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

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Contents

List of Figures

List of Tables

1 Data Cleaning

Each of more then 30 datasets have been cleaned and homogenized separately, before combing 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 $\mu g/L$. Values below limit of quantification have be set to zero.
6. Other meta-data: meta-data has been standardised.
7. Temporal resolution: The temporal resolution of the database is 1 day. Date below this resolution has been aggregated by maximum.
8. Validity Checks: Simple rules for validity checks have been implemented (e.g. no negative concentrations).

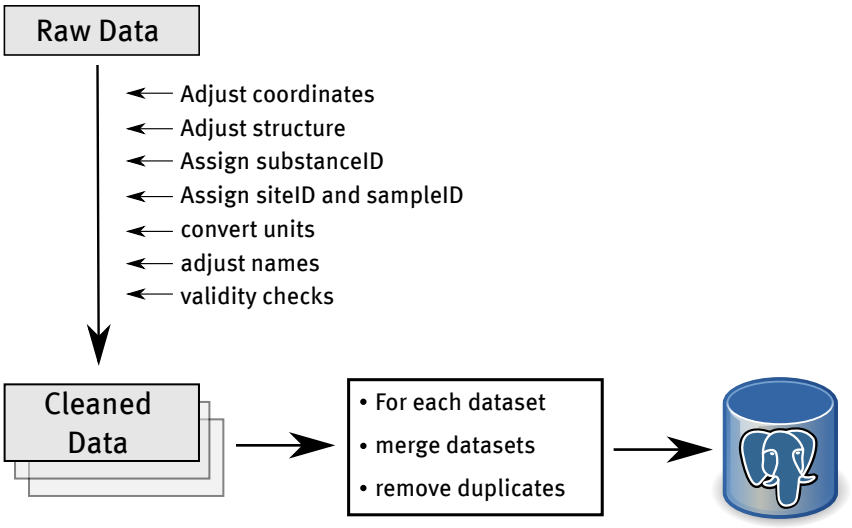


Figure S1: Overview on data cleaning steps. After cleaning data has been stored in a relational spatial PostgreSQL database.

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 Anual 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	Cypermetryn	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	Desethylterbuthylazin	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	Etrimfos	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	Haloxyfop	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	Heptachlorepoxid	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	Methyldesphenyl-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	Quinoxyfen (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	Terbuthylazin	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	Tolylfluanid	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	Pyrifenox	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	Carfentrazone-ethyl	128639-02-1	herbicide	x	x	9800.00	epa		0.31
237	Clodinafop-propargyl	105512-06-9	herbicide			2000.00	epa		
238	Cycloat	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	Methoxyfenozid	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	Quinoclamin	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	Propoxycarbazone	145026-81-9	herbicide	x	x	950866.02	chemprop	
324	Thiencarbazon-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	Metalaxyl-CA	75596-99-5	metabolite			37321.03	chemprop	
333	Metazachlordicarbonsäure		metabolite				none	
334	Metalaxyl-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	Cycloxidim	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	Pyroxsulam	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	Benzoesäure	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	Haloxyfop-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	Pelargonsäure	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	Tepraloxydim	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	Aziprotryn	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	Methoprotryn	841-06-5	herbicide			42000.00	epa	
435	Furmecyclox	60568-05-0	fungicide				none	
436	Desmethylisoproturon	34123-57-4	metabolite			18407.25	chemprop	
437	Metamitron-Desamino	36993-94-9	metabolite			61635.23	chemprop	
438	Orysastrobin	248593-16-0	fungicide			1300.00	ppdb	
439	Desethyl-2-hydroxyterbuthylazin	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	Haloxyfop-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	Chlorpyriphos 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	Thifenylsulfuron	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. Cyclobutylhexanon	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	Desethylsebuthylazin	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	

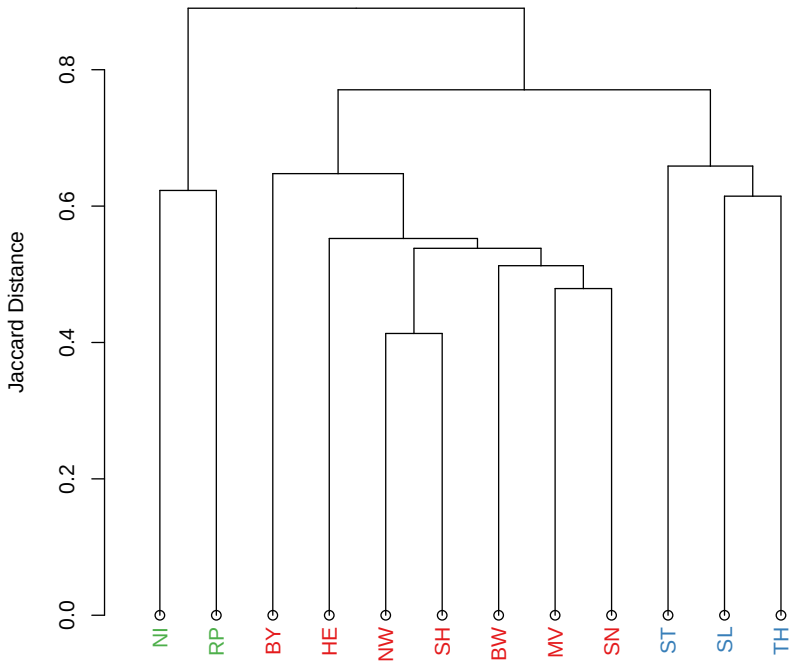


Figure S2: Complete Linkage Cluster Dendrogram of Jaccard Similarity of analysed compound spectra between federal states. Abbreviations of state names according to ISO 3166-2:DE.

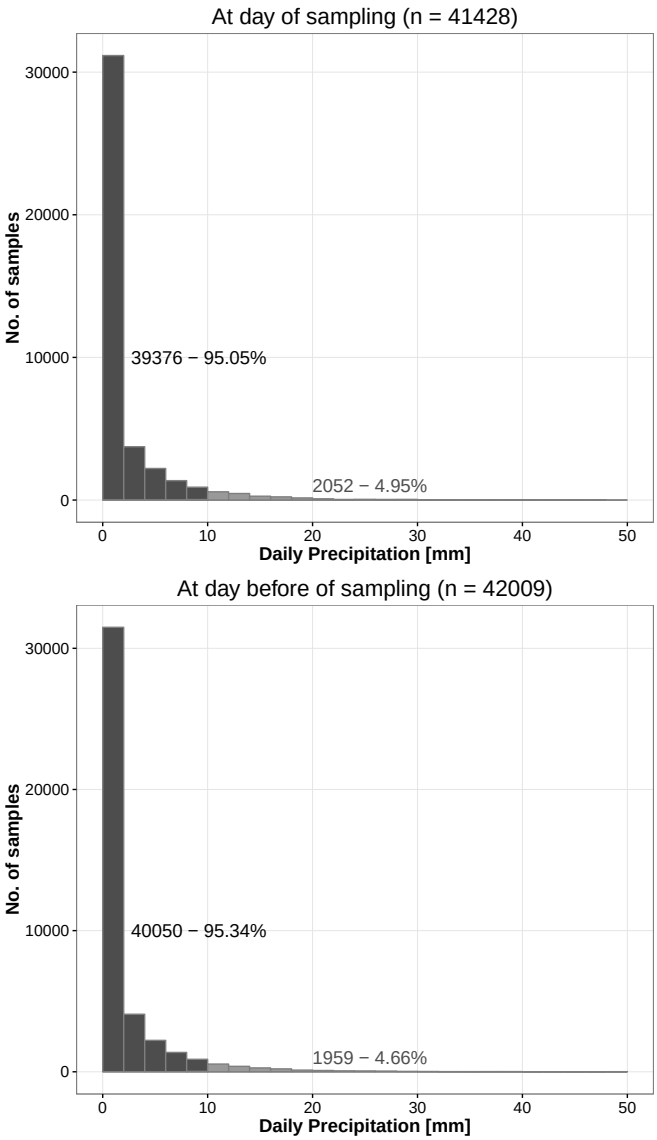


Figure S3: Distribution of precipitation at sampling occasions. top: at sampling date. bottom: at day before sampling.

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

3.1 EQS Exceedances

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

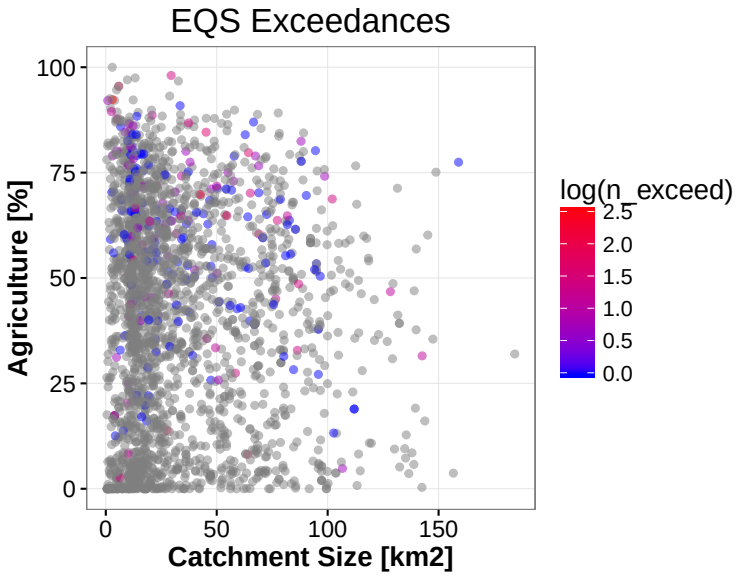
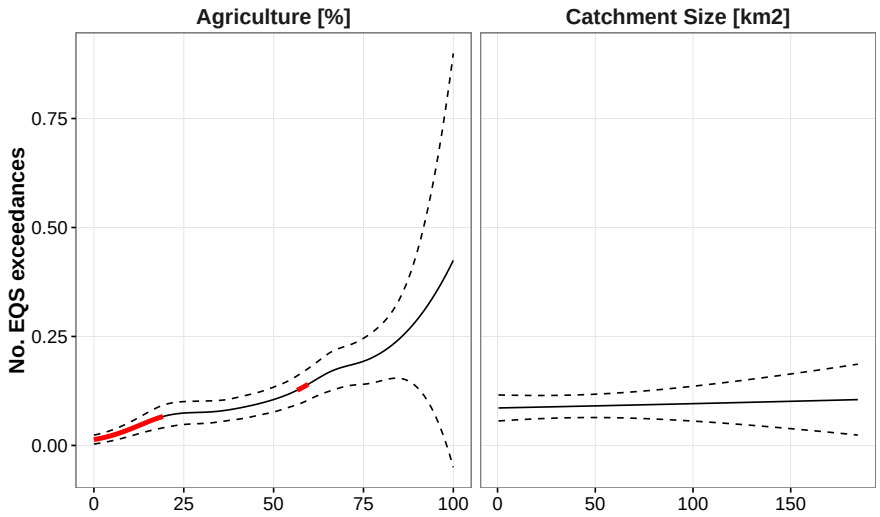


Figure S4: Raw data used for modelling EQS exceedances. Color codes the number of EQS exceedances (on a log-scale). Grey points denote sites without any exceedance.

3.2 RAC Exceedances

update refs



1.5, 2, 1, 12

Figure S5: 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.

3.3 Toxic Units

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

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

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

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

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

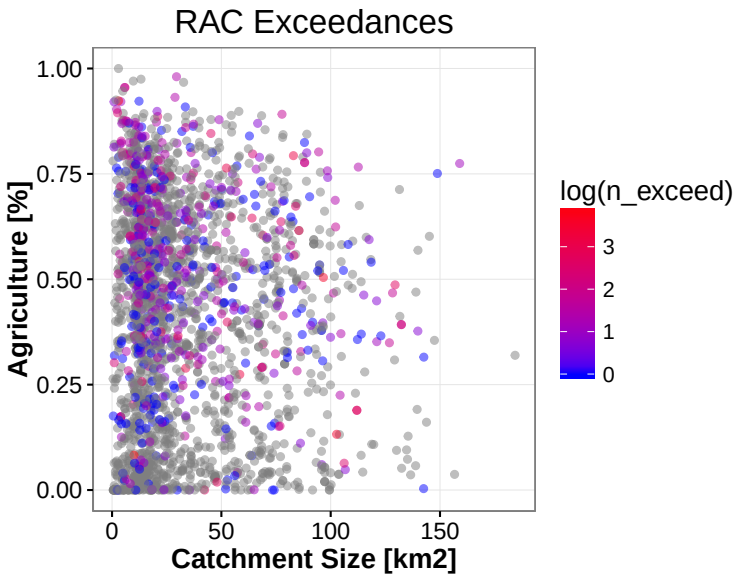


Figure S6: Raw data used for the model in equation xxx and Figure xxx of the main article. Color codes the number of RAC exceedances (on a log-scale). Grey points denote sites without any exceedance.

$$E(y_i|x_i) = P(uncensored|x_i) \times E(y_i|y_i > -8.75)) + P(censored|x_i) \times -8.75$$
$$Var(y_i) = \sigma \tag{3.3}$$

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

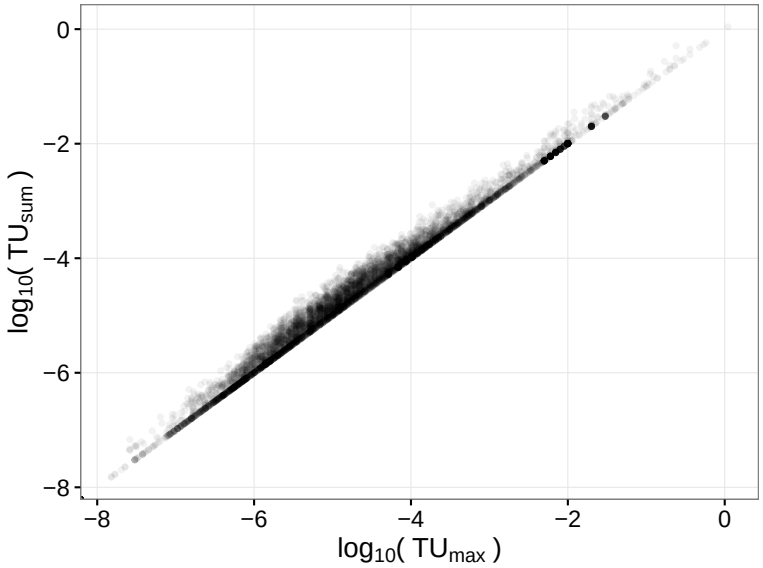


Figure S7: Correlation between $log(TU_{max})$ and $log(TU_{sum})$. n = 7067 observations with TU >0.

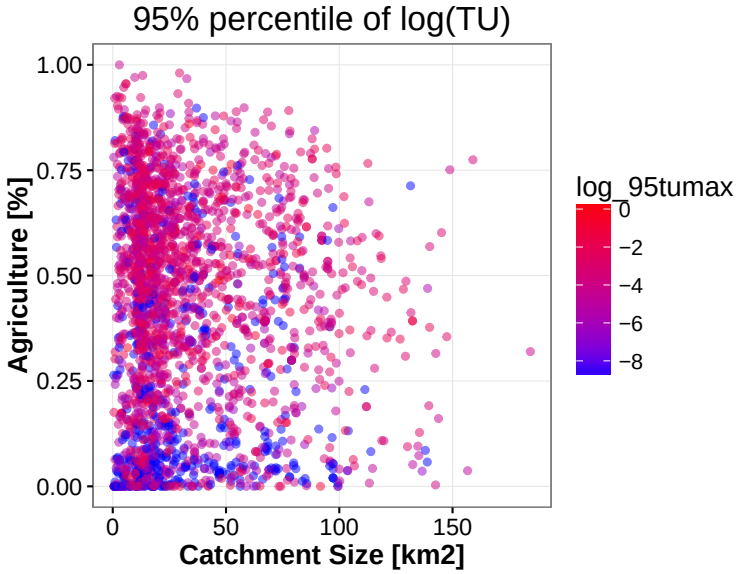


Figure S8: Raw data of effect of agriculture and catchment size on the 95th percentile of $log(TU_{max})$.

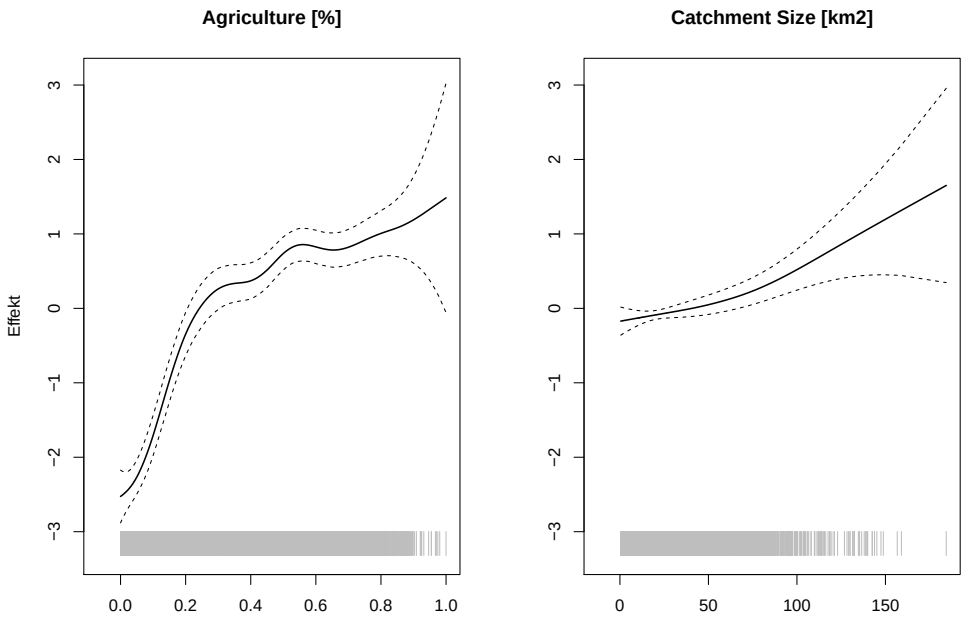


Figure S9: Effect of agriculture within the catchment (left) and catchment size (rigth) on the 95th percentile of log(TUmax). The model took censored data into account (see description above). Dashed lines denote 95% Confidence Intervals.

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