1.7	2.0	1.8	1.8	2.0	2.0	1.8
irbesartan-d6	2.0	1.9	1.7	1.6	1.6	1.7	1.9	1.7	1.6	1.9	2.1	1.7
climbazole-d4	1.4	1.3	1.3	1.3	1.3	1.3	1.4	1.3	1.4	1.3	1.3	1.4
ketoprofen-13C-d3	1.8	1.8	1.9	1.7	1.5	1.7	1.9	1.8	1.7	2.0	2.0	1.9
atorvastatin-d5	1.1	1.2	1.3	1.5	1.5	1.6	1.1	1.0	1.9	1.3	1.2	1.3
glimepiride-d5	1.1	1.1	1.2	1.4	1.7	1.5	0.9	1.0	2.0	1.1	1.0	1.2
acesulfame-d4	1.3	1.3	1.3	1.3	1.2	1.4	1.5	1.4	1.2	1.3	1.3	1.1
hydrochlorothiazide-13C-d2	1.6	1.2	1.4	1.4	1.4	1.6	1.6	1.5	1.5	1.2	1.4	1.3
furosemide-d5	1.6	1.4	1.4	1.4	1.3	1.4	1.6	1.4	1.4	1.3	1.5	1.3
clofibric acid-d4	1.5	1.4	1.4	1.3	1.4	1.4	1.5	1.5	1.4	1.4	1.4	1.3
bezafibrate-d4	1.5	1.3	1.4	1.4	1.3	1.4	1.6	1.4	1.3	1.2	1.3	1.2
valsartan-d3	1.6	1.4	1.5	1.5	1.4	1.4	1.6	1.5	1.4	1.3	1.4	1.3
bicalutamide-d4	1.0	1.0	1.2	1.2	1.4	1.3	1.1	1.0	1.9	0.9	0.9	1.1
diclofenac-13C6	1.7	1.5	1.5	1.5	1.4	1.5	1.6	1.5	1.5	1.4	1.5	1.4

Table S2. List of chemicals identified in the field.

chemical	formula	molecular weight	RT (min)
acesulfame	C4 H5 N O4 S	162.9932	1.30
acetophenone	C8 H8 O	120.0574	6.11
acetylarginine	C8 H16 N4 O3	216.1225	1.11
acridine	C13 H9 N	179.0734	3.00
adenine	C5 H5 N5	135.0548	1.12
adenosine	C10 H13 N5 O4	267.0970	1.21
amphetamine	C9 H13 N	135.1048	1.81
atenolol	C14 H22 N2 O3	266.1631	1.88
benzophenone	C13 H10 O	182.0731	6.58
benzotriazole	C6 H5 N3	119.0484	2.70
benzoylecgonine	C16 H19 N O4	289.1314	3.01
bicalutamide	C18 H14 F4 N2 O4 S	430.0613	6.18
bis(2-butoxyethyl) ether	C12 H26 O3	218.1882	7.08
bis(4-ethylbenzylidene)sorbitol	C24 H30 O6	414.2042	6.72
bis(methylbenzylidene)sorbitol	C22 H26 O6	386.1725	6.11
candesartan	C24 H20 N6 O3	440.1598	5.41
carbamazepine	C15 H12 N2 O	236.0949	4.88
choline	C5 H13 N O	103.0997	0.96
citric acid	C6 H8 O7	192.0266	0.72
climbazole	C15 H17 Cl N2 O2	292.0977	5.38
codeine	C18 H21 N O3	299.1520	2.24
coniine	C8 H17 N	127.1361	2.19
cytidine	C9 H13 N3 O5	243.0859	1.11
cytosine	C4 H5 N3 O	111.0434	1.12
d-panthenol	C9 H19 N O4	205.1315	1.68
decanamide	C10 H21 N O	171.1622	6.56
DEET	C12 H17 N O	191.1310	5.54
DL-tryptophan	C11 H12 N2 O2	204.0900	2.09
dodecamethylcyclohexasiloxane	C12 H36 O6 Si6	444.1126	9.20
ecgonine	C9 H15 N O3	185.1052	3.08
escitalopram	C20 H21 F N2 O	324.1638	4.78
fexofenadine	C32 H39 N O4	501.2881	5.42
fluconazole	C13 H12 F2 N6 O	306.1042	3.25
furosemide	C12 H11 Cl N2 O5 S	330.0081	4.69
gabapentin	C9 H17 N O2	171.1258	2.22
galaxolidone	C18 H24 O2	272.1783	2.42
guanine	C5 H5 N5 O	151.0496	1.11
guanosine	C10 H13 N5 O5	283.0921	1.22
hexamethylenetetramine	C6 H12 N4	140.1062	0.97
hydrochlorothiazide	C7 H8 Cl N3 O4 S2	296.9649	2.22
hypoxanthine	C5 H4 N4 O	136.0387	1.12
irbesartan	C25 H28 N6 O	428.2324	5.35
isoamylamine	C5 H13 N	87.1049	1.61
isoleucine	C6 H13 N O2	131.0947	1.22

kinetin	C10 H9 N5 O	215.0807	1.88
L-alanyl-L-proline	C8 H14 N2 O3	186.1006	1.09
L-phenylalanine	C9 H11 N O2	165.0791	1.60
L-tyrosine	C9 H11 N O3	181.0742	1.17
lamotrigine	C9 H7 Cl2 N5	255.0078	3.24
leucylproline	C11 H20 N2 O3	228.1473	2.08
lidocaine	C14 H22 N2 O	234.1733	2.95
losartan	C22 H23 Cl N6 O	422.1622	5.32
melamine	C3 H6 N6	126.0655	1.00
metformin	C4 H11 N5	129.1015	0.95
metoprolol	C15 H25 N O3	267.1833	3.36
mirtazapine	C17 H19 N3	265.1579	3.17
monobutyl phthalate	C12 H14 O4	222.0890	5.41
oxazepam	C15 H11 Cl N2 O2	286.0508	5.10
paracetamol	C8 H9 N O2	151.0633	1.86
PEG n5	C10 H22 O6	238.1415	1.94
PEG n6	C12 H26 O7	282.1678	2.19
PEG n7	C14 H30 O8	326.1939	2.41
PEG n8	C16 H34 O9	370.2203	2.61
perillartine	C10 H15 N O	165.1154	2.60
phenethylamine	C8 H11 N	121.0893	1.98
PPG n4	C12 H26 O5	250.1778	3.35
PPG n5	C15 H32 O6	308.2197	3.98
pregabalin	C8 H17 N O2	159.1259	2.22
propranolol	C16 H21 N O2	259.1571	4.39
pyridostigmine	C9 H12 N2 O2	180.0899	1.21
ranitidine	C13 H22 N4 O3 S	314.1411	1.96
sedanolide	C12 H18 O2	194.1307	5.83
sitagliptin	C16 H15 F6 N5 O	407.1183	3.74
sotalol	C12 H20 N2 O3 S	272.1194	1.84
sulfamethoxazole	C10 H11 N3 O3 S	253.0522	3.49
sulfapyridine	C11 H11 N3 O2 S	249.0573	2.38
thymine	C5 H6 N2 O2	126.0430	1.56
tolycaine	C15 H22 N2 O3	278.1629	2.99
tramadol	C16 H25 N O2	263.1884	3.37
triethyl phosphate	C6 H15 O4 P	182.0708	3.94
triisopropanolamine	C9 H21 N O3	191.1525	1.12
tris(2-butoxyethyl) phosphate	C18 H39 O7 P	398.2433	8.07
tropine	C8 H15 N O	141.1153	4.42
uracil	C4 H4 N2 O2	112.0274	1.12
valine	C5 H11 N O2	117.0790	0.97
valsartan	C24 H29 N5 O3	435.2274	6.14
venlafaxine	C17 H27 N O2	277.2040	4.04
xanthine	C5 H4 N4 O2	152.0327	1.17
xylenesulfonate	C8 H10 O3 S	186.0346	2.49
zolpidem	C19 H21 N3 O	307.1683	3.89
δ-valerolactam	C5 H9 N O	99.0684	1.72

Table S3. Relative mass flow during the sampling period of the chemicals with a degradation half-life of <100 d in the field.

chemical	mass flow from inflow (d^{-1}) [a]	mass flow from effluent (d^{-1}) [a]	mass flow from outflow (d^{-1}) [a]	contribution of the inflow to Σ(inflow+effluent) (%)
acesulfame	4.04E+10	2.27E+11	4.01E+11	15
amphetamine	1.8E+09	4.45E+09	4.24E+09	29
atenolol	3.61E+09	3.54E+11	1.07E+10	1
benzophenone	5.39E+10	7.47E+10	2.47E+11	42
benzotriazole	1.44E+10	1.09E+12	4.42E+11	1
benzoylecgonine	4.97E+08	1.45E+10	9.46E+08	3
choline	1.08E+12	2.21E+11	2.44E+12	83
climbazole	1.64E+09	1.76E+10	2.99E+09	9
codeine	1.34E+09	7.05E+10	4.2E+09	2
coniine	7.69E+08	3.07E+10	2.65E+09	2
D-panthenol	2.71E+10	7.11E+10	7.22E+10	28
ecgonine	2.48E+09	2.35E+11	2.39E+10	1
escitalopram	5.13E+08	1.18E+11	2.56E+09	0
fexofenadine	1.33E+09	8.27E+10	2.19E+10	2
furosemide	3.12E+09	1.74E+11	7.3E+09	2
hexamethylenetetramine	1.02E+10	4.48E+11	1.08E+11	2
hydrochlorothiazide	1.3E+09	8.6E+10	2.23E+09	1
irbesartan	7.74E+08	4.47E+10	1.58E+09	2
kinetin	1.44E+09	1.77E+11	3.07E+10	1
lamotrigine	3.46E+09	1.53E+12	4.24E+11	0
lidocaine	1.89E+09	3.93E+11	8.19E+10	0
losartan	1.27E+09	8.38E+10	1.46E+10	1
melamine	2.97E+10	5.54E+11	1.97E+11	5
metformin	1.6E+09	4.34E+11	9.37E+10	0
metoprolol	1.83E+09	9.7E+11	1.81E+10	0
oxazepam	1.96E+09	1.15E+11	3E+10	2
paracetamol	7.39E+09	1.72E+10	1.55E+10	30
PEG n5	1.17E+11	2.51E+11	1.28E+11	32
PEG n6	3.44E+10	2.75E+10	4.43E+10	56
perillartine	2.59E+09	6.65E+10	2.31E+10	4
PPG n4	3.3E+10	3.69E+11	1.18E+11	8
PPG n5	2.25E+10	2.16E+11	8.06E+10	9
pregabalin	5.3E+09	3.21E+11	2.25E+11	2
propranolol	1.86E+09	9.35E+10	5.41E+09	2
ranitidine	3.08E+09	4.49E+10	5.61E+09	6

sitagliptin	4.73E+08	4.89E+10	6.15E+09	1
sotalol	1.95E+09	1.52E+10	3.62E+09	11
sulfapyridine	2.43E+09	1.43E+11	5.37E+09	2
tramadol	1.23E+09	4.6E+11	5.63E+10	0
triisopropanolamine	4.91E+10	2.44E+11	1.07E+11	17
tropine	1.55E+10	8.02E+11	4.49E+11	2
valsartan	1.23E+09	2.01E+10	2.22E+09	6
venlafaxine	6.83E+08	5.02E+11	1.8E+10	0

[a] Unitless peak areas were used as surrogates of chemical concentration, hence the units are not mass per time and can only be evaluated on a relative basis for a given chemical.

Table S4. Comparison of chemical half-life (d) in the lab test and the field test.

chemical	lab measurements (mixture lake water / natural lake water) [a]		field measurements	
	mean	95% confidence interval	mean	rel. std. dev. (RSD)
acesulfame*	30 / 24	[26, 36] / [21, 28]	51	0.53
amphetamine*	46 /	[41, 54] /	58	0.56
atenolol*	6.5 /	[6.2, 6.8] /	3.9	0.049
benzotriazole	-- / --	[--, --] / [--, --]	68	0.16
codeine	101 / 150	[78, 142] / [98, 202]	<6.5 [b]	0.21
coniine	-- /	[--, --] /	<13	0.24
ecgonine*	5.1 / 4.9	[4.7, 5.5] / [2.9, 15]	10	0.21
escitalopram	-- /	[--, --] /	3.9	0.17
furosemide*	11 /	[9.1, 13] /	5.9	0.041
hexamethylenetetramine	-- / --	[1347, --] / [--, --]	45	0.24
hydrochlorothiazide*	36 /	[31, 41] /	<3.6	0.043
irbesartan*	10 /	[9.3, 11] /	<5.7	0.062
kinetin	92 / 135	[66, 152] / [83, 354]	25	0.17
lamotrigine	-- / --	[--, --] / [--, --]	74	0.33
lidocaine	200 / 162	[149, 306] / [133, 208]	28	0.23
losartan*	18 / 33	[15, 21] / [11, 79]	21	0.23
melamine	-- / --	[--, --] / [--, --]	39	0.28
metformin	-- / --	[1934, --] / [--, --]	15	0.38
metoprolol*	14 / 12	[13, 15] / [11, 14]	3.1	0.043
oxazepam*	105 / 119	[81, 148] / [79, 239]	37	0.18
perillartine	73 / --	[38, 1282] / [--, --]	71	0.31
PPG n4*	5.1 / 19	[4.8, 5.4] / [17, 22]	32	0.28
PPG n5*	3.7 / 24	[3.5, 4.0] / [21, 28]	34	0.31
pregabalin*	11 / 7.2	[8.9, 12] / [6.7, 8.7]	81	0.43
propranolol*	13 /	[11, 14] /	<6.8	0.083
ranitidine*	4.6 /	[3.7, 6.2] /	<17	0.055
sitagliptin	71 /	[55, 100] /	20	0.47
sulfapyridine*	2.7 /	[2.4, 3-0] /	<5.5	0.14
tramadol	401 / 731	[261, --] / [419, --]	16	0.19
tropine*	33 / 18	[29, 36] / [12, 25]	52	0.41
valsartan*	6.3 /	[4.1, 14] /	<14	0.096
venlafaxine	3818 / --	[608, --] / [--, --]	5.6	0.099

* These chemicals followed first-order dissipation kinetics in the laboratory test.

[a] -- indicates a positive slope of the dissipation curve. If the upper bound has this designation, then the dissipation half-life was not different from ∞. If the lower bound also has this designation, then there was net formation of the chemical during the incubation. If the space after the / is empty then dissipation could not be measured in the incubation with natural lake water.

[b] -- < indicates that *mean* represents an upper limit; in this case the *RSD* applies to the upper limit.

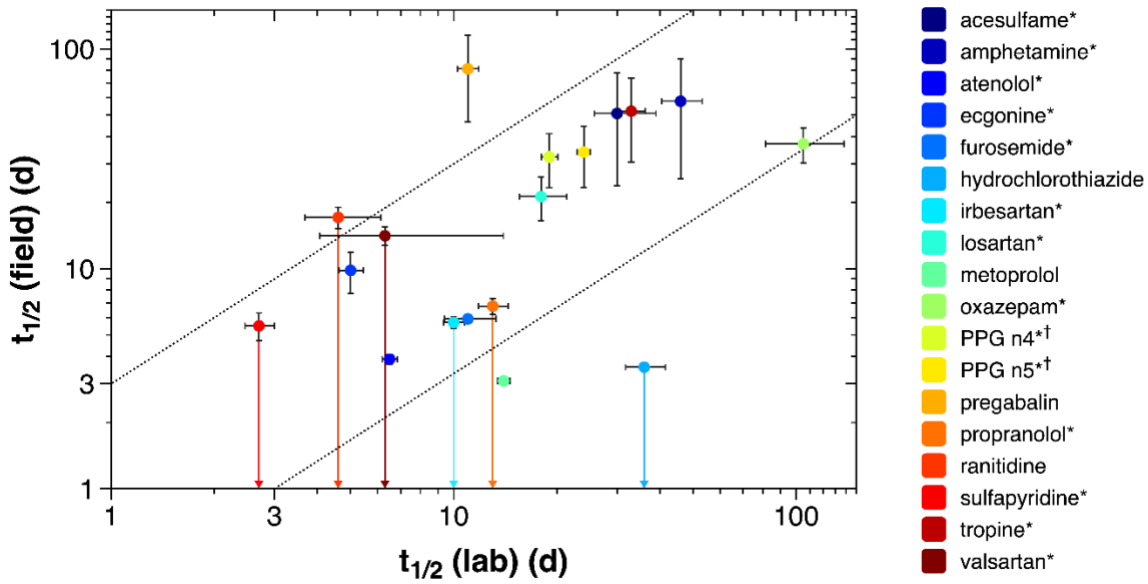

Figure S6. Field and lab half-lives ($t_{1/2}$, d) for the 18 chemicals that degraded according to first-order kinetics in the lab test. The area between the two dashed lines represents agreement between the two half-lives within a factor of 3. The * symbol next to a chemical indicates a good agreement between field and lab half-lives (central estimates differ by a factor of <3). The † symbol next to a chemical indicates the lab half-lives are from incubations of natural lake water; those for the other compounds are from incubations in mixture lake water. The error bars show the standard deviation for the field measurements and the 95% confidence interval for the lab measurements. The extended line with an arrow is used if the concentration was <LOD in outflow, in which case the calculated $t_{1/2}$ represents a maximum value.

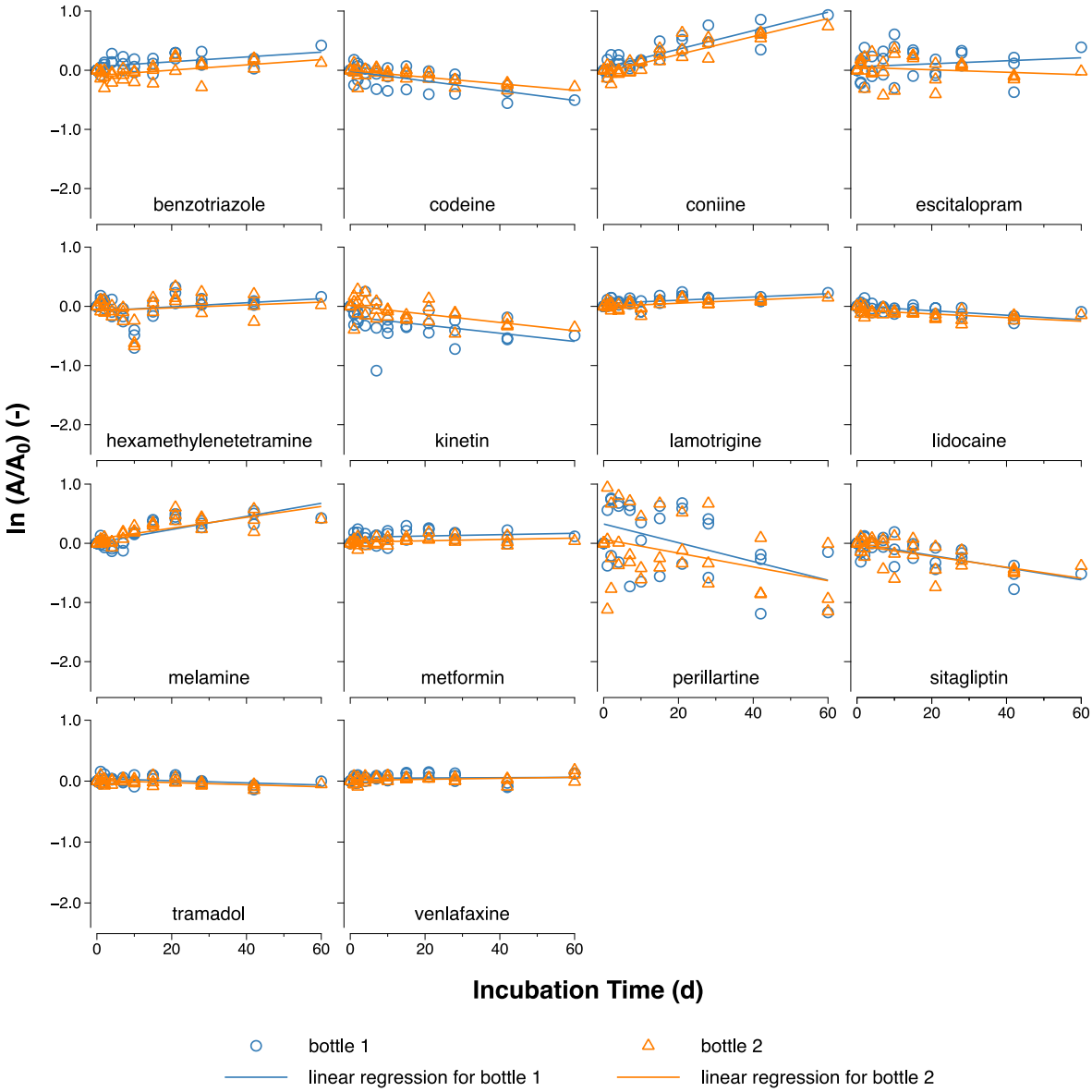

Figure S7. Concentration time trends in the lab test with mixture lake water for the 14 chemicals for which either the half-life had a high uncertainty or the 95% confidence interval of the half-life intersected infinity. All graphs share the same x and y axis. Plots are based on normalized peak areas at each time point relative to the initial peak area in each sample. Linear regressions are shown as solid lines.