

Supplemental Materials for the paper: Pesticides pollution of small streams in Germany

Eduard Szöcs, Marvin Brinke, Bilgin Karaoglan, Ralf B. Schäfer

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1 Data Cleaning

Each of more than 30 datasets have been cleaned and homogenized separately, before combining in a common database. Cleaning steps comprised (Figure S1 gives a graphical overview).

1. Structure: Structure has been adjusted to the database structure.
2. Coordinates: Coordinates have been transformed to a common Coordinate Reference System (DHDN / 3-Grad Gauss-Krüger Zone 3 (EPSG:31467) and duplicates merged.
3. Chemicals: Chemical names and identifiers have been unified using the webchem package (Szöcs, 2016).
4. Identifiers: Unique identifiers have been assigned.
5. Units: All concentrations have been converted to $\mu\text{g}/\text{L}$. Values below limit of quantification have been set to zero.
6. Other meta-data: meta-data has been standardised.
7. Temporal resolution: The temporal resolution of the database is 1 day. Data below this resolution has been aggregated by maximum.
8. Validity Checks: Simple rules for validity checks have been implemented (e.g. no negative concentrations).

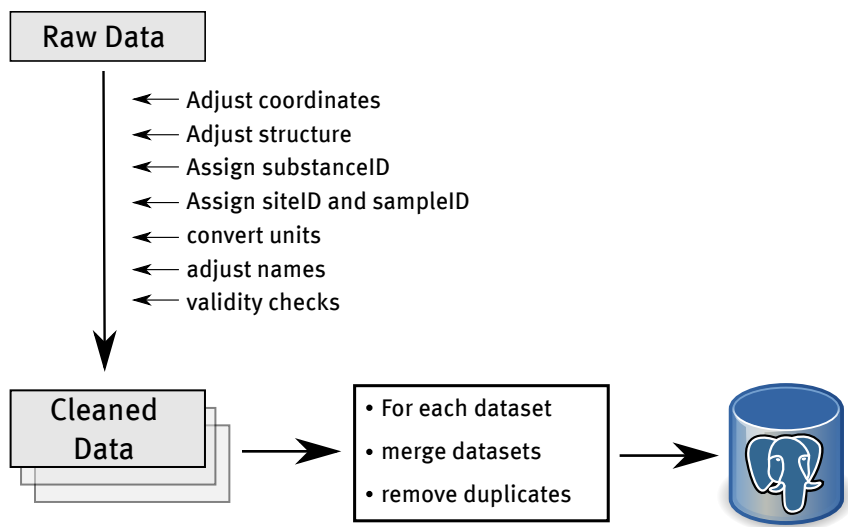


Figure S1: Overview on data cleaning steps. After cleaning data has been stored in a relational spatial PostgreSQL database.

2 Overview on compiled data

Table S1: Overview on chemical samples. Only data from running waters and grab sampling is shown. ^a: Abbreviations according to ISO 3166-2:DE. ^b: Including metabolites

state ^a	begin	end	no.sites	no.samples	no.compounds ^b
BW	2005-01-03	2014-10-02	118	4569	127
BY	2006-04-19	2013-12-18	19	297	157
HE	2007-01-15	2014-12-18	68	2512	144
MV	2005-03-08	2014-12-17	135	1535	227
NI	2014-03-24	2014-10-13	3	17	226
NW	2005-01-11	2015-01-22	1320	10985	204
RP	2005-01-05	2013-12-18	44	1277	278
SH	2005-04-26	2014-11-26	273	1419	180
SL	2005-01-03	2013-12-09	6	420	57
SN	2005-01-02	2013-12-18	917	17052	173
ST	2005-01-10	2015-03-25	46	712	93
TH	2005-01-31	2014-12-10	100	1441	76
Total	2005-01-02	2015-03-25	3049	42236	484

Table S2: Analysed chemical compounds. ^a Authorized in Germany (Source: BVL, 2015). ^b Authorized in the EU (Source: EU). ^c [ug/L]. ^d chemprop: Read-Across (Schüürmann et al., 2011); epa: US EPA (U.S. EPA, 2015); malaj:(Malaj et al., 2014); ppdb: Pesticides Properties database (Lewis et al., 2016); none: no LC50 could be found. ^e Maximum Annual Concentration Environmental Quality Standard [ug/L]. ^f Regulatory Acceptable Concentration [ug/L] (Source: German EPA).

	Name	CAS	Group	Auth. GER ^a	Auth. EU ^b	LC50 _{D.magna} ^c	Source LC50 ^d	MAC- EQS ^e	RAC ^f
1	1,3-cis-Dichlorpropen	10061-01-5	other			6483.44	chemprop		
2	1,3-trans-Dichlorpropen	10061-02-6	other			6483.44	chemprop		
3	2,4-D	94-75-7	herbicide	x	x	148281.00	malaj	1.00	1.10
4	2,4-DB	94-82-6	herbicide		x	25000.00	malaj		
5	2,4-Dichlorphenol	120-83-2	metabolite			2600.00	malaj		
6	2,4,5-T	93-76-5	herbicide			5000.00	malaj		
7	2,4,6-Trichlorphenol	88-06-2	metabolite			1710.00	malaj		
8	2,6-Dichlorobenzamid	2008-58-4	metabolite			180000.00	malaj		
9	3-Hydroxy Carbofuran	16655-82-6	metabolite			293.44	chemprop		
10	4,6-Dinitro-o-Cresol	534-52-1	insecticide			3200.00	malaj		
11	Acetochlor	34256-82-1	herbicide			8600.00	malaj		

12	Acetochlorsäure	194992-44-4	metabolite				none		
13	Acetochlorsulfonsäure	187022-11-3	metabolite			139523.68	chemprop		
14	Aclonifen	74070-46-5	herbicide	x	x	1200.00	ppdb	0.12	1.06
15	Alachlor	15972-60-8	herbicide			10000.00	malaj	0.70	
16	Aldicarb	116-06-3	insecticide			339.52	epa		
17	Aldrin	309-00-2	insecticide			28.00	malaj		
18	Ametryn	834-12-8	herbicide			28000.00	malaj		
19	AMPA	1066-51-9	metabolite				none		
20	Atrazin	1912-24-9	herbicide			54000.00	malaj	2.00	
21	Atrazin, 2-Hydroxy	2163-68-0	metabolite			36738.13	chemprop		
22	Avermectin B1a	71751-41-2	insecticide	x	x		none		
23	Azinphos-ethyl	2642-71-9	insecticide			4.00	epa		
24	Azinphos-methyl	86-50-0	insecticide			2.09	epa		
25	Azoxystrobin	131860-33-8	fungicide	x	x	254.47	epa		0.55
26	Benalaxyl	71626-11-4	fungicide	x	x	590.00	ppdb		20.00
27	Bensulfuron-methyl	83055-99-6	herbicide		x	130000.00	ppdb		
28	Bentazon	25057-89-0	herbicide	x	x	125000.00	malaj		710.00
29	Bifenox	42576-02-3	herbicide	x	x	350.00	epa	0.04	
30	Bifenthrin	82657-04-3	insecticide		x	1.53	epa		
31	Boscalid	188425-85-6	fungicide	x	x	5330.00	ppdb		12.50
32	Bromacil	314-40-9	herbicide			121000.00	malaj		
33	Bromocyclen	1715-40-8	insecticide			700.00	ppdb		
34	Bromoxynil	1689-84-5	herbicide	x	x	12500.00	malaj		3.30
35	Carbendazim	10605-21-7	fungicide			131.52	epa	0.70	0.15
36	Carbofuran	1563-66-2	insecticide			9.40	malaj		
37	Chlordan	57-74-9	insecticide			98.40	malaj		
38	Chlorfenvinphos	470-90-6	insecticide			0.25	malaj	0.30	
39	Chloridazon	1698-60-8	herbicide	x	x	132000.00	malaj		56.00
40	Chloroxuron	1982-47-4	herbicide			2950.00	epa		
41	Chlorpyrifos	2921-88-2	insecticide		x	0.10	malaj	0.10	0.00
42	Chlortoluron	15545-48-9	herbicide	x	x	67000.00	ppdb		2.30
43	Clomazon	81777-89-1	herbicide	x	x	5200.00	epa		5.70
44	Clopyralid	1702-17-6	herbicide	x	x	225000.00	malaj		1080.00
45	Clothianidin	210880-92-5	insecticide	x	x	119000.00	epa		0.01
46	Coumaphos	56-72-4	insecticide			0.19	epa		
47	Cyanazin	21725-46-2	herbicide			49000.00	malaj		
48	Cyazofamid	120116-88-3	fungicide	x	x	429.19	epa		
49	Cypermethrin	52315-07-8	insecticide	x	x	0.57	epa	0.00	0.00
50	Cyprodinil	121552-61-2	fungicide	x	x	32.00	epa		0.75
51	Demeton-O	298-03-3	insecticide				none		
52	Demeton-S	126-75-0	insecticide			22.07	chemprop		
53	Demeton-S-methyl	919-86-8	insecticide			23.00	malaj		
54	Demeton-S-methylsulfon	17040-19-6	insecticide			259.00	malaj		
55	Desethylatrazin	6190-65-4	metabolite			76529.00	malaj		
56	Desethylterbutylazin	30125-63-4	metabolite			42000.00	malaj		
57	Desisopropylatrazin	1007-28-9	metabolite			132340.00	malaj		
58	Desmetryn	1014-69-3	herbicide			26000.00	malaj		
59	Desphenyl-Chloridazon	6339-19-1	metabolite				none		
60	Diazinon	333-41-5	insecticide			1.26	epa		
61	Dichlorprop	120-36-5	herbicide			100000.00	malaj		
62	Dichlorvos	62-73-7	insecticide			0.19	malaj	0.00	
63	Dicofol	115-32-2	insecticide			140.00	ppdb		
64	Dieldrin	60-57-1	insecticide			250.00	malaj		
65	Diflufenican	83164-33-4	herbicide	x	x	4937.72	chemprop		0.03
66	Dimefuron	34205-21-5	herbicide				none		0.83
67	Dimethachlor	50563-36-5	herbicide	x	x	24000.00	ppdb		3.50
68	Dimethachlorsäure		metabolite				none		

69	Dimethachlorsulfonsäure		metabolite				none		
70	Dimethenamid	87674-68-8	herbicide			16000.00	epa		1.35
71	Dimethenamidsulfonsäure		metabolite				none		
72	Dimethoat	60-51-5	insecticide	x	x	2000.00	malaj	1.00	4.00
73	Dimethomorph	110488-70-5	fungicide	x	x	10600.00	epa		5.60
74	Dimoxystrobin	149961-52-4	fungicide	x	x	39.40	ppdb	2.00	0.03
75	Disulfoton	298-04-4	insecticide			13.00	epa		
76	Diuron	330-54-1	herbicide		x	5700.00	malaj	1.80	0.79
77	Endosulfan, alpha	959-98-8	insecticide			440.00	malaj		
78	Endosulfan, beta	33213-65-9	insecticide			550.00	epa		
79	Endrin	72-20-8	insecticide			117.00	malaj		
80	Epoxiconazol	133855-98-8	fungicide	x	x		chemprop		0.54
81	Ethofenprox	80844-07-1	insecticide	x	x	0.57	epa		
82	Ethofumesat	26225-79-6	herbicide	x	x	14000.00	malaj		24.00
83	Etrinfos	38260-54-7	insecticide			1.48	chemprop		
84	Fenhexamid	126833-17-8	fungicide	x	x		chemprop		10.10
85	Fenitrothion	122-14-5	insecticide			8.60	malaj		
86	Fenoprop	93-72-1	herbicide			4379.00	malaj		
87	Fenpropidin	67306-00-7	fungicide	x	x	540.00	ppdb		
88	Fenpropimorph	67564-91-4	fungicide	x	x	2380.00	epa	20.00	0.20
89	Fenthion	55-38-9	insecticide			12.17	epa		
90	Fenuron	101-42-8	herbicide			1679.96	chemprop		
91	Fluazifop-P-butyl	79241-46-6	herbicide			2995.84	chemprop		7.70
92	Flufenacet	142459-58-3	herbicide	x	x	30900.00	ppdb	0.20	2.40
93	Fluopicolide	239110-15-7	fungicide	x	x	1700.00	epa		
94	Fluoxastrobin	361377-29-9	fungicide	x	x	646.22	epa		
95	Fluquinconazole	136426-54-5	fungicide	x	x		chemprop		0.80
96	Fluroxypyr	69377-81-7	herbicide	x	x	100000.00	epa		16.00
97	Flurtamone	96525-23-4	herbicide	x	x	13000.00	ppdb	1.00	0.99
98	Flusilazol	85509-19-9	fungicide			3400.00	ppdb		1.10
99	Flutriafol	76674-21-0	fungicide		x	21749.83	epa		
100	Glufosinat	51276-47-2	herbicide	x	x		none		
101	Glyphosate	1071-83-6	herbicide	x	x	40000.00	malaj		100.00
102	Haloxifop	69806-34-4	herbicide			63160.93	chemprop		
103	HCH, gamma (Lindan)	58-89-9	insecticide			1600.00	malaj		
104	Heptachlor	76-44-8	insecticide			42.00	malaj	0.00	
105	Heptachlorepoxyd	1024-57-3	metabolite			240.00	malaj	0.00	
106	Heptenophos	23560-59-0	insecticide			2.20	ppdb		
107	Hexachlorbenzen	118-74-1	fungicide			5.70	malaj	0.05	
108	Hexazinon	51235-04-2	herbicide			85000.00	malaj		
109	Imidacloprid	138261-41-3	insecticide	x	x	30638.85	epa	0.10	0.01
110	Ioxynil	1689-83-4	herbicide	x		3900.00	malaj		2.70
111	Isodrin	465-73-6	insecticide			69.00	malaj		
112	Isoproturon	34123-59-6	herbicide	x	x	580.00	malaj	1.00	1.30
113	Isoxaben	82558-50-7	herbicide	x	x	1300.00	epa		
114	Kresoxim-methyl	143390-89-0	fungicide	x	x	332.00	epa		1.00
115	Lenacil	2164-08-1	herbicide	x	x	8400.00	malaj		0.65
116	Linuron	330-55-2	herbicide		x	477.00	malaj		
117	Malathion	121-75-5	insecticide		x	0.70	malaj		
118	MCPA	94-74-6	herbicide	x	x	190000.00	malaj		9.00
119	MCPB	94-81-5	herbicide		x	55000.00	malaj		
120	Mecoprop	93-65-2	herbicide		x	10000.00	epa		160.00
121	Metalaxyl	57837-19-1	fungicide		x	28000.00	malaj		46.00
122	Metaldehyd	108-62-3	other	x	x	77660.00	epa		
123	Metamitron	41394-05-2	herbicide	x	x	97000.00	malaj		38.00
124	Metazachlor	67129-08-2	herbicide	x	x	33000.00	malaj		0.88
125	Metazachlorsäure	1231244-60-2	metabolite				none		
126	Metazachlorsulfonsäure	172960-62-2	metabolite				none		
127	Metconazol	125116-23-6	fungicide	x	x	4200.00	ppdb		

128	Methabenzthiazuron	18691-97-9	herbicide			30600.00	ppdb		
129	Methamidophos	10265-92-6	insecticide			270.00	malaj		2.60
130	Methobromuron	3060-89-7	herbicide		x	44100.00	ppdb		2.00
131	Methoxychlor	72-43-5	insecticide			50.00	malaj		
132	Methyl-desphenyl-Chloridazon	17254-80-7	metabolite				none		
133	Metolachlor	51218-45-2	herbicide			15595.00	malaj		
134	Metolachlorsäure	152019-73-3	metabolite			87605.85	chemprop		
135	Metolachlorsulfonsäure	171118-09-5	metabolite			156909.76	chemprop		
136	Metoxuron	19937-59-8	herbicide			160000.00	epa		
137	Metribuzin	21087-64-9	herbicide	x	x	49000.00	malaj		0.58
138	Mevinphos	7786-34-7	insecticide			12.08	chemprop		
139	Mirex	2385-85-5	insecticide			65.00	malaj		
140	Monolinuron	1746-81-2	herbicide			32500.00	ppdb	20.00	
141	Napropamid	15299-99-7	herbicide	x	x	15229.22	epa		6.70
142	Nicosulfuron	111991-09-4	herbicide	x	x	1000000.00	epa	0.09	0.09
143	o,p-DDE	3424-82-6	metabolite			19.00	malaj		
144	o,p-DDT	789-02-6	insecticide			5.00	malaj		
145	Omethoat	1113-02-6	insecticide			21.00	malaj	2.00	
146	Oxadixyl	77732-09-3	fungicide			530000.00	epa		
147	Oxydemeton-methyl	301-12-2	insecticide			50.23	epa		1.10
148	p,p-DDD (p,p TDE)	72-54-8	insecticide			9.00	malaj		
149	p,p-DDE	72-55-9	metabolite			13.00	malaj		
150	p,p-DDT	50-29-3	insecticide			5.00	malaj		
151	Parathion-ethyl	56-38-2	insecticide			2.50	malaj		
152	Parathion-methyl	298-00-0	insecticide			7.30	malaj		
153	Penconazol	66246-88-6	fungicide	x	x	6750.00	ppdb		3.20
154	Pencycuron	66063-05-6	fungicide	x	x	666.50	chemprop		
155	Pendimethalin	40487-42-1	herbicide	x	x	280.00	malaj		0.63
156	Pethoxamid	106700-29-2	herbicide	x	x	23000.00	ppdb		1.77
157	Phenmedipham	13684-63-4	herbicide	x	x	14000.00	epa		
158	Phoxim	14816-18-3	insecticide			0.81	ppdb		0.01
159	Picolinafen	137641-05-5	herbicide	x	x	13805.30	chemprop		0.04
160	Picoxystrobin	117428-22-5	fungicide	x	x	24.00	ppdb		0.60
161	Pirimicarb	23103-98-2	insecticide	x	x	17.00	malaj		0.09
162	Prochloraz	67747-09-5	fungicide	x	x	3681.99	epa		5.00
163	Prometryn	7287-19-6	herbicide			12660.00	malaj		
164	Propamocarb	24579-73-5	fungicide	x	x	106000.00	epa		
165	Propanil	709-98-8	herbicide			3008.45	epa		
166	Propazin	139-40-2	herbicide			11000.00	malaj		
167	Propiconazol	60207-90-1	fungicide	x	x	10200.00	malaj		2.00
168	Propoxur	114-26-1	insecticide			134.64	epa		
169	Propyzamid	23950-58-5	herbicide	x	x	5600.00	malaj		34.00
170	Prosulfocarb	52888-80-9	herbicide	x	x	510.00	ppdb		3.80
171	Pyraclostrobin	175013-18-0	fungicide	x	x	32.67	epa		
172	Pyrimethanil	53112-28-0	fungicide	x	x	3040.00	epa		8.00
173	Quinmerac	90717-03-6	herbicide	x	x	86745.74	chemprop		316.00
174	Quinoxifen (5,7-dichloro-4-(p-fluorophenoxy)quinoline)	124495-18-7	fungicide	x	x	91.00	epa	2.70	
175	Sebuthylazin	7286-69-3	herbicide			34498.39	chemprop		
176	Simazin	122-34-9	herbicide			94000.00	malaj	4.00	
177	Simazin, 2-Hydroxy	2599-11-3	metabolite			165760.00	malaj		
178	Spiroxamin	118134-30-8	fungicide	x	x	4164.13	epa		0.13
179	Tebuconazol	107534-96-3	fungicide	x	x	2051.97	epa		0.58
180	Terbutryn	886-50-0	herbicide			7100.00	malaj	0.34	
181	Terbutylazin	5915-41-3	herbicide	x	x	5000.00	epa		1.20
182	Thiacloprid	111988-49-9	insecticide	x	x	44516.96	epa		0.00
183	Thiamethoxam	153719-23-4	insecticide	x	x	106000.00	epa		0.04

184	Thifensulfuron-methyl	79277-27-3	herbicide			470000.00	ppdb	
185	Tolclofos-methyl	57018-04-9	fungicide	x	x	48000.00	ppdb	
186	Tolyfluanid	731-27-1	fungicide			190.00	epa	
187	trans-Chlordan	5103-74-2	insecticide			153.23	chemprop	
188	Triadimenol	55219-65-3	fungicide	x	x	2500.00	epa	3.40
189	Triazophos	24017-47-8	insecticide			12.92	epa	0.03
190	Tribenuron	106040-48-6	herbicide	x	x	1765007.38	chemprop	
191	Trichlorfon	52-68-6	insecticide			1.28	epa	
192	Trifloxystrobin	141517-21-7	fungicide	x	x	136.83	epa	0.09
193	Trifluralin	1582-09-8	herbicide			245.00	malaj	
194	Tritosulfuron	142469-14-5	herbicide	x	x		none	
195	Tefluthrin	79538-32-2	insecticide	x	x	0.11	epa	
196	tau-Fluvalinat	102851-06-9	insecticide	x	x	0.94	epa	0.03
197	Sulcotrion	99105-77-8	herbicide	x	x	430221.57	chemprop	5.00
198	Methiocarb	2032-65-7	insecticide	x	x	19.00	epa	0.01
199	Mesotrion	104206-82-8	herbicide	x	x	840000.00	epa	
200	Fluazifop	69335-91-7	herbicide			31317.92	chemprop	
201	Fenoxaprop	95617-09-7	herbicide			1260.00	ppdb	
202	Esfenvalerat	66230-04-4	insecticide	x	x	0.27	epa	
203	Dinoterb	1420-07-1	herbicide			2552.17	chemprop	
204	Dicamba	1918-00-9	herbicide	x	x	110300.00	malaj	180.00
205	Deltamethrin	52918-63-5	insecticide	x	x	0.15	epa	
206	Cyhalothrin (Summe Isomere)	91465-08-6	insecticide	x	x	0.24	epa	
207	Cyfluthrin (Summe Isomere)	68359-37-5	insecticide			0.43	epa	
208	Chlormequat	7003-89-6	other	x	x		none	
209	Thiometon	640-15-3	insecticide			70.40	chemprop	
210	Quintozen	82-68-8	fungicide			770.00	malaj	
211	Vinclozolin	50471-44-8	fungicide			3650.00	ppdb	
212	Dichlofluanid	1085-98-9	fungicide			1050.00	epa	
213	Iprodion	36734-19-7	fungicide	x	x	1010.05	epa	
214	Dinoseb	88-85-7	herbicide			240.00	malaj	
215	Kresoximsäure		metabolite				none	
216	Quizalofop	76578-12-6	herbicide			57700.00	ppdb	
217	Acifluorfen	50594-66-6	herbicide			28000.00	ppdb	
218	Diclofop	40843-25-2	herbicide		x	709.06	epa	
219	Flamprop	58667-63-3	herbicide				none	
220	Fludioxonil	131341-86-1	fungicide	x	x	900.00	epa	0.50
221	Anthranilsäureisopropylamid	30391-89-0	metabolite				none	
222	Diflubenzuron	35367-38-5	insecticide		x	3.76	epa	
223	Pyrifeno	88283-41-4	fungicide			3600.00	ppdb	
224	Difenoconazol	119446-68-3	fungicide	x	x	15.15	epa	0.36
225	Amidosulfuron	120923-37-7	herbicide	x	x	36000.00	ppdb	
226	Triasulfuron	82097-50-5	herbicide	x	x		chemprop	
227	Metsulfuron	79510-48-8	herbicide	x	x		chemprop	
228	Rimsulfuron	122931-48-0	herbicide	x	x		chemprop	0.46
229	Triflusulfuron	135990-29-3	herbicide	x	x		chemprop	
230	Methidathion	950-37-8	insecticide			8.73	epa	
231	Triflumuron	64628-44-0	insecticide		x	1.60	ppdb	
232	Fluazinam	79622-59-6	fungicide	x	x	199.90	epa	0.26
233	Oxamyl	23135-22-0	insecticide		x	1665.36	epa	
234	Acibenzolar-S-methyl	135158-54-2	fungicide		x	2900.00	epa	
235	Bromuconazol	116255-48-2	fungicide		x	869.77	epa	
236	Carfentrazon-ethyl	128639-02-1	herbicide	x	x	9800.00	epa	0.31
237	Clodinafop-propargyl	105512-06-9	herbicide			2000.00	epa	
238	Cycloa	1134-23-2	herbicide			24000.00	epa	
239	Cyflufenamid	180409-60-3	fungicide	x	x		none	
240	Diniconazol	83657-24-3	fungicide			7400.00	ppdb	

241	Fenamidon	161326-34-7	fungicide	x	x	96.19	epa	
242	Fenbuconazol	114369-43-6	fungicide		x	2300.00	epa	
243	Fosthiazat	98886-44-3	other	x	x	414.25	epa	
244	Fuberidazol	3878-19-1	fungicide	x	x	4700.00	ppdb	
245	Hexaconazol	79983-71-4	fungicide			3549.63	epa	
246	Hexythiazox	78587-05-0	insecticide	x	x	7155.49	chemprop	
247	Indoxacarb	173584-44-6	insecticide	x	x	45.54	epa	
248	Mandipropamid	374726-62-2	fungicide	x	x	7100.00	ppdb	7.60
249	Metrafenon	220899-03-6	fungicide	x	x		none	
250	Oxadiazon	19666-30-9	herbicide		x	1935.29	epa	
251	Proquinazid	189278-12-4	fungicide	x	x	287.00	ppdb	
252	Tebufenpyrad	119168-77-3	insecticide	x	x	40.20	epa	
253	Tetraconazol	112281-77-3	fungicide	x	x	3873.84	epa	
254	Zoxamid	156052-68-5	fungicide	x	x	780.00	epa	
255	Hexaflumuron	86479-06-3	insecticide			0.11	epa	
256	Neburon	555-37-3	herbicide			557.72	chemprop	
257	Cyproconazol	94361-06-5	fungicide	x	x	26000.00	epa	
258	Fenarimol	60168-88-9	fungicide			6800.00	epa	
259	Iprovalicarb	140923-17-7	fungicide	x	x	17891.50	chemprop	189.00
260	Myclobutanil	88671-89-0	fungicide	x	x	11000.00	epa	2.40
261	Acetamiprid	135410-20-7	insecticide	x	x	50000.00	epa	0.24
262	Chlorfluazuron	71422-67-8	insecticide			0.91	ppdb	
263	Cyromazin	66215-27-8	insecticide		x	32349.03	epa	
264	Etaconazol	60207-93-4	fungicide			9276.38	chemprop	
265	Ethidimuron	30043-49-3	herbicide				none	
266	Fenpyroximat	134098-61-6	insecticide	x	x	22.00	ppdb	
267	Flazasulfuron	104040-78-0	herbicide	x	x	13223.50	chemprop	
268	Flufenoxuron	101463-69-8	insecticide			0.04	ppdb	
269	Mepronil	55814-41-0	fungicide			10000.00	epa	
270	Methomyl	16752-77-5	insecticide		x	7.60	malaj	
271	Methoxyfenozyd	161050-58-4	insecticide	x	x	3700.00	epa	
272	Pirimicarb-desmethyl	30614-22-3	metabolite			62.44	chemprop	
273	Spirodiclofen	148477-71-8	insecticide	x	x		none	
274	Spiromesifen	283594-90-1	insecticide		x	92.30	epa	
275	Tebufenozid	112410-23-8	insecticide	x	x	3800.00	malaj	
276	Thiabendazol	148-79-8	fungicide	x	x	761.18	epa	
277	Triflumizol	99387-89-0	fungicide		x	2110.00	ppdb	
278	Triforin	26644-46-2	fungicide			13811.28	epa	
279	Triticonazol	131983-72-7	fungicide	x	x	7600.00	epa	
280	Teflubenzuron	83121-18-0	insecticide		x	2.80	ppdb	
281	Triadimefon	43121-43-3	fungicide			7450.34	epa	
282	cis-Chlordan	5103-71-9	insecticide			153.23	chemprop	
283	Monuron	150-68-5	herbicide			14358.54	chemprop	
284	Propachlor	1918-16-7	herbicide			10097.83	epa	
285	Fluazifop-butyl	69806-50-4	herbicide			316000.00	ppdb	
286	Carbetamid	16118-49-3	herbicide		x	81000.00	ppdb	
287	Propetamphos	31218-83-4	insecticide			6.86	epa	
288	Triallat	2303-17-5	herbicide		x	115.58	epa	
289	Dichlobenil	1194-65-6	herbicide			6200.00	malaj	
290	Propham	122-42-9	herbicide			23000.00	ppdb	
291	Endosulfansulfat	1031-07-8	metabolite			1023.68	epa	
292	Beflubutamid	113614-08-7	herbicide	x	x	1640.00	ppdb	
293	Flurochloridon	61213-25-0	herbicide		x	5100.00	ppdb	
294	Iodosulfuron	185119-76-0	herbicide	x	x		chemprop	0.08
295	Metosulam	139528-85-1	herbicide	x	x	8876593.52	chemprop	
296	Triclopyr	55335-06-3	herbicide	x	x	132900.00	epa	
297	Florasulam	145701-23-1	herbicide	x	x	40074.93	epa	
298	Famoxadone	131807-57-3	fungicide	x	x	11.80	epa	
299	Folpet	133-07-3	fungicide	x	x	314.86	epa	

300	Procymidon	32809-16-8	fungicide				none	
301	Thiophanat-methyl	23564-05-8	fungicide	x	x	10719.28	epa	
302	Fluometuron	2164-17-2	herbicide		x	4626.07	epa	
303	Bupirimat	41483-43-6	fungicide		x	7142.95	chemprop	
304	Carboxin	5234-68-4	fungicide		x	69359.93	epa	
305	Chlorantraniliprole	500008-45-7	insecticide	x	x	11.07	epa	0.35
306	Dinotefuran	165252-70-0	insecticide			327252.17	epa	
307	Fenazaquin	120928-09-8	insecticide	x	x	4.10	malaj	
308	Fenoxycarb	72490-01-8	insecticide		x	400.00	epa	
309	Flupyrsulfuron	150315-10-9	herbicide	x	x		none	
310	Foramsulfuron	173159-57-4	herbicide	x	x	100000.00	ppdb	0.95
311	Imazosulfuron	122548-33-8	herbicide	x	x	32000.00	epa	
312	Mesosulfuron	400852-66-6	herbicide	x	x		none	
313	Prothioconazol-desthio	120983-64-4	metabolite				none	
314	Quinoclamín	2797-51-5	herbicide	x	x	2150.00	ppdb	
315	Sulfosulfuron	141776-32-1	herbicide		x		chemprop	
316	Triazoxid	72459-58-6	fungicide	x	x	7200.00	ppdb	
317	Tribenuron-methyl	101200-48-0	herbicide			894000.00	ppdb	
318	Ametoctradin	865318-97-4	fungicide	x	x		none	
319	Clodinafop	114420-56-3	herbicide	x	x		none	
320	Cyclanilide	113136-77-9	other			8062.26	epa	
321	Mepanipyrim	110235-47-7	fungicide	x	x	630.00	ppdb	
322	Profoxydim	139001-49-3	herbicide		x	18100.00	ppdb	
323	Propoxycarbazon	145026-81-9	herbicide	x	x	950866.02	chemprop	
324	Thiencazabon-methyl	317815-83-1	herbicide	x	x	99297.53	epa	
325	Fluopyram	658066-35-4	fungicide	x	x	25483.33	epa	5.12
326	Flutolanil	66332-96-5	fungicide	x	x	8246.21	epa	
327	Chlorthalonil-SA		metabolite				none	
328	Dimethachlor-CA		metabolite				none	
329	Dimethenamid-CA		metabolite				none	
330	Dimethenamid-SA		metabolite				none	
331	Flufenacet-SA		metabolite				none	
332	Metaxyl-CA	75596-99-5	metabolite			37321.03	chemprop	
333	Metazachlordicarbonsäure		metabolite				none	
334	Metaxyl-CA2	104390-56-9	metabolite				none	
335	Azoxystrobin-CA		metabolite				none	
336	Thiacloprid-SA		metabolite				none	
337	Trifloxystrobin-CA2		metabolite				none	
338	Clethodim	99129-21-2	herbicide	x	x		epa	
339	Cycloxydim	101205-02-1	herbicide	x	x		none	
340	Imazamox	114311-32-9	herbicide	x	x	122000.00	epa	
341	Imazapic	104098-48-8	herbicide				none	
342	Imazaquin	81335-37-7	herbicide		x	280000.00	epa	
343	Imazethapyr	81335-77-5	herbicide			331662.48	epa	
344	Meptyldinocap	131-72-6	fungicide		x		none	
345	Tralkoxydim	87820-88-0	herbicide		x	14720.73	epa	
346	Saflufenacil	372137-35-4	herbicide			98200.00	epa	
347	Valifenalate	283159-90-0	fungicide	x	x		none	
348	Fluxapyroxad	907204-31-3	fungicide	x	x	104000.00	epa	
349	Isopyrazam	881685-58-1	fungicide	x	x	44.00	ppdb	
350	Penflufen	494793-67-8	fungicide		x		none	
351	Pyroxulam	422556-08-9	herbicide	x	x	100000.00	epa	
352	Fipronil	120068-37-3	insecticide		x	118.82	epa	0.00
353	Hexachlorophen	70-30-4	other				none	
354	(E)-7-(Z)-9-Dodecadienylacetat	55774-32-8	other	x	x		none	
355	(Z)-9-Dodecenylacetat	16974-11-1	other	x	x	2600.00	ppdb	
356	1-Decanol	112-30-1	other	x	x	6510.00	epa	
357	1-Methylcyclopropen	3100-04-7	other	x	x		none	

358	Acequinocyl	57960-19-7	insecticide	x	x	2.70	epa	9.00
359	alpha-Cypermethrin	67375-30-8	insecticide	x	x	0.30	ppdb	
360	Aminopyralid	150114-71-9	herbicide	x	x	98600.00	epa	
361	Amisulbrom	348635-87-0	fungicide	x	x	37.00	ppdb	
362	Azadirachtin (Neem)	11141-17-6	insecticide	x	x	622.58	epa	
363	Benthiavalicarb	413615-35-7	fungicide	x	x		none	
364	Benzoesaure	65-85-0	fungicide	x	x	293257.57	epa	
365	Bifenazate	149877-41-8	insecticide	x	x	500.00	epa	
366	Bixafen	581809-46-3	fungicide	x	x	1200.00	ppdb	0.46
367	Bromadiolon	28772-56-7	other		x	2000.00	ppdb	
368	Captan	133-06-2	fungicide	x	x	7100.00	malaj	5.00
369	Chlorpropham	101-21-3	herbicide	x	x	3700.00	epa	
370	Chlorthalonil	1897-45-6	fungicide	x	x	100.82	epa	
371	Cinidon-ethyl	142891-20-1	herbicide			59200.00	ppdb	
372	Clofentezin	74115-24-5	insecticide		x	44.56	epa	
373	Codlemone (Codlelure)	33956-49-9	other	x	x	2800.00	epa	
374	Cymoxanil	57966-95-7	fungicide	x	x	2616.85	epa	4.40
375	Daminozid	1596-84-5	other	x	x	99742.17	epa	
376	Deiquat	2764-72-9	herbicide	x	x	1392.94	epa	
377	Desmedipham	13684-56-5	herbicide	x	x	450.00	malaj	
378	Dichlorprop-P	15165-67-0	herbicide	x	x	3821.30	epa	
379	Difenacoum	56073-07-5	other		x	520.00	ppdb	
380	Dimethenamid-P	163515-14-8	herbicide	x	x	12000.00	epa	1.35
381	Dithianon	3347-22-6	fungicide	x	x	260.00	ppdb	0.78
382	Dodin	2439-10-3	fungicide	x	x	48.32	epa	5.33
383	Fenoxaprop-p-ethyl	71283-80-2	herbicide			4134.71	chemprop	
384	Flonicamid	158062-67-0	insecticide	x	x	98600.00	epa	310.00
385	Fluazifop-P	83066-88-0	herbicide	x	x	31317.92	chemprop	146.00
386	Flumioxazin	103361-09-7	herbicide	x	x	5500.00	epa	
387	Fluroxypyr- methylheptyl	81406-37-3	herbicide				none	0.31
388	Fosetyl	15845-66-6	fungicide	x	x		none	
389	gamma-Cyhalothrin	76703-62-3	insecticide	x	x	2.91	epa	
390	Haloxypop-P	95977-29-0	herbicide	x	x		none	
391	Hymexazol	10004-44-1	fungicide	x	x	30800.00	epa	
392	Imazalil	35554-44-0	fungicide	x	x	3540.00	epa	
393	Isoxaflutole	141112-29-0	herbicide	x	x	1500.00	epa	
394	Mancozeb	8018-01-7	fungicide	x	x	910.17	epa	0.22
395	Maneb	12427-38-2	fungicide	x	x	346.41	epa	
396	Mepiquat	15302-91-7	other	x	x		none	
397	Metaflumizone	139968-49-3	insecticide	x	x	920.52	epa	
398	Metalaxyl-M	70630-17-0	fungicide	x	x	84682.67	epa	46.00
399	Metiram	9006-42-2	fungicide	x	x	573.97	epa	
400	Metsulfuron-methyl	74223-64-6	herbicide				chemprop	
401	Milbemectin	51596-11-3	insecticide	x	x	64.81	epa	
402	Paclobutrazol	76738-62-0	other	x	x	15839.70	epa	
403	Pelargonsaure	112-05-0	herbicide	x	x	96000.00	epa	
404	Penoxsulam	219714-96-2	herbicide	x	x	94110.73	epa	
405	Picloram	1918-02-1	herbicide	x	x	54852.97	epa	
406	Pinoxaden	243973-20-8	herbicide	x			none	
407	Pirimiphos-methyl	29232-93-7	insecticide	x	x	0.22	epa	
408	Prohexadion	88805-35-0	other	x	x		none	
409	Propaquizafop	111479-05-1	herbicide	x	x	1252.20	chemprop	
410	Prosulfuron	94125-34-5	herbicide	x	x		chemprop	
411	Prothioconazol	178928-70-6	fungicide	x	x	1200.00	epa	1.71
412	Pymetrozin	123312-89-0	insecticide	x	x	87000.00	ppdb	
413	Pyraflufen	129630-17-7	herbicide	x	x		none	
414	Pyridat	55512-33-9	herbicide	x	x	1080.00	epa	

415	Silthiofam	175217-20-6	fungicide	x	x	14000.00	ppdb	
416	Spinosad	168316-95-8	insecticide	x	x	6500.00	epa	0.06
417	Sulfurylfluorid	2699-79-8	insecticide	x	x	620.00	ppdb	
418	Tembotrione	335104-84-2	herbicide	x	x	48900.00	epa	
419	Tepraloxymid	149979-41-9	herbicide	x	x	7400.00	epa	
420	Thiram	137-26-8	fungicide	x	x	11.00	malaj	0.11
421	Topramezone	210631-68-8	herbicide	x		99995.00	epa	0.90
422	Trinexapac-ethyl	95266-40-3	other	x	x	40445.07	chemprop	
423	Warfarin	81-81-2	other			57770.44	epa	
424	Aziprotrryn	4658-28-0	herbicide			26000.00	epa	
425	Chlorsulfuron	64902-72-3	herbicide				chemprop	
426	Norflurazon	27314-13-2	herbicide			15000.00	epa	
427	Primisulfuron-methyl	86209-51-0	herbicide			260000.00	ppdb	
428	Pyrazophos	13457-18-6	fungicide			0.36	ppdb	
429	Quinalphos	13593-03-8	insecticide			0.21	epa	
430	Secbumeton	26259-45-0	herbicide			3992.00	malaj	
431	Tebutam	35256-85-0	herbicide				none	
432	Fluchloralin	33245-39-5	herbicide			669.33	epa	
433	Furalaxyl	57646-30-7	fungicide			39000.00	ppdb	
434	Methoprotrryn	841-06-5	herbicide			42000.00	epa	
435	Furmecyclox	60568-05-0	fungicide				none	
436	Desmethyldisoproturon	34123-57-4	metabolite			18407.25	chemprop	
437	Metamitron-Desamino	36993-94-9	metabolite			61635.23	chemprop	
438	Orysastobin	248593-16-0	fungicide			1300.00	ppdb	
439	Desethyl-2-hydroxyterbutylazin	66753-06-8	metabolite			59384.47	chemprop	
440	Icaridinsäure		metabolite				none	
441	Desaminometribuzin	35045-02-4	metabolite				none	
442	Karbutylat	4849-32-5	herbicide				none	
443	Crimidin	535-89-7	other				none	
444	Buturon	3766-60-7	herbicide				none	
445	Chlorbromuron	13360-45-7	herbicide			12342.32	chemprop	
446	Fenoxaprop-p	113158-40-0	herbicide	x	x	6247.76	epa	
447	Fenamiphos	22224-92-6	insecticide		x	2.11	epa	
448	Isophenphos	25311-71-1	insecticide			4.01	epa	
449	4,4-Methoxychlor	2132-70-9	insecticide				none	
450	oxi-Chlordan	27304-13-8	metabolite			1300.00	epa	
451	3-Trifluormethylanilin	98-16-8	metabolite			2700.00	epa	
452	1-(3,4-Dichlorphenyl)urea	2327-02-8	metabolite			8372.59	chemprop	
453	1-(4-Isopropylphenyl)urea	56046-17-4	metabolite			22814.20	chemprop	
454	Telodrin	297-78-9	insecticide			8.00	malaj	
455	Terbumeton	33693-04-8	herbicide			40000.00	malaj	
456	Nitenpyram	120738-89-8	insecticide				none	
457	Permethrin	52645-53-1	insecticide			0.60	malaj	
458	Quizalofop-ethyl	76578-14-8	herbicide			3700.00	epa	
459	Mefenpyr-diethyl	135591-00-3	other	x		5600.00	epa	
460	Iodosulfuron-methyl	144550-06-1	herbicide				none	
461	Haloxypop-ethoxyethyl	87237-48-7	herbicide				none	
462	Desmethyldiuron	3567-62-2	metabolite			2142.31	chemprop	
463	Cloquintocet-mexyl	99607-70-2	other		x	820.00	epa	
464	Chlorpyrifos methyl	5598-13-0	insecticide		x	0.94	epa	
465	Ethirimol	23947-60-6	fungicide			53000.00	ppdb	
466	Desethylsimazin	6190-65-4	metabolite				none	
467	Nitrofen	1836-75-5	herbicide			217.00	malaj	
468	Thiophenylsulfuron	79277-67-1	herbicide	x	x		none	
469	Acrinathrin	101007-06-1	insecticide		x	53000.00	ppdb	
470	Betacypermethrin	65731-84-2	insecticide		x	53000.00	ppdb	

471	4-tert. Cyclobutylhex-anon	98-53-3	metabolite				none	
472	Pirimiphos-ethyl	23505-41-1	insecticide				none	
473	Pyrethrum	8003-34-7	insecticide	x	x	17.03	epa	0.01
474	Pyridaben	96489-71-3	insecticide		x	0.82	epa	
475	Iodosulfuron-methyl-sodium	144550-36-7	herbicide				none	
476	Benazolin	3813-05-6	herbicide				none	
477	Chloramben	133-90-4	herbicide			53000.00	ppdb	
478	Chlorfenac	85-34-7	herbicide				none	
479	Desethylsebutylazin	37019-18-4	metabolite				none	
480	Prometon	1610-18-0	herbicide			41167.00	malaj	
481	Atraton	1610-17-9	herbicide				none	
482	Terbutylazin-Metabolit SYN 545666		metabolite				none	
483	2-Hydroxydesethylatrazin	19988-24-0	metabolite				none	
484	Terbutylazin-Metabolit CGA 324007	309923-18-0	metabolite				none	

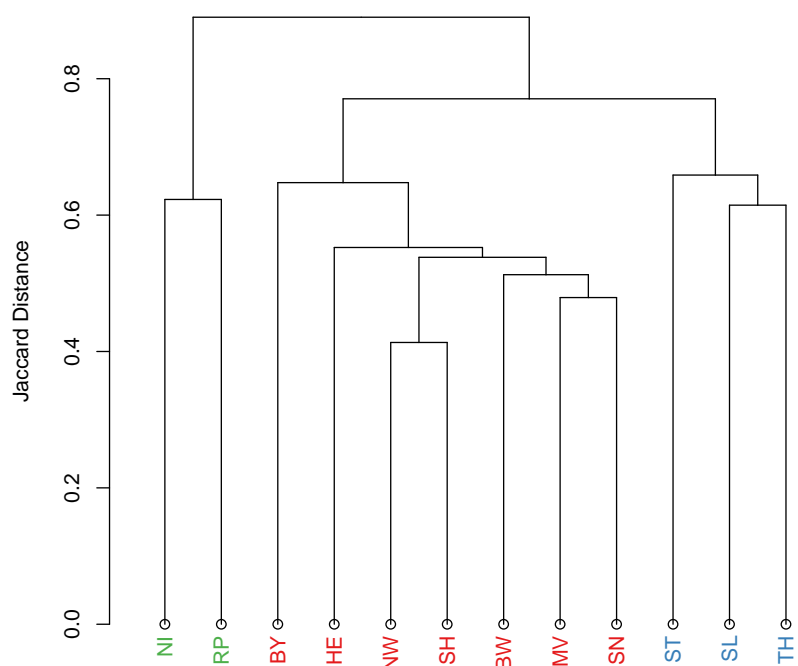


Figure S2: Complete Linkage Cluster Dendrogram of Jaccard Similarity of analysed compound spectra between federal states. Abbreviations of state names according to ISO 3166-2:DE.

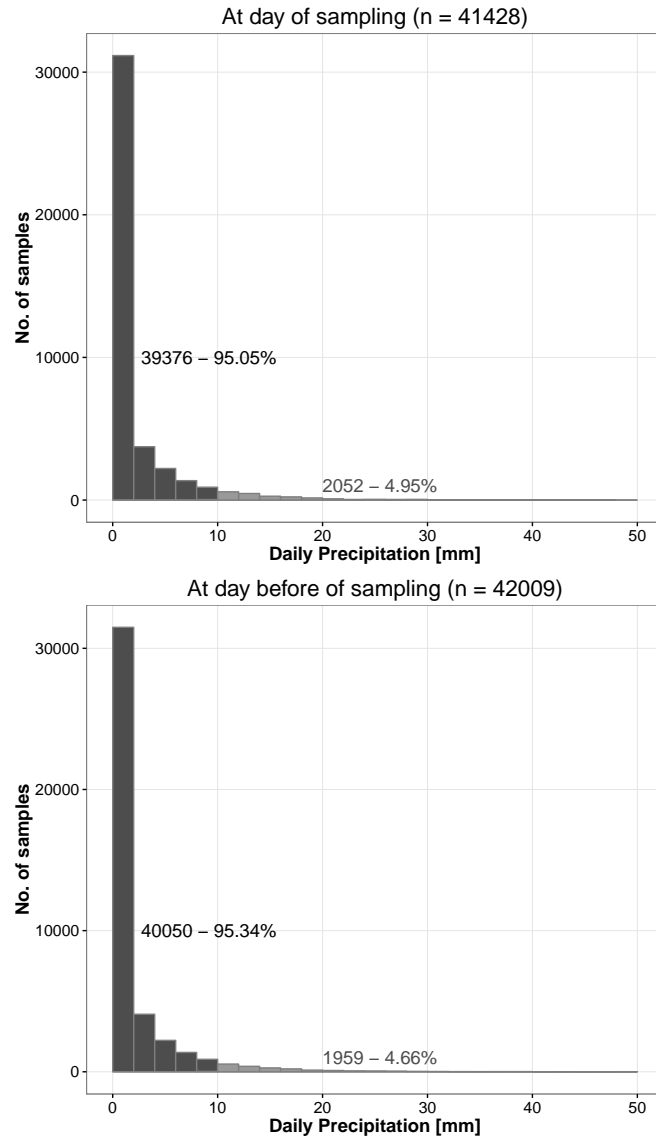


Figure S3: Distribution of precipitation at sampling occasions. top: at sampling date.
bottom: at day before sampling.

3 Are small agricultural waters more polluted compared to bigger streams?

3.1 RAC Exceedances

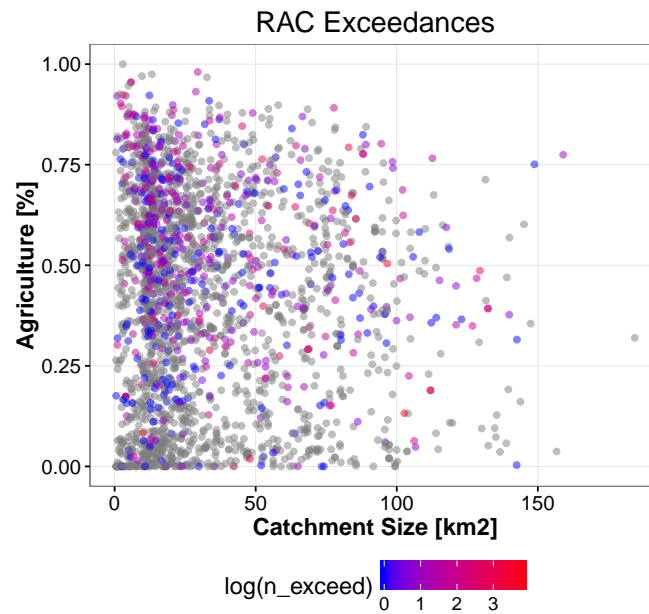


Figure S4: Raw data used for the model in equation xxx and Figure xxx of the main article. Color codes the number of RAC exceedances (on a log-scale). Grey points are sites without any exceedance.

update
refs

3.2 Toxic Units

We modeled the 95th percentile of TU_{max} on a logarithmic scale assuming a Normal distribution:

$$\begin{aligned} \log(TU_{max}) &\sim \text{Normal}(\mu_i, \sigma) \\ \log(\mu_i) &= \beta_0 + f_1(Agri_i) + f_2(Size_i) \end{aligned} \quad (3.1)$$

where TU_{maxi} is 95th percentile of TU_{max} at site i , $Agri_i$ the proportion of agriculture within the catchment and $Size_i$ the catchment size of the site. f_1 and f_2 are smoothing functions.

Because of samples at low polluted sites contained only values below the limit of quantification (LOQ) the derived TU_{max} were also left censored (at a value of $10^{-8.75}$), thus we have

$$\log(TU_{max\ i}) = \begin{cases} \beta_0 + f_1(Agri_i) + f_2(Size_i) + \epsilon_i, & \text{if } \log(TU_{max}) > -8.75 \\ -8.75, & \text{if } \log(TU_{max}) \leq -8.75. \end{cases} \quad (3.2)$$

Instead of assuming a fixed value for the data $< \text{LOQ}$, we use a model taking this censoring into account (Helsel, 2006) with the expected value being a mixture of censored and uncensored data.

$$\begin{aligned} E(y_i|x_i) &= P(\text{uncensored}|x_i) \times E(y_i|y_i > -8.75) + P(\text{censored}|x_i) \times -8.75 \\ \text{Var}(y_i) &= \sigma \end{aligned} \quad (3.3)$$

With y_i being $\log(TU_{max\ i})$ and x_i the predictor functions $f_1(Agri_i) + f_2(Size_i)$. $P(\text{censored}|x_i)$ is the probability of censoring at given predictors and $E(y_i|y_i > -8.75)$ the expected value given non-censoring. Further, we assumed constant variance. This model was fitted using the `gamlss` package (Stasinopoulos and Rigby, 2007).

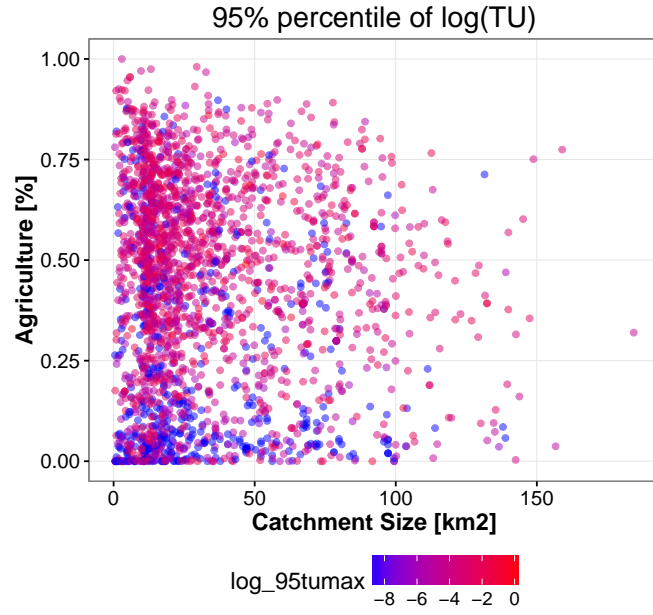


Figure S5: Raw data of effect of agriculture and catchment size on the 95th percentile of $\log(TU_{max})$.

3.3 EQS Exceedances

We modeled the number of EQS exceedances (No) the same way as RAC exceedances (see main article).

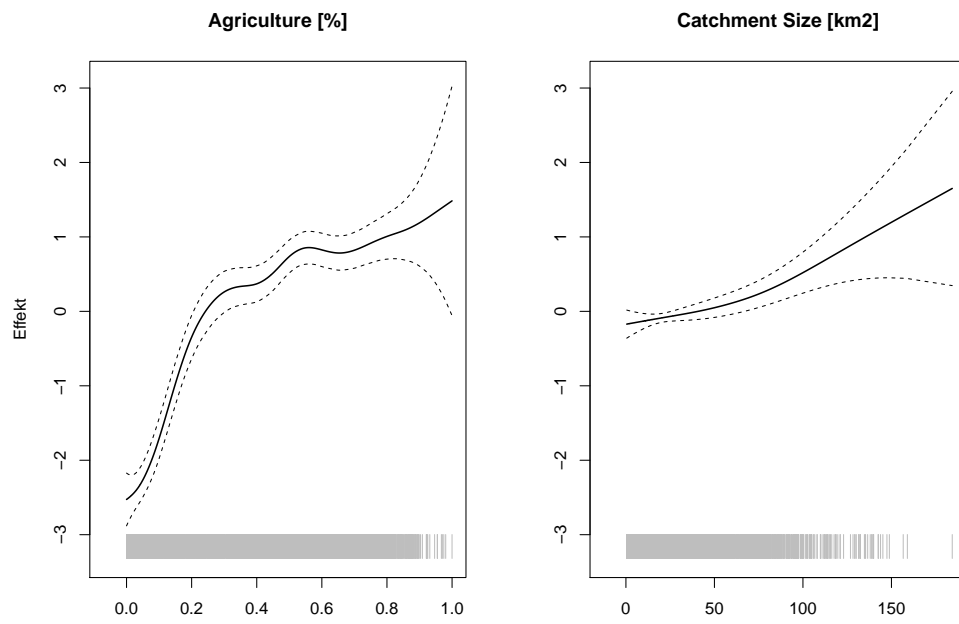


Figure S6: Effect of agriculture within the catchment (left) and catchment size (right) on the 95th percentile of $\log(\text{TUmax})$. The model took censored data into account (see description above). Dashed lines denote 95% Confidence Intervals.

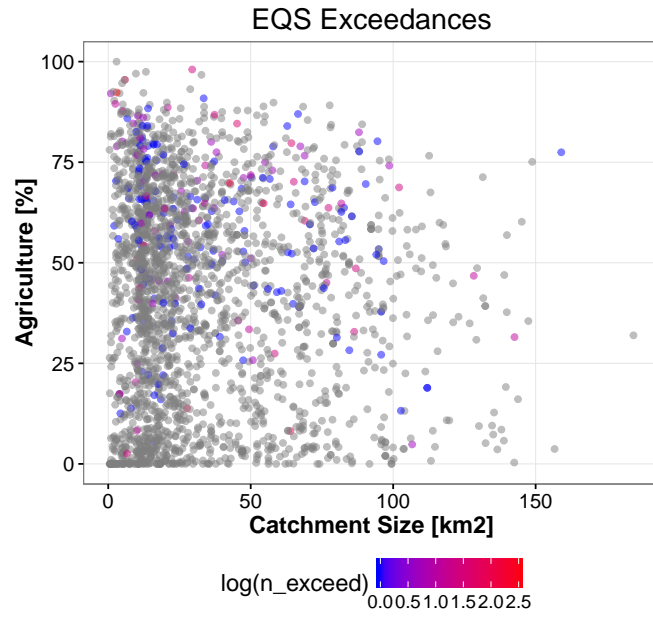


Figure S7: Raw data used for modelling EQS exceedances. Color codes the number of EQS exceedances (on a log-scale). Grey points are sites without any exceedance.

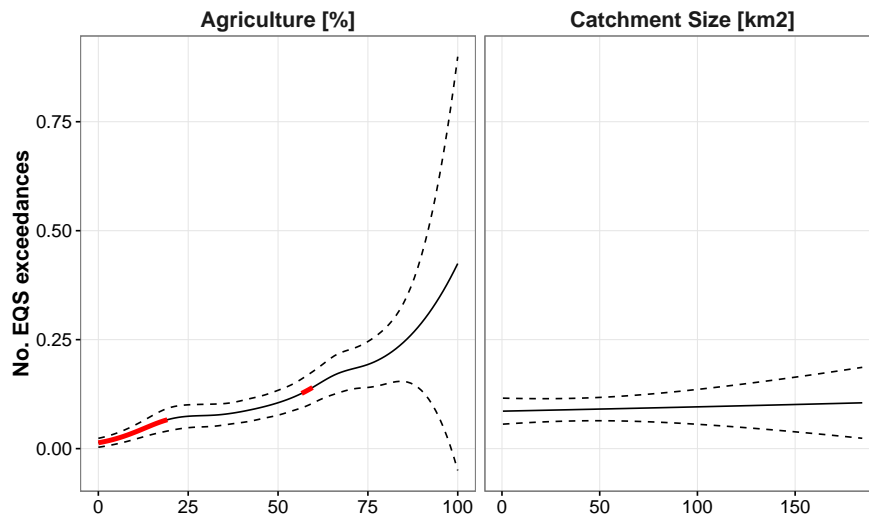


Figure S8: Effect of agriculture within the catchment (left) and catchment size (right) on the number of EQS exceedances. Red line marks statistically significant changes. Dashed lines denote 95% Confidence Intervals.

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