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

More then 30 datasets have been cleaned and homogenized separately, before combing into 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).

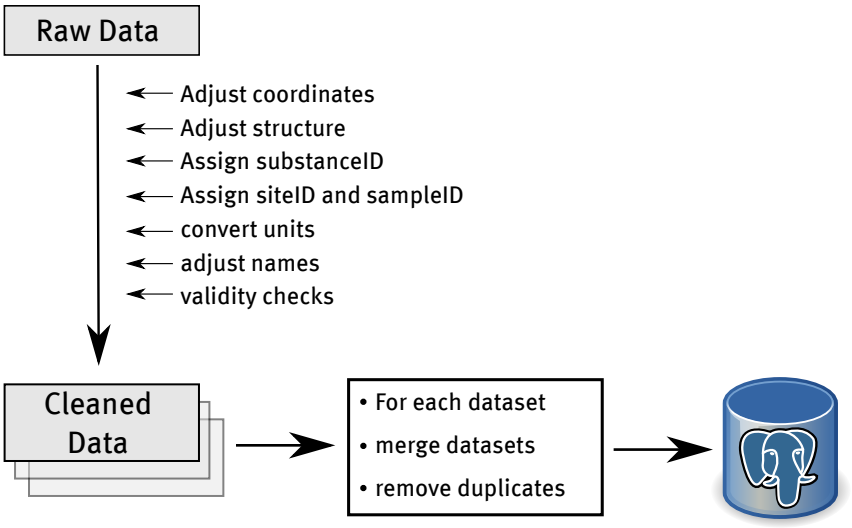

Figure S1: Overview on data cleaning steps. After cleaning data has been stored in a relational spatial PostgreSQL database.

2 Catchment size - stream width relationships

We studied the relationship between catchment size based on three datasets containing this informations: Data delivered by the federal state Thuringia, Voß et al. (2015) and Fernández et al. (2015) (both from Rhineland-Palatinate). We fitted to each dataset separately and to the combined dataset a power-function. The resulting models are shown in Figure S2.

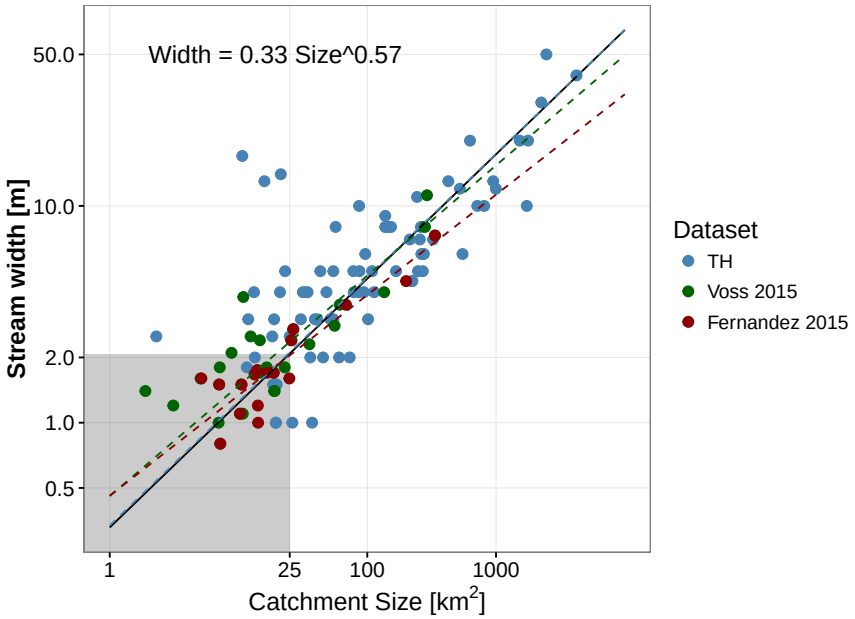

Figure S2: Relationship between catchment size and stream width. A power function has been fitted to each dataset separately and the combined dataset (black line and equation). The gray rectangle marks the estimated with for a catchment size of 25km^2.

3 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

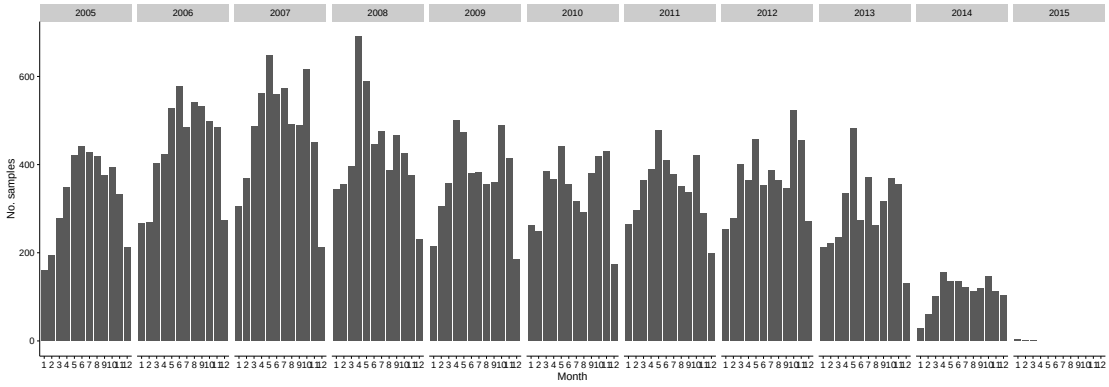

Figure S3: Number of sampling occasions per year and month.

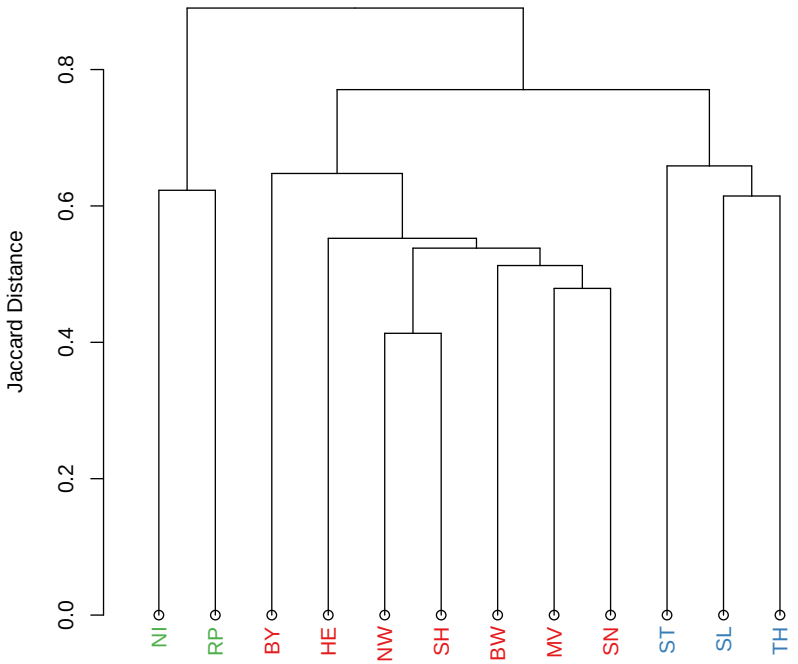

Figure S4: Complete Linkage Cluster Dendrogram of Jaccard Similarity of analysed compound spectra between federal states. Abbreviations of state names according to ISO 3166-2:DE.

Table S2: Overview on pesticides in the database. [a] Authorized in Germany (Source: BVL, 2015). [b] Authorized in the EU (Source: EU). [c] Regulatory Acceptable Concentration [ug/L] (Source: German EPA).

	Name	CAS	Group	Auth. GER[a]	Auth. EU[b]	RAC [c]
1	1,3-cis-Dichlorpropen	10061-01-5	other			
2	1,3-trans-Dichlorpropen	10061-02-6	other			
3	2,4-D	94-75-7	herbicide	x	x	1.10
4	2,4-DB	94-82-6	herbicide		x	
5	2,4-Dichlorphenol	120-83-2	metabolite			
6	2,4,5-T	93-76-5	herbicide			
7	2,4,6-Trichlorphenol	88-06-2	metabolite			
8	2,6-Dichlorobenzamid	2008-58-4	metabolite			
9	3-Hydroxy Carbofuran	16655-82-6	metabolite			
10	4,6-Dinitro-o-Cresol	534-52-1	insecticide			
11	Acetochlor	34256-82-1	herbicide			
12	Acetochlorsäure	194992-44-4	metabolite			

13	Acetochlorsulfonsäure	187022-11-3	metabolite			
14	Aclonifen	74070-46-5	herbicide	x	x	1.06
15	Alachlor	15972-60-8	herbicide			
16	Aldicarb	116-06-3	insecticide			
17	Aldrin	309-00-2	insecticide			
18	Ametryn	834-12-8	herbicide			
19	AMPA	1066-51-9	metabolite			
20	Atrazin	1912-24-9	herbicide			
21	Atrazin, 2-Hydroxy	2163-68-0	metabolite			
22	Avermectin B1a	71751-41-2	insecticide	x	x	
23	Azinphos-ethyl	2642-71-9	insecticide			
24	Azinphos-methyl	86-50-0	insecticide			
25	Azoxystrobin	131860-33-8	fungicide	x	x	0.55
26	Benalaxyl	71626-11-4	fungicide	x	x	20.00
27	Bensulfuron-methyl	83055-99-6	herbicide		x	
28	Bentazon	25057-89-0	herbicide	x	x	710.00
29	Bifenox	42576-02-3	herbicide	x	x	
30	Bifenthrin	82657-04-3	insecticide		x	
31	Boscalid	188425-85-6	fungicide	x	x	12.50
32	Bromacil	314-40-9	herbicide			
33	Bromocyclen	1715-40-8	insecticide			
34	Bromoxynil	1689-84-5	herbicide	x	x	3.30
35	Carbendazim	10605-21-7	fungicide			0.15
36	Carbofuran	1563-66-2	insecticide			
37	Chlordan	57-74-9	insecticide			
38	Chlorfenvinphos	470-90-6	insecticide			
39	Chloridazon	1698-60-8	herbicide	x	x	56.00
40	Chloroxuron	1982-47-4	herbicide			
41	Chlorpyrifos	2921-88-2	insecticide		x	0.00
42	Chlortoluron	15545-48-9	herbicide	x	x	2.30
43	Clomazon	81777-89-1	herbicide	x	x	5.70
44	Clopyralid	1702-17-6	herbicide	x	x	1080.00
45	Clothianidin	210880-92-5	insecticide	x	x	0.01
46	Coumaphos	56-72-4	insecticide			
47	Cyanazin	21725-46-2	herbicide			
48	Cyazofamid	120116-88-3	fungicide	x	x	
49	Cypermetryn	52315-07-8	insecticide	x	x	0.00
50	Cyprodinil	121552-61-2	fungicide	x	x	0.75
51	Demeton-O	298-03-3	insecticide			
52	Demeton-S	126-75-0	insecticide			
53	Demeton-S-methyl	919-86-8	insecticide			
54	Demeton-S-methylsulfon	17040-19-6	insecticide			
55	Desethylatrazin	6190-65-4	metabolite			
56	Desethylterbuthylazin	30125-63-4	metabolite			
57	Desisopropylatrazin	1007-28-9	metabolite			
58	Desmetryn	1014-69-3	herbicide			
59	Desphenyl-Chloridazon	6339-19-1	metabolite			
60	Diazinon	333-41-5	insecticide			
61	Dichlorprop	120-36-5	herbicide			
62	Dichlorvos	62-73-7	insecticide			
63	Dicofol	115-32-2	insecticide			
64	Dieldrin	60-57-1	insecticide			
65	Diflufenican	83164-33-4	herbicide	x	x	0.03
66	Dimefuron	34205-21-5	herbicide			0.83
67	Dimethachlor	50563-36-5	herbicide	x	x	3.50
68	Dimethachlorsäure		metabolite			
69	Dimethachlorsulfonsäure		metabolite			

70	Dimethenamid	87674-68-8	herbicide			1.35
71	Dimethenamidsulfonsäure		metabolite			
72	Dimethoat	60-51-5	insecticide	x	x	4.00
73	Dimethomorph	110488-70-5	fungicide	x	x	5.60
74	Dimoxystrobin	149961-52-4	fungicide	x	x	0.03
75	Disulfoton	298-04-4	insecticide			
76	Diuron	330-54-1	herbicide		x	0.79
77	Endosulfan, alpha	959-98-8	insecticide			
78	Endosulfan, beta	33213-65-9	insecticide			
79	Endrin	72-20-8	insecticide			
80	Epoxiconazol	133855-98-8	fungicide	x	x	0.54
81	Ethofenprox	80844-07-1	insecticide	x	x	
82	Ethofumesat	26225-79-6	herbicide	x	x	24.00
83	Etrimfos	38260-54-7	insecticide			
84	Fenhexamid	126833-17-8	fungicide	x	x	10.10
85	Fenitrothion	122-14-5	insecticide			
86	Fenoprop	93-72-1	herbicide			
87	Fenpropidin	67306-00-7	fungicide	x	x	
88	Fenpropimorph	67564-91-4	fungicide	x	x	0.20
89	Fenthion	55-38-9	insecticide			
90	Fenuron	101-42-8	herbicide			
91	Fluazifop-P-butyl	79241-46-6	herbicide			7.70
92	Flufenacet	142459-58-3	herbicide	x	x	2.40
93	Fluopicolide	239110-15-7	fungicide	x	x	
94	Fluoxastrobin	361377-29-9	fungicide	x	x	
95	Fluquinconazole	136426-54-5	fungicide	x	x	0.80
96	Fluroxypyr	69377-81-7	herbicide	x	x	16.00
97	Flurtamone	96525-23-4	herbicide	x	x	0.99
98	Flusilazol	85509-19-9	fungicide			1.10
99	Flutriafol	76674-21-0	fungicide		x	
100	Glufosinat	51276-47-2	herbicide	x	x	
101	Glyphosate	1071-83-6	herbicide	x	x	100.00
102	Haloxyfop	69806-34-4	herbicide			
103	HCH, gamma (Lindan)	58-89-9	insecticide			
104	Heptachlor	76-44-8	insecticide			
105	Heptachlorepoxid	1024-57-3	metabolite			
106	Heptenophos	23560-59-0	insecticide			
107	Hexachlorbenzen	118-74-1	fungicide			
108	Hexazinon	51235-04-2	herbicide			
109	Imidacloprid	138261-41-3	insecticide	x	x	0.01
110	Ioxynil	1689-83-4	herbicide	x		2.70
111	Isodrin	465-73-6	insecticide			
112	Isoproturon	34123-59-6	herbicide	x	x	1.30
113	Isoxaben	82558-50-7	herbicide	x	x	
114	Kresoxim-methyl	143390-89-0	fungicide	x	x	1.00
115	Lenacil	2164-08-1	herbicide	x	x	0.65
116	Linuron	330-55-2	herbicide		x	
117	Malathion	121-75-5	insecticide		x	
118	MCPA	94-74-6	herbicide	x	x	9.00
119	MCPB	94-81-5	herbicide		x	
120	Mecoprop	93-65-2	herbicide		x	160.00
121	Metalaxyl	57837-19-1	fungicide		x	46.00
122	Metaldehyd	108-62-3	other	x	x	
123	Metamitron	41394-05-2	herbicide	x	x	38.00
124	Metazachlor	67129-08-2	herbicide	x	x	0.88
125	Metazachlorsäure	1231244-60-2	metabolite			
126	Metazachlorsulfonsäure	172960-62-2	metabolite			
127	Metconazol	125116-23-6	fungicide	x	x	
128	Methabenzthiazuron	18691-97-9	herbicide			

129	Methamidophos	10265-92-6	insecticide			2.60
130	Methobromuron	3060-89-7	herbicide		x	2.00
131	Methoxychlor	72-43-5	insecticide			
132	Methyldesphenyl-Chloridazon	17254-80-7	metabolite			
133	Metolachlor	51218-45-2	herbicide			
134	Metolachlorsäure	152019-73-3	metabolite			
135	Metolachlorsulfonsäure	171118-09-5	metabolite			
136	Metoxuron	19937-59-8	herbicide			
137	Metribuzin	21087-64-9	herbicide	x	x	0.58
138	Mevinphos	7786-34-7	insecticide			
139	Mirex	2385-85-5	insecticide			
140	Monolinuron	1746-81-2	herbicide			
141	Napropamid	15299-99-7	herbicide	x	x	6.70
142	Nicosulfuron	111991-09-4	herbicide	x	x	0.09
143	o,p-DDE	3424-82-6	metabolite			
144	o,p-DDT	789-02-6	insecticide			
145	Omethoat	1113-02-6	insecticide			
146	Oxadixyl	77732-09-3	fungicide			
147	Oxydemeton-methyl	301-12-2	insecticide			1.10
148	p,p-DDD (p,p TDE)	72-54-8	insecticide			
149	p,p-DDE	72-55-9	metabolite			
150	p,p-DDT	50-29-3	insecticide			
151	Parathion-ethyl	56-38-2	insecticide			
152	Parathion-methyl	298-00-0	insecticide			
153	Penconazol	66246-88-6	fungicide	x	x	3.20
154	Pencycuron	66063-05-6	fungicide	x	x	
155	Pendimethalin	40487-42-1	herbicide	x	x	0.63
156	Pethoxamid	106700-29-2	herbicide	x	x	1.77
157	Phenmedipham	13684-63-4	herbicide	x	x	
158	Phoxim	14816-18-3	insecticide			0.01
159	Picolinafen	137641-05-5	herbicide	x	x	0.04
160	Picoxystrobin	117428-22-5	fungicide	x	x	0.60
161	Pirimicarb	23103-98-2	insecticide	x	x	0.09
162	Prochloraz	67747-09-5	fungicide	x	x	5.00
163	Prometryn	7287-19-6	herbicide			
164	Propamocarb	24579-73-5	fungicide	x	x	
165	Propanil	709-98-8	herbicide			
166	Propazin	139-40-2	herbicide			
167	Propiconazol	60207-90-1	fungicide	x	x	2.00
168	Propoxur	114-26-1	insecticide			
169	Propyzamid	23950-58-5	herbicide	x	x	34.00
170	Prosulfocarb	52888-80-9	herbicide	x	x	3.80
171	Pyraclostrobin	175013-18-0	fungicide	x	x	
172	Pyrimethanil	53112-28-0	fungicide	x	x	8.00
173	Quinmerac	90717-03-6	herbicide	x	x	316.00
174	Quinoxyfen (5,7-dichloro-4-(p-fluorophenoxy)quinoline)	124495-18-7	fungicide	x	x	
175	Sebuthylazin	7286-69-3	herbicide			
176	Simazin	122-34-9	herbicide			
177	Simazin, 2-Hydroxy	2599-11-3	metabolite			
178	Spiroxamin	118134-30-8	fungicide	x	x	0.13
179	Tebuconazol	107534-96-3	fungicide	x	x	0.58
180	Terbutryn	886-50-0	herbicide			
181	Terbuthylazin	5915-41-3	herbicide	x	x	1.20
182	Thiacloprid	111988-49-9	insecticide	x	x	0.00
183	Thiamethoxam	153719-23-4	insecticide	x	x	0.04
184	Thifensulfuron-methyl	79277-27-3	herbicide			

185	Tolclofos-methyl	57018-04-9	fungicide	x	x	
186	Tolylfluanid	731-27-1	fungicide			
187	trans-Chlordan	5103-74-2	insecticide			
188	Triadimenol	55219-65-3	fungicide	x	x	3.40
189	Triazophos	24017-47-8	insecticide			0.03
190	Tribenuron	106040-48-6	herbicide	x	x	
191	Trichlorfon	52-68-6	insecticide			
192	Trifloxystrobin	141517-21-7	fungicide	x	x	0.09
193	Trifluralin	1582-09-8	herbicide			
194	Tritosulfuron	142469-14-5	herbicide	x	x	
195	Tefluthrin	79538-32-2	insecticide	x	x	
196	tau-Fluvalinat	102851-06-9	insecticide	x	x	0.03
197	Sulcotrion	99105-77-8	herbicide	x	x	
198	Methiocarb	2032-65-7	insecticide	x	x	0.01
199	Mesotrion	104206-82-8	herbicide	x	x	
200	Fluazifop	69335-91-7	herbicide			
201	Fenoxaprop	95617-09-7	herbicide			
202	Esfenvalerat	66230-04-4	insecticide	x	x	
203	Dinoterb	1420-07-1	herbicide			
204	Dicamba	1918-00-9	herbicide	x	x	180.00
205	Deltamethrin	52918-63-5	insecticide	x	x	
206	Cyhalothrin (Summe Isomere)	91465-08-6	insecticide	x	x	
207	Cyfluthrin (Summe Isomere)	68359-37-5	insecticide			
208	Chlormequat	7003-89-6	other	x	x	
209	Thiometon	640-15-3	insecticide			
210	Quintozen	82-68-8	fungicide			
211	Vinclozolin	50471-44-8	fungicide			
212	Dichlofluanid	1085-98-9	fungicide			
213	Iprodion	36734-19-7	fungicide	x	x	
214	Dinoseb	88-85-7	herbicide			
215	Kresoximsäure		metabolite			
216	Quizalofop	76578-12-6	herbicide			
217	Acifluorfen	50594-66-6	herbicide			
218	Diclofop	40843-25-2	herbicide		x	
219	Flamprop	58667-63-3	herbicide			
220	Fludioxonil	131341-86-1	fungicide	x	x	0.50
221	Anthranilsäureisopropylamid	30391-89-0	metabolite			
222	Diflubenzuron	35367-38-5	insecticide		x	
223	Pyrifenox	88283-41-4	fungicide			
224	Difenoconazol	119446-68-3	fungicide	x	x	0.36
225	Amidosulfuron	120923-37-7	herbicide	x	x	
226	Triasulfuron	82097-50-5	herbicide	x	x	
227	Metsulfuron	79510-48-8	herbicide	x	x	
228	Rimsulfuron	122931-48-0	herbicide	x	x	0.46
229	Triflusulfuron	135990-29-3	herbicide	x	x	
230	Methidathion	950-37-8	insecticide			
231	Triflumuron	64628-44-0	insecticide		x	
232	Fluazinam	79622-59-6	fungicide	x	x	0.26
233	Oxamyl	23135-22-0	insecticide		x	
234	Acibenzolar-S-methyl	135158-54-2	fungicide		x	
235	Bromuconazol	116255-48-2	fungicide		x	
236	Carfentrazone-ethyl	128639-02-1	herbicide	x	x	0.31
237	Clodinafop-propargyl	105512-06-9	herbicide			
238	Cycloat	1134-23-2	herbicide			
239	Cyflufenamid	180409-60-3	fungicide	x	x	
240	Diniconazol	83657-24-3	fungicide			
241	Fenamidon	161326-34-7	fungicide	x	x	

242	Fenbuconazol	114369-43-6	fungicide		x	
243	Fosthiazat	98886-44-3	other	x	x	
244	Fuberidazol	3878-19-1	fungicide	x	x	
245	Hexaconazol	79983-71-4	fungicide			
246	Hexythiazox	78587-05-0	insecticide	x	x	
247	Indoxacarb	173584-44-6	insecticide	x	x	
248	Mandipropamid	374726-62-2	fungicide	x	x	7.60
249	Metrafenon	220899-03-6	fungicide	x	x	
250	Oxadiazon	19666-30-9	herbicide		x	
251	Proquinazid	189278-12-4	fungicide	x	x	
252	Tebufenpyrad	119168-77-3	insecticide	x	x	
253	Tetraconazol	112281-77-3	fungicide	x	x	
254	Zoxamid	156052-68-5	fungicide	x	x	
255	Hexaflumuron	86479-06-3	insecticide			
256	Neburon	555-37-3	herbicide			
257	Cyproconazol	94361-06-5	fungicide	x	x	
258	Fenarimol	60168-88-9	fungicide			
259	Iprovalicarb	140923-17-7	fungicide	x	x	189.00
260	Myclobutanil	88671-89-0	fungicide	x	x	2.40
261	Acetamiprid	135410-20-7	insecticide	x	x	0.24
262	Chlorfluazuron	71422-67-8	insecticide			
263	Cyromazin	66215-27-8	insecticide		x	
264	Etaconazol	60207-93-4	fungicide			
265	Ethidimuron	30043-49-3	herbicide			
266	Fenpyroximat	134098-61-6	insecticide	x	x	
267	Flazasulfuron	104040-78-0	herbicide	x	x	
268	Flufenoxuron	101463-69-8	insecticide			
269	Mepronil	55814-41-0	fungicide			
270	Methomyl	16752-77-5	insecticide		x	
271	Methoxyfenozid	161050-58-4	insecticide	x	x	
272	Pirimicarb-desmethyl	30614-22-3	metabolite			
273	Spirodiclofen	148477-71-8	insecticide	x	x	
274	Spiromesifen	283594-90-1	insecticide		x	
275	Tebufenozid	112410-23-8	insecticide	x	x	
276	Thiabendazol	148-79-8	fungicide	x	x	
277	Triflumizol	99387-89-0	fungicide		x	
278	Triforin	26644-46-2	fungicide			
279	Triticonazol	131983-72-7	fungicide	x	x	
280	Teflubenzuron	83121-18-0	insecticide		x	
281	Triadimefon	43121-43-3	fungicide			
282	cis-Chlordan	5103-71-9	insecticide			
283	Monuron	150-68-5	herbicide			
284	Propachlor	1918-16-7	herbicide			
285	Fluazifop-butyl	69806-50-4	herbicide			
286	Carbetamid	16118-49-3	herbicide		x	
287	Propetamphos	31218-83-4	insecticide			
288	Triallat	2303-17-5	herbicide		x	
289	Dichlobenil	1194-65-6	herbicide			
290	Propham	122-42-9	herbicide			
291	Endosulfansulfat	1031-07-8	metabolite			
292	Beflubutamid	113614-08-7	herbicide	x	x	
293	Flurochloridon	61213-25-0	herbicide		x	
294	Iodosulfuron	185119-76-0	herbicide	x	x	0.08
295	Metosulam	139528-85-1	herbicide	x	x	
296	Triclopyr	55335-06-3	herbicide	x	x	
297	Florasulam	145701-23-1	herbicide	x	x	
298	Famoxadone	131807-57-3	fungicide	x	x	
299	Folpet	133-07-3	fungicide	x	x	
300	Procymidon	32809-16-8	fungicide			

301	Thiophanat-methyl	23564-05-8	fungicide	x	x	
302	Fluometuron	2164-17-2	herbicide		x	
303	Bupirimat	41483-43-6	fungicide		x	
304	Carboxin	5234-68-4	fungicide		x	
305	Chlorantraniliprole	500008-45-7	insecticide	x	x	0.35
306	Dinotefuran	165252-70-0	insecticide			
307	Fenazaquin	120928-09-8	insecticide	x	x	
308	Fenoxycarb	72490-01-8	insecticide		x	
309	Flupyrsulfuron	150315-10-9	herbicide	x	x	
310	Foramsulfuron	173159-57-4	herbicide	x	x	0.95
311	Imazosulfuron	122548-33-8	herbicide	x	x	
312	Mesosulfuron	400852-66-6	herbicide	x	x	
313	Prothioconazol-desthio	120983-64-4	metabolite			
314	Quinoclamin	2797-51-5	herbicide	x	x	
315	Sulfosulfuron	141776-32-1	herbicide		x	
316	Triazoxid	72459-58-6	fungicide	x	x	
317	Tribenuron-methyl	101200-48-0	herbicide			
318	Ametoctradin	865318-97-4	fungicide	x	x	
319	Clodinafop	114420-56-3	herbicide	x	x	
320	Cyclanilide	113136-77-9	other			
321	Mepanipyrim	110235-47-7	fungicide	x	x	
322	Profoxydim	139001-49-3	herbicide		x	
323	Propoxycarbazone	145026-81-9	herbicide	x	x	
324	Thiencarbazon-methyl	317815-83-1	herbicide	x	x	
325	Fluopyram	658066-35-4	fungicide	x	x	5.12
326	Flutolanil	66332-96-5	fungicide	x	x	
327	Chlorthalonil-SA		metabolite			
328	Dimethachlor-CA		metabolite			
329	Dimethenamid-CA		metabolite			
330	Dimethenamid-SA		metabolite			
331	Flufenacet-SA		metabolite			
332	Metalaxyl-CA	75596-99-5	metabolite			
333	Metazachlordicarbonsäure		metabolite			
334	Metalaxyl-CA2	104390-56-9	metabolite			
335	Azoxystrobin-CA		metabolite			
336	Thiacloprid-SA		metabolite			
337	Trifloxystrobin-CA2		metabolite			
338	Clethodim	99129-21-2	herbicide	x	x	
339	Cycloxidim	101205-02-1	herbicide	x	x	
340	Imazamox	114311-32-9	herbicide	x	x	
341	Imazapic	104098-48-8	herbicide			
342	Imazaquin	81335-37-7	herbicide		x	
343	Imazethapyr	81335-77-5	herbicide			
344	Meptyldinocap	131-72-6	fungicide		x	
345	Tralkoxydim	87820-88-0	herbicide		x	
346	Saflufenacil	372137-35-4	herbicide			
347	Valifenalate	283159-90-0	fungicide	x	x	
348	Fluxapyroxad	907204-31-3	fungicide	x	x	
349	Isopyrazam	881685-58-1	fungicide	x	x	
350	Penflufen	494793-67-8	fungicide		x	
351	Pyroxsulam	422556-08-9	herbicide	x	x	
352	Fipronil	120068-37-3	insecticide		x	0.00
353	Hexachlorophen	70-30-4	other			
354	(E)7-(Z)9-Dodecadienylacetat	55774-32-8	other	x	x	
355	(Z)-9-Dodecenylacetat	16974-11-1	other	x	x	
356	1-Decanol	112-30-1	other	x	x	
357	1-Methylcyclopropen	3100-04-7	other	x	x	
358	Acequinocyl	57960-19-7	insecticide	x	x	9.00

359	alpha-Cypermethrin	67375-30-8	insecticide	x	x	
360	Aminopyralid	150114-71-9	herbicide	x	x	
361	Amisulbrom	348635-87-0	fungicide	x	x	
362	Azadirachtin (Neem)	11141-17-6	insecticide	x	x	
363	Benthiavalicarb	413615-35-7	fungicide	x	x	
364	Benzoesäure	65-85-0	fungicide	x	x	
365	Bifenazate	149877-41-8	insecticide	x	x	
366	Bixafen	581809-46-3	fungicide	x	x	0.46
367	Bromadiolon	28772-56-7	other		x	
368	Captan	133-06-2	fungicide	x	x	5.00
369	Chlorpropham	101-21-3	herbicide	x	x	
370	Chlorthalonil	1897-45-6	fungicide	x	x	
371	Cinidon-ethyl	142891-20-1	herbicide			
372	Clofentezin	74115-24-5	insecticide		x	
373	Codlemone (Codlelure)	33956-49-9	other	x	x	
374	Cymoxanil	57966-95-7	fungicide	x	x	4.40
375	Daminozid	1596-84-5	other	x	x	
376	Deiquat	2764-72-9	herbicide	x	x	
377	Desmedipham	13684-56-5	herbicide	x	x	
378	Dichlorprop-P	15165-67-0	herbicide	x	x	
379	Difenacoum	56073-07-5	other		x	
380	Dimethenamid-P	163515-14-8	herbicide	x	x	1.35
381	Dithianon	3347-22-6	fungicide	x	x	0.78
382	Dodin	2439-10-3	fungicide	x	x	5.33
383	Fenoxaprop-p-ethyl	71283-80-2	herbicide			
384	Flonicamid	158062-67-0	insecticide	x	x	310.00
385	Fluazifop-P	83066-88-0	herbicide	x	x	146.00
386	Flumioxazin	103361-09-7	herbicide	x	x	
387	Fluroxypyr-methylheptyl	81406-37-3	herbicide			
388	Fosetyl	15845-66-6	fungicide	x	x	
389	gamma-Cyhalothrin	76703-62-3	insecticide	x	x	
390	Haloxyfop-P	95977-29-0	herbicide	x	x	
391	Hymexazol	10004-44-1	fungicide	x	x	
392	Imazalil	35554-44-0	fungicide	x	x	
393	Isoxaflutole	141112-29-0	herbicide	x	x	
394	Mancozeb	8018-01-7	fungicide	x	x	0.22
395	Maneb	12427-38-2	fungicide	x	x	
396	Mepiquat	15302-91-7	other	x	x	
397	Metaflumizone	139968-49-3	insecticide	x	x	
398	Metalaxyl-M	70630-17-0	fungicide	x	x	46.00
399	Metiram	9006-42-2	fungicide	x	x	
400	Metsulfuron-methyl	74223-64-6	herbicide			
401	Milbemectin	51596-11-3	insecticide	x	x	
402	Paclobutrazol	76738-62-0	other	x	x	
403	Pelargonsäure	112-05-0	herbicide	x	x	
404	Penoxsulam	219714-96-2	herbicide	x	x	
405	Picloram	1918-02-1	herbicide	x	x	
406	Pinoxaden	243973-20-8	herbicide	x		
407	Pirimiphos-methyl	29232-93-7	insecticide	x	x	
408	Prohexadion	88805-35-0	other	x	x	
409	Propaquizafop	111479-05-1	herbicide	x	x	
410	Prosulfuron	94125-34-5	herbicide	x	x	
411	Prothioconazol	178928-70-6	fungicide	x	x	1.71
412	Pymetrozin	123312-89-0	insecticide	x	x	
413	Pyraflufen	129630-17-7	herbicide	x	x	
414	Pyridat	55512-33-9	herbicide	x	x	
415	Silthiofam	175217-20-6	fungicide	x	x	

416	Spinosad	168316-95-8	insecticide	x	x	0.06
417	Sulfurylfluorid	2699-79-8	insecticide	x	x	
418	Tembotrione	335104-84-2	herbicide	x	x	
419	Tepraloxydim	149979-41-9	herbicide	x	x	
420	Thiram	137-26-8	fungicide	x	x	0.11
421	Topramezone	210631-68-8	herbicide	x		0.90
422	Trinexapac-ethyl	95266-40-3	other	x	x	
423	Warfarin	81-81-2	other			
424	Aziprotryn	4658-28-0	herbicide			
425	Chlorsulfuron	64902-72-3	herbicide			
426	Norflurazon	27314-13-2	herbicide			
427	Primisulfuron-methyl	86209-51-0	herbicide			
428	Pyrazophos	13457-18-6	fungicide			
429	Quinalphos	13593-03-8	insecticide			
430	Secbumeton	26259-45-0	herbicide			
431	Tebutam	35256-85-0	herbicide			
432	Fluchloralin	33245-39-5	herbicide			
433	Furalaxyl	57646-30-7	fungicide			
434	Methoprotryn	841-06-5	herbicide			
435	Furmecyclox	60568-05-0	fungicide			
436	Desmethylisoproturon	34123-57-4	metabolite			
437	Metamitron-Desamino	36993-94-9	metabolite			
438	Orysastrobin	248593-16-0	fungicide			
439	Desethyl-2-hydroxyterbuthylazin	66753-06-8	metabolite			
440	Icaridinsäure		metabolite			
441	Desaminometribuzin	35045-02-4	metabolite			
442	Karbutylat	4849-32-5	herbicide			
443	Crimidin	535-89-7	other			
444	Buturon	3766-60-7	herbicide			
445	Chlorbromuron	13360-45-7	herbicide			
446	Fenoxaprop-p	113158-40-0	herbicide	x	x	
447	Fenamiphos	22224-92-6	insecticide		x	
448	Isophenphos	25311-71-1	insecticide			
449	4,4-Methoxychlor	2132-70-9	insecticide			
450	oxi-Chlordan	27304-13-8	metabolite			
451	3-Trifluormethylanilin	98-16-8	metabolite			
452	1-(3,4-Dichlorphenyl)urea	2327-02-8	metabolite			
453	1-(4-Isopropylphenyl)urea	56046-17-4	metabolite			
454	Telodrin	297-78-9	insecticide			
455	Terbumeton	33693-04-8	herbicide			
456	Nitenpyram	120738-89-8	insecticide			
457	Permethrin	52645-53-1	insecticide			
458	Quizalofop-ethyl	76578-14-8	herbicide			
459	Mefenpyr-diethyl	135591-00-3	other	x		
460	Iodosulfuron-methyl	144550-06-1	herbicide			
461	Haloxyfop-ethoxyethyl	87237-48-7	herbicide			
462	Desmethyldiuron	3567-62-2	metabolite			
463	Cloquintocet-mexyl	99607-70-2	other		x	
464	Chlorpyriphos methyl	5598-13-0	insecticide		x	
465	Ethirimol	23947-60-6	fungicide			
466	Desethylsimazin	6190-65-4	metabolite			
467	Nitrofen	1836-75-5	herbicide			
468	Thifenylsulfuron	79277-67-1	herbicide	x	x	
469	Acrinathrin	101007-06-1	insecticide		x	
470	Betacypermethrin	65731-84-2	insecticide		x	

471	4-tert. Cyclobutylhexanon	98-53-3	metabolite			
472	Pirimiphos-ethyl	23505-41-1	insecticide			
473	Pyrethrum	8003-34-7	insecticide	x	x	0.01
474	Pyridaben	96489-71-3	insecticide		x	
475	Iodosulfuron-methyl-sodium	144550-36-7	herbicide			
476	Benazolin	3813-05-6	herbicide			
477	Chloramben	133-90-4	herbicide			
478	Chlorfenac	85-34-7	herbicide			
479	Desethylsebuthylazin	37019-18-4	metabolite			
480	Prometon	1610-18-0	herbicide			
481	Atraton	1610-17-9	herbicide			
482	Terbutylazin-Metabolit SYN 545666		metabolite			
483	2-Hydroxydesethylatrazin	19988-24-0	metabolite			
484	Terbutylazin-Metabolit CGA 324007	309923-18-0	metabolite			

4 Thresholds for agricultural land use and catchment size

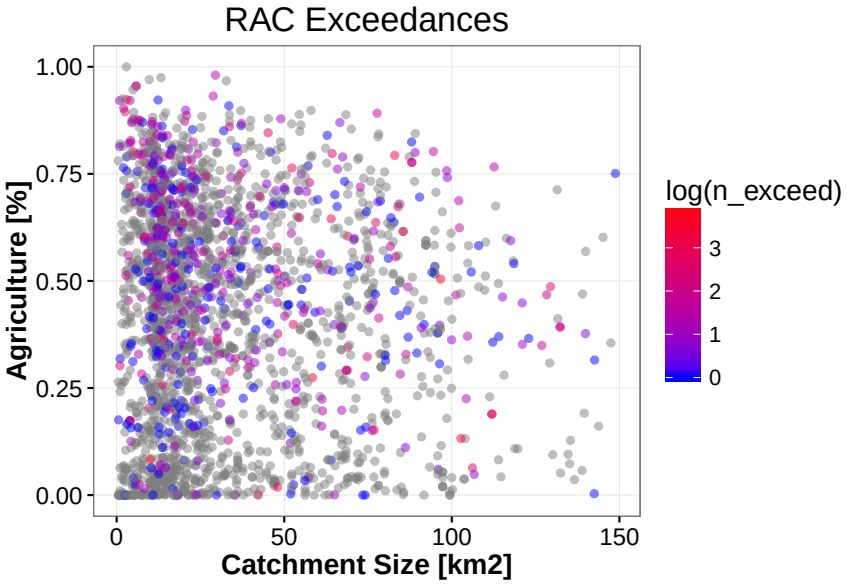

Figure S5: Raw data used for the model in equation 2 and Figure 3 of the main article. Color codes the number of RAC exceedances (on a log-scale). Grey points denote sites without any exceedance.

5 Effect of precipitation and season on RQ

Table S3: 24 pesticides for which we modelled the relationship with precipitation and seasonality. Order is the same as in Figure 5 of the articles. See Table S4 for model coefficients.

	Compound	CAS	Group	%>LOQ	no. > LOQ	total no.
1	Azoxystrobin	131860-33-8	fungicide	9.65	676	7002
2	Bentazon	25057-89-0	herbicide	19.09	2417	12660
3	Boscalid	188425-85-6	fungicide	23.24	2278	9802
4	Carbendazim	10605-21-7	fungicide	17.15	655	3819
5	Chlorpyrifos	2921-88-2	insecticide	6.38	956	14986
6	Clothianidin	210880-92-5	insecticide	6.74	158	2345
7	Diflufenican	83164-33-4	herbicide	12.71	1999	15729
8	Dimethenamid	87674-68-8	herbicide	6.17	588	9536
9	Dimoxystrobin	149961-52-4	fungicide	6.70	218	3252
10	Diuron	330-54-1	herbicide	12.24	2277	18610
11	Ethofumesat	26225-79-6	herbicide	5.11	1036	20290
12	Flufenacet	142459-58-3	herbicide	5.93	803	13549
13	Glyphosate	1071-83-6	herbicide	40.07	1412	3524
14	Imidacloprid	138261-41-3	insecticide	6.29	197	3133
15	Isoproturon	34123-59-6	herbicide	21.99	4216	19171
16	MCPA	94-74-6	herbicide	12.61	1638	12986
17	Mecoprop	93-65-2	herbicide	12.32	1569	12732
18	Metazachlor	67129-08-2	herbicide	9.67	2130	22029
19	Nicosulfuron	111991-09-4	herbicide	5.54	280	5053
20	Penconazol	66246-88-6	fungicide	5.94	297	5004
21	Propiconazol	60207-90-1	fungicide	7.29	1054	14458
22	Quinmerac	90717-03-6	herbicide	13.50	975	7223
23	Tebuconazol	107534-96-3	fungicide	6.01	1006	16735
24	Terbuthylazin	5915-41-3	herbicide	14.99	3395	22652

Table S4: Raw data for figure 5 in the main article. Bold values denote coefficients where the CI encompasses zero.

	Compound	effect	$precip_0$	$precip_{-1}$	$season_{Q2}$	$season_{Q3}$	$season_{Q4}$
1	Azoxystrobin	μ	**0.05** (0.03 - 0.06)	**0.02** (0.01 - 0.03)	**0.21** (0.02 - 0.4)	0.16 (-0.03 - 0.35)	-0.1 (-0.32 - 0.12)
2	Bentazon	μ	0 (0 - 0.01)	0 (-0.01 - 0.01)	**0.46** (0.38 - 0.54)	**0.28** (0.2 - 0.37)	-0.02 (-0.11 - 0.07)
3	Boscalid	μ	0.01 (0 - 0.01)	**0.02** (0.02 - 0.03)	**0.23** (0.14 - 0.31)	**0.13** (0.05 - 0.22)	**0.12** (0.03 - 0.22)
4	Carbendazim	μ	-0.01 (-0.02 - 0)	**0.03** (0.02 - 0.04)	**0.33** (0.16 - 0.5)	0.13 (-0.04 - 0.3)	-0.09 (-0.28 - 0.1)
5	Chlorpyrifos	μ	0.01 (0 - 0.02)	0 (-0.01 - 0.01)	**0.2** (0.1 - 0.29)	0.02 (-0.08 - 0.12)	0.06 (-0.05 - 0.17)

6	Clothianidin	μ	0 (-0.02 - 0.02)	0 (-0.02 - 0.03)	**-0.25** (-0.47 - -0.04)	-0.03 (-0.28 - 0.22)	**0.86** (0.59 - 1.12)
7	Diflufenican	μ	-0.01 (-0.02 - 0)	**0.01** (0.01 - 0.02)	**-0.45** (-0.54 - -0.37)	**-0.51** (-0.61 - -0.42)	**-0.14** (-0.22 - -0.06)
8	Dimethenamid	μ	**-0.03** (-0.04 - -0.01)	**0.03** (0.02 - 0.04)	**0.2** (0.03 - 0.37)	**0.2** (0.02 - 0.37)	-0.02 (-0.2 - 0.15)
9	Dimoxystrobin	μ	**0.03** (0.01 - 0.05)	0.02 (-0.01 - 0.05)	**0.77** (0.43 - 1.12)	**0.89** (0.5 - 1.28)	**1.17** (0.76 - 1.58)
10	Diuron	μ	0 (-0.01 - 0)	0.01 (0 - 0.01)	**0.26** (0.14 - 0.37)	**0.2** (0.09 - 0.32)	0.01 (-0.12 - 0.13)
11	Ethofumesat	μ	0.01 (0 - 0.02)	0 (-0.01 - 0.01)	**0.62** (0.46 - 0.78)	-0.04 (-0.21 - 0.14)	0.1 (-0.1 - 0.3)
12	Flufenacet	μ	0 (-0.01 - 0.01)	0 (-0.01 - 0.01)	0.02 (-0.11 - 0.16)	**0.4** (0.24 - 0.56)	0.08 (-0.01 - 0.18)
13	Glyphosate	μ	-0.01 (-0.02 - 0.01)	**0.02** (0.01 - 0.03)	**0.19** (0.01 - 0.36)	**0.55** (0.37 - 0.72)	0.17 (-0.02 - 0.36)
14	Imidacloprid	μ	0.01 (-0.01 - 0.04)	0 (-0.01 - 0.02)	**0.4** (0.14 - 0.66)	**0.57** (0.31 - 0.83)	**0.51** (0.22 - 0.81)
15	Isoproturon	μ	0 (-0.01 - 0)	**0.04** (0.03 - 0.05)	**0.23** (0.15 - 0.32)	**-0.18** (-0.28 - -0.08)	**0.46** (0.37 - 0.54)
16	MCPA	μ	0.01 (0 - 0.02)	**0.02** (0.01 - 0.02)	**0.87** (0.67 - 1.07)	**0.6** (0.39 - 0.81)	**0.44** (0.21 - 0.66)
17	Mecoprop	μ	0.01 (0 - 0.02)	0 (0 - 0.01)	**0.68** (0.54 - 0.81)	**0.5** (0.35 - 0.64)	**0.2** (0.04 - 0.35)
18	Metazachlor	μ	**-0.02** (-0.03 - -0.01)	**0.03** (0.02 - 0.04)	0.04 (-0.08 - 0.16)	**0.74** (0.64 - 0.84)	**0.24** (0.13 - 0.34)
19	Nicosulfuron	μ	-0.01 (-0.03 - 0.01)	**-0.02** (-0.04 - -0.01)	**0.93** (0.65 - 1.2)	**1.03** (0.75 - 1.31)	0.13 (-0.16 - 0.42)
20	Penconazol	μ	**0.03** (0.01 - 0.05)	0.02 (0 - 0.04)	**1.55** (1.26 - 1.84)	**1.99** (1.69 - 2.28)	**0.68** (0.37 - 0.98)
21	Propiconazol	μ	0.01 (0 - 0.02)	**0.02** (0.01 - 0.03)	**0.48** (0.34 - 0.62)	**0.38** (0.23 - 0.52)	**0.39** (0.23 - 0.54)
22	Quinmerac	μ	-0.02 (-0.03 - 0)	**0.03** (0.02 - 0.04)	-0.02 (-0.18 - 0.13)	**0.62** (0.45 - 0.78)	**0.44** (0.3 - 0.58)
23	Tebuconazol	μ	0 (-0.01 - 0.01)	**0.02** (0.01 - 0.03)	**0.21** (0.09 - 0.33)	-0.08 (-0.21 - 0.06)	0 (-0.14 - 0.14)
24	Terbuthylazin	μ	**0.01** (0.01 - 0.02)	**0.02** (0.01 - 0.02)	**0.85** (0.75 - 0.94)	**0.33** (0.23 - 0.43)	0.1 (-0.01 - 0.21)
25	Azoxystrobin	π	0 (-0.02 - 0.02)	**0.03** (0.01 - 0.06)	**1.09** (0.79 - 1.39)	**1.31** (1.01 - 1.62)	0.27 (-0.07 - 0.6)
26	Bentazon	π	0 (-0.02 - 0.02)	-0.01 (-0.02 - 0.01)	**0.71** (0.52 - 0.91)	**0.37** (0.16 - 0.58)	-0.01 (-0.23 - 0.2)
27	Boscalid	π	0 (-0.01 - 0.02)	**0.07** (0.06 - 0.09)	**0.72** (0.52 - 0.92)	**0.7** (0.49 - 0.9)	0.21 (0 - 0.42)
28	Carbendazim	π	0.01 (-0.01 - 0.04)	**0.03** (0.01 - 0.06)	**1.12** (0.81 - 1.44)	**1.38** (1.06 - 1.7)	**0.38** (0.04 - 0.72)
29	Chlorpyrifos	π	0.02 (0 - 0.04)	0.02 (0 - 0.03)	**0.54** (0.32 - 0.75)	-0.04 (-0.26 - 0.19)	-0.16 (-0.4 - 0.07)
30	Clothianidin	π	0 (-0.04 - 0.04)	0.04 (0 - 0.08)	-0.01 (-0.53 - 0.5)	**-0.74** (-1.33 - -0.16)	**-1.03** (-1.62 - -0.43)
31	Diflufenican	π	0.02 (0 - 0.03)	**0.04** (0.03 - 0.06)	**-0.59** (-0.77 - -0.42)	**-1.29** (-1.48 - -1.09)	**-0.19** (-0.36 - -0.01)
32	Dimethenamid	π	-0.01 (-0.04 - 0.01)	**0.04** (0.02 - 0.05)	**0.74** (0.45 - 1.02)	**0.65** (0.36 - 0.95)	**0.51** (0.21 - 0.82)
33	Dimoxystrobin	π	**0.05** (0.02 - 0.09)	**0.05** (0.01 - 0.08)	**0.99** (0.49 - 1.48)	0.07 (-0.5 - 0.63)	-0.17 (-0.74 - 0.4)
34	Diuron	π	**0.02** (0.01 - 0.03)	**0.04** (0.03 - 0.05)	**2.15** (1.93 - 2.36)	**2.07** (1.85 - 2.29)	**1.14** (0.91 - 1.37)

35	Ethofumesat	π	0.02 (0 - 0.03)	**0.04** (0.02 - 0.05)	**2.1** (1.85 - 2.35)	**0.85** (0.58 - 1.13)	0.15 (-0.15 - 0.46)
36	Flufenacet	π	0.02 (0 - 0.04)	**0.08** (0.07 - 0.09)	**-1.31** (-1.58 - -1.04)	**-1.71** (-2.03 - -1.39)	**0.81** (0.6 - 1.01)
37	Glyphosate	π	0.02 (0 - 0.05)	**0.08** (0.05 - 0.1)	**1.56** (1.23 - 1.89)	**2** (1.67 - 2.34)	**1.22** (0.87 - 1.57)
38	Imidacloprid	π	0 (-0.06 - 0.06)	-0.01 (-0.06 - 0.04)	**1.53** (0.84 - 2.21)	**1.65** (0.96 - 2.35)	0.58 (-0.18 - 1.34)
39	Isoproturon	π	0.01 (0 - 0.02)	**0.04** (0.03 - 0.05)	**0.59** (0.46 - 0.72)	**-0.32** (-0.46 - -0.18)	**1** (0.87 - 1.13)
40	MCPA	π	0 (-0.02 - 0.01)	**0.06** (0.04 - 0.07)	**2.47** (2.22 - 2.72)	**1.93** (1.66 - 2.19)	**0.99** (0.71 - 1.27)
41	Mecoprop	π	0.01 (0 - 0.03)	**0.06** (0.05 - 0.08)	**1.39** (1.18 - 1.6)	**1.05** (0.83 - 1.27)	**0.28** (0.05 - 0.51)
42	Metazachlor	π	0 (-0.01 - 0.01)	**0.05** (0.04 - 0.06)	**-0.44** (-0.61 - -0.26)	**0.66** (0.5 - 0.81)	**0.75** (0.59 - 0.9)
43	Nicosulfuron	π	0.04 (0 - 0.08)	**0.05** (0.02 - 0.09)	**0.79** (0.33 - 1.25)	**0.73** (0.26 - 1.2)	**0.51** (0.03 - 0.99)
44	Penconazol	π	0.03 (-0.05 - 0.11)	**0.1** (0.03 - 0.17)	**2.22** (1.37 - 3.06)	**3.58** (2.72 - 4.44)	**2.07** (1.18 - 2.95)
45	Propiconazol	π	0.01 (-0.01 - 0.03)	**0.06** (0.05 - 0.08)	**1.18** (0.91 - 1.46)	**1.07** (0.78 - 1.35)	**0.57** (0.28 - 0.87)
46	Quinmerac	π	-0.01 (-0.03 - 0.01)	**0.05** (0.04 - 0.07)	**-0.4** (-0.66 - -0.15)	**-0.29** (-0.56 - -0.02)	**1.03** (0.8 - 1.26)
47	Tebuconazol	π	**0.03** (0.01 - 0.05)	**0.03** (0.02 - 0.05)	**0.69** (0.46 - 0.92)	**0.47** (0.23 - 0.72)	0.22 (-0.04 - 0.47)
48	Terbuthylazin	π	0 (-0.01 - 0.02)	**0.05** (0.04 - 0.06)	**1.41** (1.27 - 1.55)	**1.39** (1.25 - 1.53)	**0.44** (0.29 - 0.6)

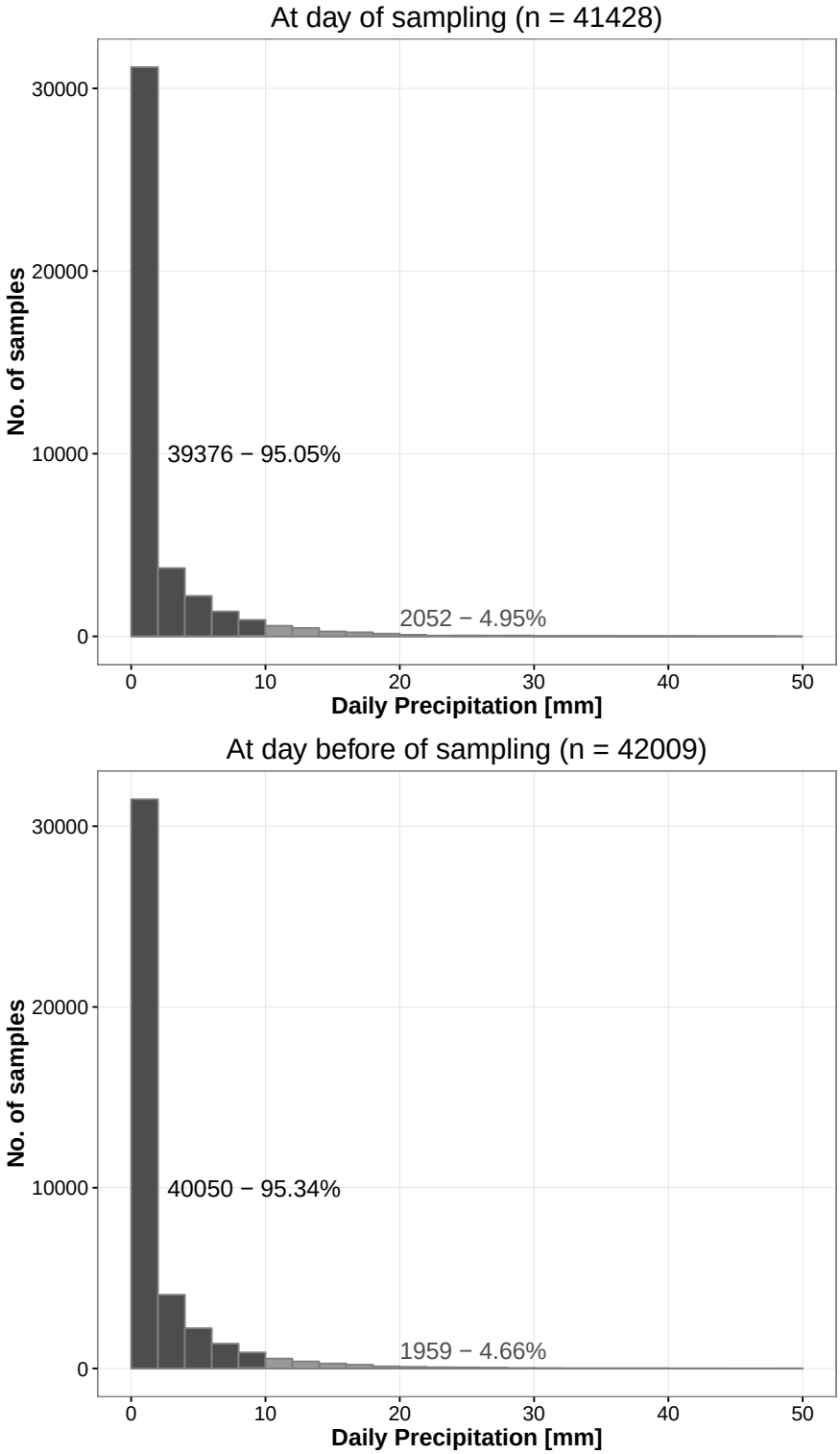

Figure S6: Distribution of precipitation at sampling occasions. top: at sampling date. bottom: at day before sampling.

6 Pesticides in small water bodies

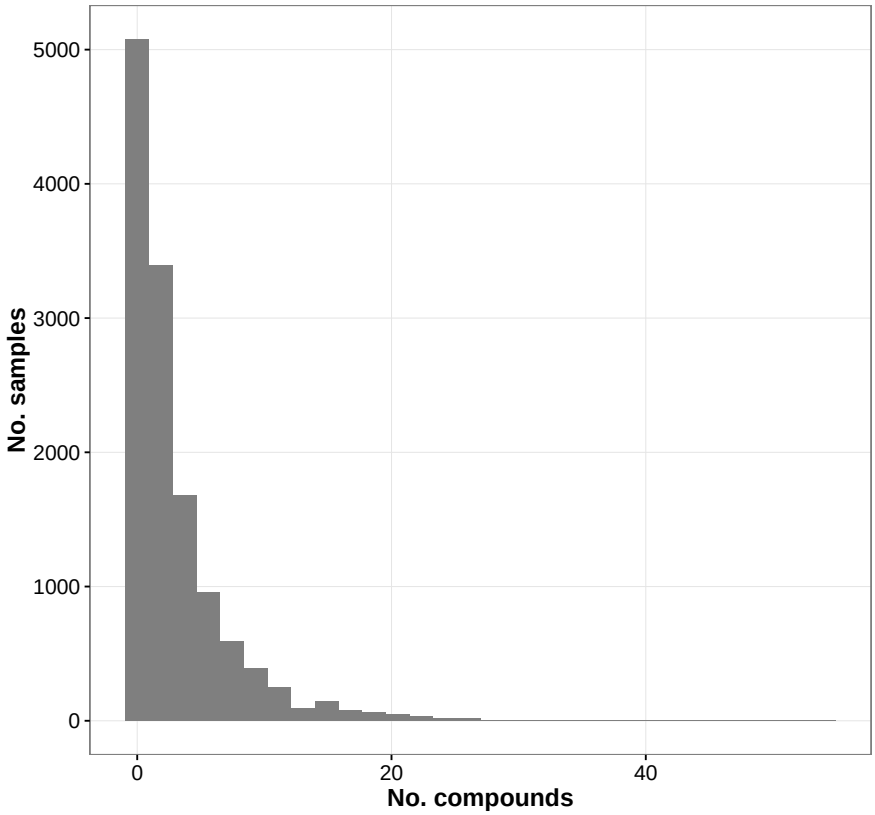

Figure S7: Distribution the number of quantified compounds in the samples from small water bodies.

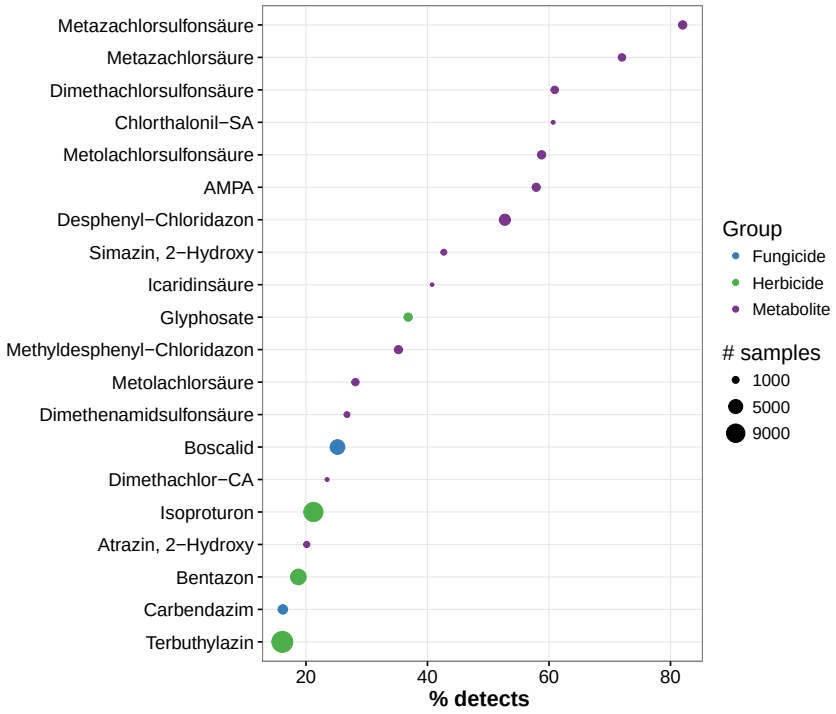

Figure S8: Proportion of samples with detects in SWB. Only Compounds with more than 100 samples and 15% of detects are show.

Bibliography

Fernández, D., Voss, K., Bundschuh, M., Zubrod, J. P., and Schäfer, R. B. (2015). Effects of fungicides on decomposer communities and litter decomposition in vineyard streams. *Science of The Total Environment*, 533:40–48.

Szöcs, E. (2016). webchem: webchem v0.1.0. DOI: 10.5281/zenodo.46930.

Voß, K., Fernández, D., and Schäfer, R. (2015). Organic matter breakdown in streams in a region of contrasting anthropogenic land use. *Science of The Total Environment*, 527-528:179–184.