Supplemental Materials for the paper: Pesticide exposure in small streams in Germany

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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).

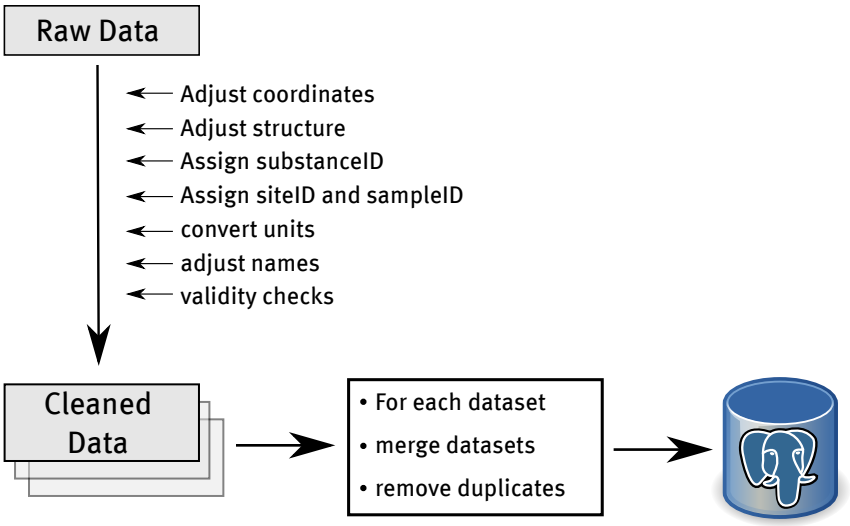

Figure S1: Overview on data cleaning steps. After cleaning data has been stored in a relational spatial PostgreSQL database.

2 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	2005-03-10	2014-10-02	7	172	98
BY	2006-04-19	2013-12-17	13	218	155
HE	2007-01-15	2014-12-18	65	2411	144
MV	2005-03-08	2014-12-17	130	1503	227
NI	2014-03-24	2014-10-13	1	7	226
NW	2005-01-18	2015-01-22	1139	8536	198
RP	2008-01-02	2013-12-18	7	341	236
SH	2005-04-26	2014-11-26	269	1380	180
SL	2005-01-03	2013-11-25	2	104	57
SN	2005-01-02	2013-12-18	606	9141	173
ST	2005-01-24	2015-03-19	30	416	88
TH	2005-06-16	2014-12-08	32	514	63
Total	2005-01-02	2015-03-19	2301	24743	478

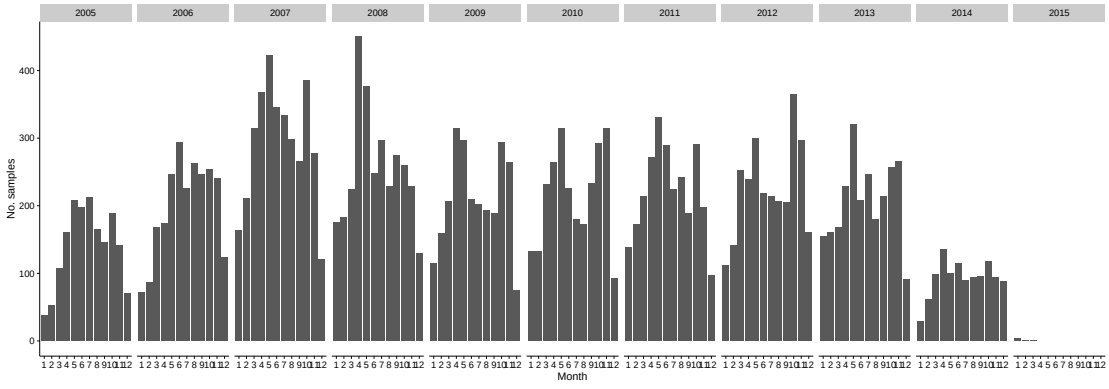

Figure S2: Number of sampling occasions per year and month.

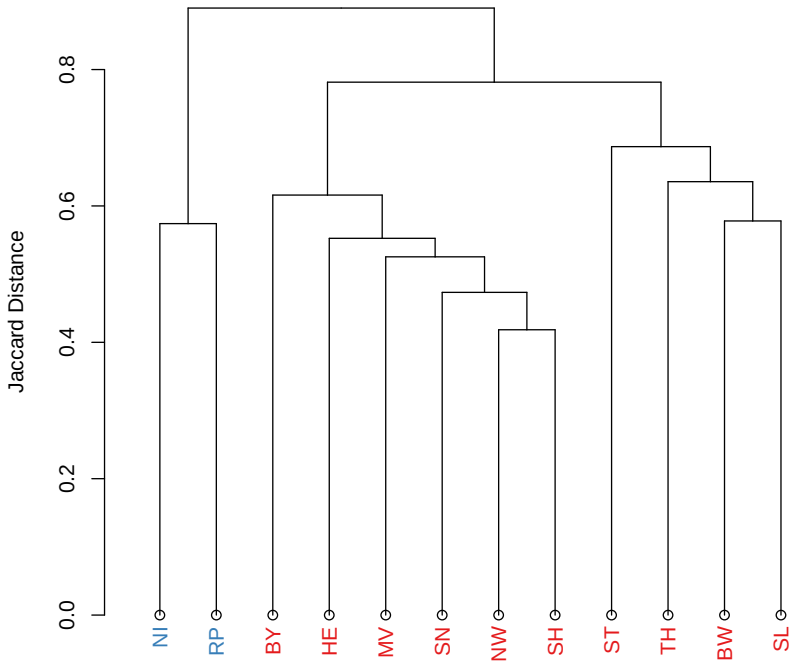

Figure S3: Complete Linkage Cluster Dendrogram of Jaccard Similarity of analysed compound spectra between federal states. Abbreviations of state names according to ISO 3166-2:DE.

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	Bromoxynil	1689-84-5	herbicide	x	x	3.30
2	Ioxynil	1689-83-4	herbicide	x		2.70
3	Bentazon	25057-89-0	herbicide	x	x	710.00
4	Methoxychlor	72-43-5	insecticide			
5	Thiometon	640-15-3	insecticide			
6	Quintozen	82-68-8	fungicide			
7	Vinclozolin	50471-44-8	fungicide			
8	Pyrazophos	13457-18-6	fungicide			
9	Quinalphos	13593-03-8	insecticide			
10	Quinoxyfen (5,7-dichloro-4-(p-fluorophenoxy)quinoline)	124495-18-7	fungicide	x	x	
11	2,4-DB	94-82-6	herbicide		x	

12	2,4,5-T	93-76-5	herbicide			
13	Alachlor	15972-60-8	herbicide			
14	Ametryn	834-12-8	herbicide			
15	Atrazin	1912-24-9	herbicide			
16	Azinphos-ethyl	2642-71-9	insecticide			
17	Bromacil	314-40-9	herbicide			
18	Chlorfenvinphos	470-90-6	insecticide			
19	Chloridazon	1698-60-8	herbicide	x	x	56.00
20	Chloroxuron	1982-47-4	herbicide			
21	Chlorpyrifos	2921-88-2	insecticide		x	0.00
22	Chlortoluron	15545-48-9	herbicide	x	x	2.30
23	Cyanazin	21725-46-2	herbicide			
24	Cypermetryn	52315-07-8	insecticide	x	x	0.00
25	Desethylatrazin	6190-65-4	metabolite			
26	Desethylterbuthylazin	30125-63-4	metabolite			
27	Desisopropylatrazin	1007-28-9	metabolite			
28	Desmetryn	1014-69-3	herbicide			
29	Diazinon	333-41-5	insecticide			
30	Dichlorprop	120-36-5	herbicide			
31	Dichlorvos	62-73-7	insecticide			
32	Dicofol	115-32-2	insecticide			
33	Diflufenican	83164-33-4	herbicide	x	x	0.03
34	Dimethoat	60-51-5	insecticide	x	x	4.00
35	Disulfoton	298-04-4	insecticide			
36	Diuron	330-54-1	herbicide		x	0.79
37	Etrimfos	38260-54-7	insecticide			
38	Fenitrothion	122-14-5	insecticide			
39	Fenoprop	93-72-1	herbicide			
40	Fenpropimorph	67564-91-4	fungicide	x	x	0.20
41	Fenthion	55-38-9	insecticide			
42	Flurtamone	96525-23-4	herbicide	x	x	0.99
43	Hexazinon	51235-04-2	herbicide			
44	Isoproturon	34123-59-6	herbicide	x	x	1.30
45	Linuron	330-55-2	herbicide		x	
46	Malathion	121-75-5	insecticide		x	
47	MCPA	94-74-6	herbicide	x	x	9.00
48	MCPB	94-81-5	herbicide		x	
49	Mecoprop	93-65-2	herbicide		x	160.00
50	Metalaxyl	57837-19-1	fungicide		x	46.00
51	Metamitron	41394-05-2	herbicide	x	x	38.00
52	Metazachlor	67129-08-2	herbicide	x	x	0.88
53	Methabenzthiazuron	18691-97-9	herbicide			
54	Methobromuron	3060-89-7	herbicide		x	2.00
55	Metolachlor	51218-45-2	herbicide			
56	Metoxuron	19937-59-8	herbicide			
57	Mevinphos	7786-34-7	insecticide			
58	Monolinuron	1746-81-2	herbicide			
59	Napropamid	15299-99-7	herbicide	x	x	6.70
60	Oxadixyl	77732-09-3	fungicide			
61	Parathion-ethyl	56-38-2	insecticide			
62	Parathion-methyl	298-00-0	insecticide			
63	Penconazol	66246-88-6	fungicide	x	x	3.20
64	Pendimethalin	40487-42-1	herbicide	x	x	0.63
65	Pirimicarb	23103-98-2	insecticide	x	x	0.09
66	Prometryn	7287-19-6	herbicide			
67	Propazin	139-40-2	herbicide			
68	Propiconazol	60207-90-1	fungicide	x	x	2.00
69	Sebuthylazin	7286-69-3	herbicide			
70	Simazin	122-34-9	herbicide			

71	Tebuconazol	107534-96-3	fungicide	x	x	0.58
72	Terbutryn	886-50-0	herbicide			
73	Terbuthylazin	5915-41-3	herbicide	x	x	1.20
74	Tolclofos-methyl	57018-04-9	fungicide	x	x	
75	Triazophos	24017-47-8	insecticide			0.03
76	Trifluralin	1582-09-8	herbicide			
77	Dicamba	1918-00-9	herbicide	x	x	180.00
78	Propetamphos	31218-83-4	insecticide			
79	Aziprotryn	4658-28-0	herbicide			
80	Norflurazon	27314-13-2	herbicide			
81	Secbumeton	26259-45-0	herbicide			
82	Tebutam	35256-85-0	herbicide			
83	2,4-D	94-75-7	herbicide	x	x	1.10
84	4,6-Dinitro-o-Cresol	534-52-1	insecticide			
85	Azinphos-methyl	86-50-0	insecticide			
86	Azoxystrobin	131860-33-8	fungicide	x	x	0.55
87	Carbofuran	1563-66-2	insecticide			
88	Epoxiconazol	133855-98-8	fungicide	x	x	0.54
89	Ethofumesat	26225-79-6	herbicide	x	x	24.00
90	Flufenacet	142459-58-3	herbicide	x	x	2.40
91	Lenacil	2164-08-1	herbicide	x	x	0.65
92	Metribuzin	21087-64-9	herbicide	x	x	0.58
93	Phenmedipham	13684-63-4	herbicide	x	x	
94	Picolinafen	137641-05-5	herbicide	x	x	0.04
95	Propanil	709-98-8	herbicide			
96	Dinoterb	1420-07-1	herbicide			
97	Dinoseb	88-85-7	herbicide			
98	Clodinafop	114420-56-3	herbicide	x	x	
99	2,6-Dichlorobenzamid	2008-58-4	metabolite			
100	Aclonifen	74070-46-5	herbicide	x	x	1.06
101	AMPA	1066-51-9	metabolite			
102	Atrazin, 2-Hydroxy	2163-68-0	metabolite			
103	Benalaxyl	71626-11-4	fungicide	x	x	20.00
104	Bensulfuron-methyl	83055-99-6	herbicide		x	
105	Bifenox	42576-02-3	herbicide	x	x	
106	Boscalid	188425-85-6	fungicide	x	x	12.50
107	Carbendazim	10605-21-7	fungicide			0.15
108	Clomazon	81777-89-1	herbicide	x	x	5.70
109	Clopyralid	1702-17-6	herbicide	x	x	1080.00
110	Clothianidin	210880-92-5	insecticide	x	x	0.01
111	Cyprodinil	121552-61-2	fungicide	x	x	0.75
112	Dimefuron	34205-21-5	herbicide			0.83
113	Dimethachlor	50563-36-5	herbicide	x	x	3.50
114	Endosulfan, alpha	959-98-8	insecticide			
115	Endosulfan, beta	33213-65-9	insecticide			
116	Fenhexamid	126833-17-8	fungicide	x	x	10.10
117	Fenpropidin	67306-00-7	fungicide	x	x	
118	Fenuron	101-42-8	herbicide			
119	Fluopicolide	239110-15-7	fungicide	x	x	
120	Fluroxypyr	69377-81-7	herbicide	x	x	16.00
121	Flusilazol	85509-19-9	fungicide			1.10
122	Glufosinat	51276-47-2	herbicide	x	x	
123	Glyphosate	1071-83-6	herbicide	x	x	100.00
124	Haloxyfop	69806-34-4	herbicide			
125	HCH, gamma (Lindan)	58-89-9	insecticide			
126	Imidacloprid	138261-41-3	insecticide	x	x	0.01
127	Kresoxim-methyl	143390-89-0	fungicide	x	x	1.00
128	Metolachlorsäure	152019-73-3	metabolite			
129	Metolachlorsulfonsäure	171118-09-5	metabolite			

130	Nicosulfuron	111991-09-4	herbicide	x	x	0.09
131	Picoxystrobin	117428-22-5	fungicide	x	x	0.60
132	Prochloraz	67747-09-5	fungicide	x	x	5.00
133	Prosulfocarb	52888-80-9	herbicide	x	x	3.80
134	Quinmerac	90717-03-6	herbicide	x	x	316.00
135	Triadimenol	55219-65-3	fungicide	x	x	3.40
136	Fluazifop	69335-91-7	herbicide			
137	Fenoxaprop	95617-09-7	herbicide			
138	Esfenvalerat	66230-04-4	insecticide	x	x	
139	Cyhalothrin (Summe Isomere)	91465-08-6	insecticide	x	x	
140	Cyfluthrin (Summe Isomere)	68359-37-5	insecticide			
141	Acifluorfen	50594-66-6	herbicide			
142	Diclofop	40843-25-2	herbicide		x	
143	Flamprop	58667-63-3	herbicide			
144	Diflubenzuron	35367-38-5	insecticide		x	
145	Difenoconazol	119446-68-3	fungicide	x	x	0.36
146	Amidosulfuron	120923-37-7	herbicide	x	x	
147	Triasulfuron	82097-50-5	herbicide	x	x	
148	Triflusulfuron	135990-29-3	herbicide	x	x	
149	Methidathion	950-37-8	insecticide			
150	Cyproconazol	94361-06-5	fungicide	x	x	
151	Ethidimuron	30043-49-3	herbicide			
152	Monuron	150-68-5	herbicide			
153	Carbetamid	16118-49-3	herbicide		x	
154	Triallat	2303-17-5	herbicide		x	
155	Dichlobenil	1194-65-6	herbicide			
156	Endosulfansulfat	1031-07-8	metabolite			
157	Flurochloridon	61213-25-0	herbicide		x	
158	Triclopyr	55335-06-3	herbicide	x	x	
159	Fenoxycarb	72490-01-8	insecticide		x	
160	Desmedipham	13684-56-5	herbicide	x	x	
161	Flumioxazin	103361-09-7	herbicide	x	x	
162	Fluroxypyr-methylheptyl	81406-37-3	herbicide			
163	Metsulfuron-methyl	74223-64-6	herbicide			
164	Picloram	1918-02-1	herbicide	x	x	
165	Propaquizafop	111479-05-1	herbicide	x	x	
166	Prosulfuron	94125-34-5	herbicide	x	x	
167	Chlorsulfuron	64902-72-3	herbicide			
168	Primisulfuron-methyl	86209-51-0	herbicide			
169	Desmethylisoproturon	34123-57-4	metabolite			
170	Desethyl-2-hydroxyterbuthylazin	66753-06-8	metabolite			
171	1-(3,4-Dichlorphenyl)urea	2327-02-8	metabolite			
172	1-(4-Isopropylphenyl)urea	56046-17-4	metabolite			
173	Terbumeton	33693-04-8	herbicide			
174	Permethrin	52645-53-1	insecticide			
175	Mefenpyr-diethyl	135591-00-3	other	x		
176	Iodosulfuron-methyl	144550-06-1	herbicide			
177	Desmethyldiuron	3567-62-2	metabolite			
178	Desethylsimazin	6190-65-4	metabolite			
179	Thifenylsulfuron	79277-67-1	herbicide	x	x	
180	Benazolin	3813-05-6	herbicide			
181	Chloramben	133-90-4	herbicide			
182	Chlorfenac	85-34-7	herbicide			

183	Desethylsebuthylazin	37019-18-4	metabolite			
184	Atraton	1610-17-9	herbicide			
185	Terbutylazin-Metabolit SYN 545666		metabolite			
186	2-Hydroxydesethylatrazin	19988-24-0	metabolite			
187	Terbutylazin-Metabolit CGA 324007	309923-18-0	metabolite			
188	Aldrin	309-00-2	insecticide			
189	Chlordan	57-74-9	insecticide			
190	Coumaphos	56-72-4	insecticide			
191	Demeton-S	126-75-0	insecticide			
192	Desphenyl-Chloridazon	6339-19-1	metabolite			
193	Dieldrin	60-57-1	insecticide			
194	Dimethomorph	110488-70-5	fungicide	x	x	5.60
195	Dimoxystrobin	149961-52-4	fungicide	x	x	0.03
196	Endrin	72-20-8	insecticide			
197	Heptachlor	76-44-8	insecticide			
198	Heptachlorepoxid	1024-57-3	metabolite			
199	Isodrin	465-73-6	insecticide			
200	Omethoat	1113-02-6	insecticide			
201	p,p-DDT	50-29-3	insecticide			
202	Pethoxamid	106700-29-2	herbicide	x	x	1.77
203	Pyraclostrobin	175013-18-0	fungicide	x	x	
204	Pyrimethanil	53112-28-0	fungicide	x	x	8.00
205	Spiroxamin	118134-30-8	fungicide	x	x	0.13
206	Thiacloprid	111988-49-9	insecticide	x	x	0.00
207	Tolylfluanid	731-27-1	fungicide			
208	trans-Chlordan	5103-74-2	insecticide			
209	Tritosulfuron	142469-14-5	herbicide	x	x	
210	Methiocarb	2032-65-7	insecticide	x	x	0.01
211	Iprodion	36734-19-7	fungicide	x	x	
212	Anthranilsäureisopropylamid	30391-89-0	metabolite			
213	Tebufenozid	112410-23-8	insecticide	x	x	
214	cis-Chlordan	5103-71-9	insecticide			
215	Propham	122-42-9	herbicide			
216	Cycloxidim	101205-02-1	herbicide	x	x	
217	Bixafen	581809-46-3	fungicide	x	x	0.46
218	Dimethenamid-P	163515-14-8	herbicide	x	x	1.35
219	Dithianon	3347-22-6	fungicide	x	x	0.78
220	Fenoxaprop-p-ethyl	71283-80-2	herbicide			
221	Isoxaflutole	141112-29-0	herbicide	x	x	
222	Prothioconazol	178928-70-6	fungicide	x	x	1.71
223	Fluchloralin	33245-39-5	herbicide			
224	Furalaxyl	57646-30-7	fungicide			
225	Methoprotryn	841-06-5	herbicide			
226	Furmecyclox	60568-05-0	fungicide			
227	Metamitron-Desamino	36993-94-9	metabolite			
228	Orysastrobin	248593-16-0	fungicide			
229	Icaridinsäure		metabolite			
230	Desaminometribuzin	35045-02-4	metabolite			
231	Fenoxaprop-p	113158-40-0	herbicide	x	x	
232	Aldicarb	116-06-3	insecticide			
233	Bifenthrin	82657-04-3	insecticide		x	
234	Demeton-S-methyl	919-86-8	insecticide			
235	Demeton-S-methylsulfon	17040-19-6	insecticide			
236	Dimethachlorsulfonsäure		metabolite			

237	Dimethenamid	87674-68-8	herbicide			1.35
238	Hexachlorbenzen	118-74-1	fungicide			
239	Metazachlorsäure	1231244-60-2	metabolite			
240	Metazachlorsulfonsäure	172960-62-2	metabolite			
241	Methyldesphenyl-Chloridazon	17254-80-7	metabolite			
242	Mirex	2385-85-5	insecticide			
243	o,p-DDE	3424-82-6	metabolite			
244	o,p-DDT	789-02-6	insecticide			
245	Oxydemeton-methyl	301-12-2	insecticide			1.10
246	p,p-DDD (p,p TDE)	72-54-8	insecticide			
247	Propamocarb	24579-73-5	fungicide	x	x	
248	Propoxur	114-26-1	insecticide			
249	Propyzamid	23950-58-5	herbicide	x	x	34.00
250	Thifensulfuron-methyl	79277-27-3	herbicide			
251	Trichlorfon	52-68-6	insecticide			
252	Sulcotrion	99105-77-8	herbicide	x	x	
253	Pyrifenox	88283-41-4	fungicide			
254	Rimsulfuron	122931-48-0	herbicide	x	x	0.46
255	Oxamyl	23135-22-0	insecticide		x	
256	Hexaconazol	79983-71-4	fungicide			
257	Tebufenpyrad	119168-77-3	insecticide	x	x	
258	Fenarimol	60168-88-9	fungicide			
259	Myclobutanil	88671-89-0	fungicide	x	x	2.40
260	Triadimefon	43121-43-3	fungicide			
261	Propachlor	1918-16-7	herbicide			
262	Fluazifop-butyl	69806-50-4	herbicide			
263	Procymidon	32809-16-8	fungicide			
264	Fluometuron	2164-17-2	herbicide		x	
265	Bupirimat	41483-43-6	fungicide		x	
266	Mepanipyrim	110235-47-7	fungicide	x	x	
267	Chlorthalonil-SA		metabolite			
268	Dimethachlor-CA		metabolite			
269	Chlorpropham	101-21-3	herbicide	x	x	
270	Fluazifop-P	83066-88-0	herbicide	x	x	146.00
271	Buturon	3766-60-7	herbicide			
272	Isophenphos	25311-71-1	insecticide			
273	Telodrin	297-78-9	insecticide			
274	Quizalofop-ethyl	76578-14-8	herbicide			
275	Chlorpyriphos methyl	5598-13-0	insecticide		x	
276	Ethirimol	23947-60-6	fungicide			
277	Nitrofen	1836-75-5	herbicide			
278	Betacypermethrin	65731-84-2	insecticide		x	
279	Pirimiphos-ethyl	23505-41-1	insecticide			
280	Pyrethrum	8003-34-7	insecticide	x	x	0.01
281	Pyridaben	96489-71-3	insecticide		x	
282	Ethofenprox	80844-07-1	insecticide	x	x	
283	Fluquinconazole	136426-54-5	fungicide	x	x	0.80
284	Methamidophos	10265-92-6	insecticide			2.60
285	Trifloxystrobin	141517-21-7	fungicide	x	x	0.09
286	Tefluthrin	79538-32-2	insecticide	x	x	
287	Deltamethrin	52918-63-5	insecticide	x	x	
288	Dichlofluanid	1085-98-9	fungicide			
289	Fludioxonil	131341-86-1	fungicide	x	x	0.50
290	Indoxacarb	173584-44-6	insecticide	x	x	
291	Folpet	133-07-3	fungicide	x	x	
292	alpha-Cypermethrin	67375-30-8	insecticide	x	x	
293	Captan	133-06-2	fungicide	x	x	5.00
294	Chlorthalonil	1897-45-6	fungicide	x	x	

295	Fenamiphos	22224-92-6	insecticide		x	
296	Acrinathrin	101007-06-1	insecticide		x	
297	4-tert. Cyclobutylhexanon	98-53-3	metabolite			
298	Avermectin B1a	71751-41-2	insecticide	x	x	
299	Cyazofamid	120116-88-3	fungicide	x	x	
300	Fluoxastrobin	361377-29-9	fungicide	x	x	
301	Isoxaben	82558-50-7	herbicide	x	x	
302	Metaldehyd	108-62-3	other	x	x	
303	Metconazol	125116-23-6	fungicide	x	x	
304	Pencycuron	66063-05-6	fungicide	x	x	
305	Thiamethoxam	153719-23-4	insecticide	x	x	0.04
306	tau-Fluvalinat	102851-06-9	insecticide	x	x	0.03
307	Mesotrion	104206-82-8	herbicide	x	x	
308	Chlormequat	7003-89-6	other	x	x	
309	Quizalofop	76578-12-6	herbicide			
310	Fluazinam	79622-59-6	fungicide	x	x	0.26
311	Carfentrazone-ethyl	128639-02-1	herbicide	x	x	0.31
312	Cyflufenamid	180409-60-3	fungicide	x	x	
313	Fenamidon	161326-34-7	fungicide	x	x	
314	Fosthiazat	98886-44-3	other	x	x	
315	Fuberidazol	3878-19-1	fungicide	x	x	
316	Hexythiazox	78587-05-0	insecticide	x	x	
317	Mandipropamid	374726-62-2	fungicide	x	x	7.60
318	Metrafenon	220899-03-6	fungicide	x	x	
319	Proquinazid	189278-12-4	fungicide	x	x	
320	Tetraconazol	112281-77-3	fungicide	x	x	
321	Zoxamid	156052-68-5	fungicide	x	x	
322	Iprovalicarb	140923-17-7	fungicide	x	x	189.00
323	Acetamiprid	135410-20-7	insecticide	x	x	0.24
324	Fenpyroximat	134098-61-6	insecticide	x	x	
325	Flazasulfuron	104040-78-0	herbicide	x	x	
326	Methoxyfenozid	161050-58-4	insecticide	x	x	
327	Spirodiclofen	148477-71-8	insecticide	x	x	
328	Thiabendazol	148-79-8	fungicide	x	x	
329	Triticonazol	131983-72-7	fungicide	x	x	
330	Beflubutamid	113614-08-7	herbicide	x	x	
331	Iodosulfuron	185119-76-0	herbicide	x	x	0.08
332	Metosulam	139528-85-1	herbicide	x	x	
333	Florasulam	145701-23-1	herbicide	x	x	
334	Famoxadone	131807-57-3	fungicide	x	x	
335	Thiophanat-methyl	23564-05-8	fungicide	x	x	
336	Chlorantraniliprole	500008-45-7	insecticide	x	x	0.35
337	Fenazaquin	120928-09-8	insecticide	x	x	
338	Flupyrsulfuron	150315-10-9	herbicide	x	x	
339	Foramsulfuron	173159-57-4	herbicide	x	x	0.95
340	Imazosulfuron	122548-33-8	herbicide	x	x	
341	Mesosulfuron	400852-66-6	herbicide	x	x	
342	Quinoclamin	2797-51-5	herbicide	x	x	
343	Sulfosulfuron	141776-32-1	herbicide		x	
344	Triazoxid	72459-58-6	fungicide	x	x	
345	Tribenuron-methyl	101200-48-0	herbicide			
346	Ametoctradin	865318-97-4	fungicide	x	x	
347	Propoxycarbazone	145026-81-9	herbicide	x	x	
348	Thiencarbazon-methyl	317815-83-1	herbicide	x	x	
349	Flutolanil	66332-96-5	fungicide	x	x	
350	Clethodim	99129-21-2	herbicide	x	x	
351	Imazamox	114311-32-9	herbicide	x	x	
352	Pyroxsulam	422556-08-9	herbicide	x	x	

353	(E)7-(Z)9-Dodecadienylacetat	55774-32-8	other	x	x	
354	(Z)-9-Dodecenylacetat	16974-11-1	other	x	x	
355	1-Decanol	112-30-1	other	x	x	
356	1-Methylcyclopropen	3100-04-7	other	x	x	
357	Acequinocyl	57960-19-7	insecticide	x	x	9.00
358	Aminopyralid	150114-71-9	herbicide	x	x	
359	Amisulbrom	348635-87-0	fungicide	x	x	
360	Azadirachtin (Neem)	11141-17-6	insecticide	x	x	
361	Benthiavalicarb	413615-35-7	fungicide	x	x	
362	Benzoesäure	65-85-0	fungicide	x	x	
363	Bifenazate	149877-41-8	insecticide	x	x	
364	Bromadiolon	28772-56-7	other		x	
365	Cinidon-ethyl	142891-20-1	herbicide			
366	Clofentezin	74115-24-5	insecticide		x	
367	Codlemone (Codlelure)	33956-49-9	other	x	x	
368	Cymoxanil	57966-95-7	fungicide	x	x	4.40
369	Daminozid	1596-84-5	other	x	x	
370	Deiquat	2764-72-9	herbicide	x	x	
371	Dichlorprop-P	15165-67-0	herbicide	x	x	
372	Difenacoum	56073-07-5	other		x	
373	Dodin	2439-10-3	fungicide	x	x	5.33
374	Flonicamid	158062-67-0	insecticide	x	x	310.00
375	Fosetyl	15845-66-6	fungicide	x	x	
376	gamma-Cyhalothrin	76703-62-3	insecticide	x	x	
377	Haloxyfop-P	95977-29-0	herbicide	x	x	
378	Hymexazol	10004-44-1	fungicide	x	x	
379	Imazalil	35554-44-0	fungicide	x	x	
380	Mancozeb	8018-01-7	fungicide	x	x	0.22
381	Maneb	12427-38-2	fungicide	x	x	
382	Mepiquat	15302-91-7	other	x	x	
383	Metaflumizone	139968-49-3	insecticide	x	x	
384	Metalaxyl-M	70630-17-0	fungicide	x	x	46.00
385	Metiram	9006-42-2	fungicide	x	x	
386	Milbemectin	51596-11-3	insecticide	x	x	
387	Paclobutrazol	76738-62-0	other	x	x	
388	Pelargonsäure	112-05-0	herbicide	x	x	
389	Penoxsulam	219714-96-2	herbicide	x	x	
390	Pinoxaden	243973-20-8	herbicide	x		
391	Pirimiphos-methyl	29232-93-7	insecticide	x	x	
392	Prohexadion	88805-35-0	other	x	x	
393	Pymetrozin	123312-89-0	insecticide	x	x	
394	Pyraflufen	129630-17-7	herbicide	x	x	
395	Pyridat	55512-33-9	herbicide	x	x	
396	Silthiofam	175217-20-6	fungicide	x	x	
397	Spinosad	168316-95-8	insecticide	x	x	0.06
398	Sulfurylfluorid	2699-79-8	insecticide	x	x	
399	Tembotrione	335104-84-2	herbicide	x	x	
400	Tepraloxydim	149979-41-9	herbicide	x	x	
401	Thiram	137-26-8	fungicide	x	x	0.11
402	Topramezone	210631-68-8	herbicide	x		0.90
403	Trinexapac-ethyl	95266-40-3	other	x	x	
404	Warfarin	81-81-2	other			
405	1,3-cis-Dichlorpropen	10061-01-5	other			
406	1,3-trans-Dichlorpropen	10061-02-6	other			
407	Bromocyclen	1715-40-8	insecticide			
408	Heptenophos	23560-59-0	insecticide			

409	p,p-DDE	72-55-9	metabolite			
410	Clodinafop-propargyl	105512-06-9	herbicide			
411	Neburon	555-37-3	herbicide			
412	Metalaxyl-CA2	104390-56-9	metabolite			
413	Thiacloprid-SA		metabolite			
414	Karbutylat	4849-32-5	herbicide			
415	Crimidin	535-89-7	other			
416	Chlorbromuron	13360-45-7	herbicide			
417	oxi-Chlordan	27304-13-8	metabolite			
418	Nitenpyram	120738-89-8	insecticide			
419	2,4-Dichlorphenol	120-83-2	metabolite			
420	2,4,6-Trichlorphenol	88-06-2	metabolite			
421	Demeton-O	298-03-3	insecticide			
422	Chlorfluazuron	71422-67-8	insecticide			
423	Cyromazin	66215-27-8	insecticide		x	
424	Carboxin	5234-68-4	fungicide		x	
425	Dinotefuran	165252-70-0	insecticide			
426	Prothioconazol-desthio	120983-64-4	metabolite			
427	Cyclanilide	113136-77-9	other			
428	Profoxydim	139001-49-3	herbicide		x	
429	Fluopyram	658066-35-4	fungicide	x	x	5.12
430	Dimethenamid-CA		metabolite			
431	Dimethenamid-SA		metabolite			
432	Flufenacet-SA		metabolite			
433	Metalaxyl-CA	75596-99-5	metabolite			
434	Metazachlordicarbonsäure		metabolite			
435	Saflufenacil	372137-35-4	herbicide			
436	Valifenalate	283159-90-0	fungicide	x	x	
437	Fluxapyroxad	907204-31-3	fungicide	x	x	
438	Isopyrazam	881685-58-1	fungicide	x	x	
439	Penflufen	494793-67-8	fungicide		x	
440	Fipronil	120068-37-3	insecticide		x	0.00
441	Hexachlorophen	70-30-4	other			
442	Flutriafol	76674-21-0	fungicide		x	
443	Kresoximsäure		metabolite			
444	Metsulfuron	79510-48-8	herbicide	x	x	
445	Triflumuron	64628-44-0	insecticide		x	
446	Cycloat	1134-23-2	herbicide			
447	Diniconazol	83657-24-3	fungicide			
448	Hexaflumuron	86479-06-3	insecticide			
449	Oxadiazon	19666-30-9	herbicide		x	
450	Etaconazol	60207-93-4	fungicide			
451	Flufenoxuron	101463-69-8	insecticide			
452	Mepronil	55814-41-0	fungicide			
453	Methomyl	16752-77-5	insecticide		x	
454	Pirimicarb-desmethyl	30614-22-3	metabolite			
455	Spiromesifen	283594-90-1	insecticide		x	
456	Triflumizol	99387-89-0	fungicide		x	
457	Triforin	26644-46-2	fungicide			
458	Teflubenzuron	83121-18-0	insecticide		x	
459	Azoxystrobin-CA		metabolite			
460	Trifloxystrobin-CA2		metabolite			
461	Imazapic	104098-48-8	herbicide			
462	Imazaquin	81335-37-7	herbicide		x	
463	Imazethapyr	81335-77-5	herbicide			
464	Meptyldinocap	131-72-6	fungicide		x	
465	Tralkoxydim	87820-88-0	herbicide		x	
466	Fluazifop-P-butyl	79241-46-6	herbicide			7.70
467	Phoxim	14816-18-3	insecticide			0.01

468	Haloxyfop-ethoxyethyl	87237-48-7	herbicide		
469	Cloquintocet-mexyl	99607-70-2	other		x
470	3-Hydroxy Carbofuran	16655-82-6	metabolite		
471	Acetochlor	34256-82-1	herbicide		
472	Acetochlorsäure	194992-44-4	metabolite		
473	Acetochlorsulfonsäure	187022-11-3	metabolite		
474	Dimethachlorsäure		metabolite		
475	Dimethenamidsulfonsäure		metabolite		
476	Simazin, 2-Hydroxy	2599-11-3	metabolite		
477	Tribenuron	106040-48-6	herbicide	x	x
478	Iodosulfuron-methyl-sodium	144550-36-7	herbicide		

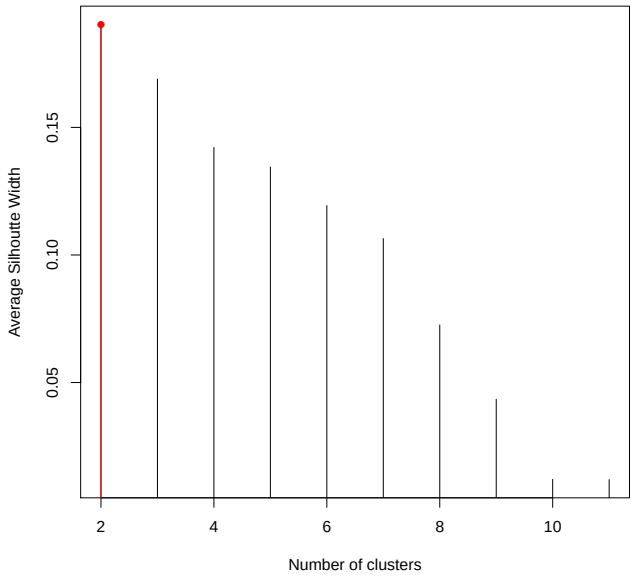

Figure S4: Average silhouette width for different cluster sizes. Two clusters showed maximum silhouette width.

3 Thresholds for agricultural land use and catchment size

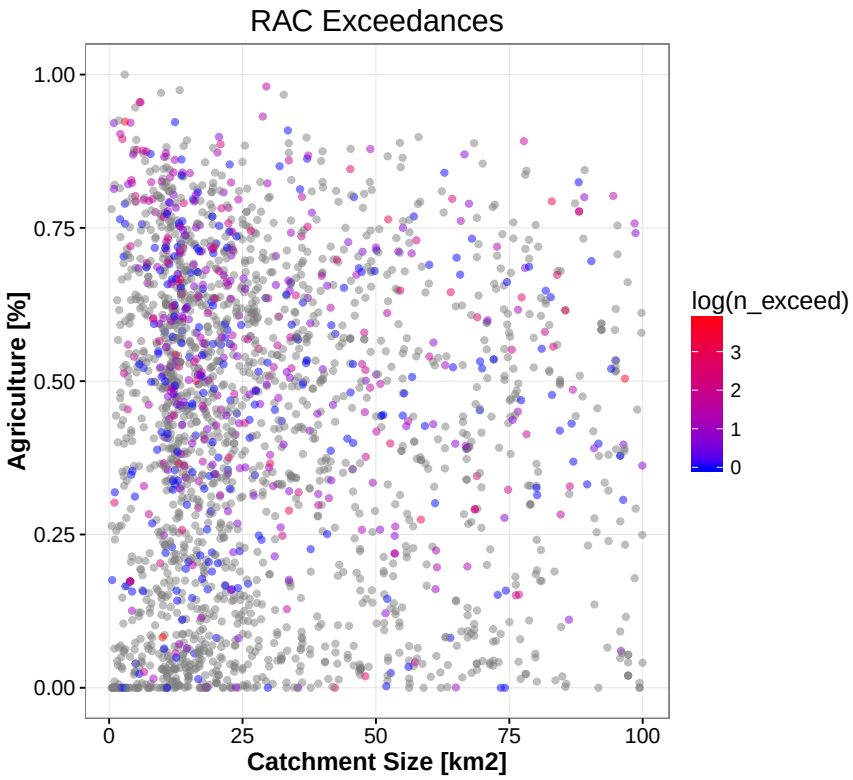

Figure S5: Raw data used for the model in equation 2 and Figure 3 of the main article. Color codes the number of RAC exceedances (on a log-scale). Grey points denote sites without any exceedance.

4 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	9.58	644	6723
2	Bentazon	25057-89-0	herbicide	19.43	2313	11905
3	Boscalid	188425-85-6	fungicide	23.00	2175	9455
4	Carbendazim	10605-21-7	fungicide	16.10	582	3615
5	Chlorpyrifos	2921-88-2	insecticide	6.17	865	14026
6	Clothianidin	210880-92-5	insecticide	6.30	141	2237
7	Diflufenican	83164-33-4	herbicide	12.63	1867	14784
8	Dimethenamid	87674-68-8	herbicide	6.14	563	9168
9	Dimoxystrobin	149961-52-4	fungicide	6.83	216	3164
10	Diuron	330-54-1	herbicide	12.07	2138	17708
11	Ethofumesat	26225-79-6	herbicide	5.10	998	19552
12	Flufenacet	142459-58-3	herbicide	5.97	772	12923
13	Glyphosate	1071-83-6	herbicide	40.73	1389	3410
14	Imidacloprid	138261-41-3	insecticide	5.88	176	2992
15	Isoproturon	34123-59-6	herbicide	21.84	3984	18239
16	MCPA	94-74-6	herbicide	12.81	1567	12237
17	Mecoprop	93-65-2	herbicide	12.21	1463	11984
18	Metazachlor	67129-08-2	herbicide	9.23	1930	20907
19	Nicosulfuron	111991-09-4	herbicide	5.33	263	4934
20	Propiconazol	60207-90-1	fungicide	5.67	772	13622
21	Quinmerac	90717-03-6	herbicide	13.46	939	6974
22	Tebuconazol	107534-96-3	fungicide	6.08	968	15924
23	Terbuthylazin	5915-41-3	herbicide	14.59	3142	21540

Table S4: Coefficients and CI from per compound models. Bold values denote coefficients where the CI for precipitation encompasses zero. Coefficients are on the link scale (log for μ and logit for ν).

	Compound	effect	*log precip*$_0$	*log precip*$_{-1}$	Quarter 1	Quarter 2	Quarter 3	Quarter 4
1	Azoxystrobin	μ	**0.23**	0.04	-3.39	-3.02	-3.16	-3.47
			(0.15 - 0.31)	(-0.03 - 0.12)	(-3.56 - -3.22)	(-3.14 - -2.89)	(-3.29 - -3.03)	(-3.63 - -3.3)
2	Bentazon	μ	-0.03	0.02	-9.74	-9.25	-9.42	-9.74
			(-0.07 - 0)	(-0.02 - 0.05)	(-9.81 - -9.67)	(-9.31 - -9.2)	(-9.48 - -9.36)	(-9.81 - -9.68)
3	Boscalid	μ	**0.06**	**0.1**	-6.72	-6.42	-6.51	-6.58
			(0.02 - 0.1)	(0.06 - 0.13)	(-6.79 - -6.64)	(-6.49 - -6.36)	(-6.58 - -6.45)	(-6.65 - -6.5)
4	Carbendazim	μ	**-0.1**	**0.16**	-2.42	-1.95	-2.11	-2.32
			(-0.16 - -0.03)	(0.09 - 0.22)	(-2.58 - -2.27)	(-2.05 - -1.84)	(-2.22 - -2)	(-2.46 - -2.18)
5	Chlorpyrifos	μ	**0.08**	-0.03	0.95	1.1	1	1.05
			(0.04 - 0.13)	(-0.08 - 0.01)	(0.88 - 1.03)	(1.03 - 1.17)	(0.93 - 1.08)	(0.96 - 1.14)

6	Clothianidin	μ	0.08	-0.1	0.94	0.67	1.02	1.55
			(-0.04 - 0.19)	(-0.21 - 0.02)	(0.77 - 1.12)	(0.49 - 0.84)	(0.8 - 1.25)	(1.32 - 1.78)
7	Diflufenican	μ	-0.02	**0.05**	-0.56	-1.01	-1.08	-0.71
			(-0.06 - 0.02)	(0.02 - 0.09)	(-0.62 - -0.5)	(-1.07 - -0.94)	(-1.16 - -1)	(-0.77 - -0.65)
8	Dimethenamid	μ	**-0.1**	0.05	-4.01	-3.79	-3.72	-4.02
			(-0.17 - -0.03)	(-0.01 - 0.12)	(-4.16 - -3.86)	(-3.89 - -3.68)	(-3.84 - -3.61)	(-4.14 - -3.9)
9	Dimoxystrobin	μ	**0.35**	0.02	-1.17	-0.42	-0.07	-0.02
			(0.2 - 0.5)	(-0.15 - 0.19)	(-1.44 - -0.89)	(-0.64 - -0.2)	(-0.39 - 0.25)	(-0.35 - 0.31)
10	Diuron	μ	0	**0.07**	-2.72	-2.43	-2.48	-2.64
			(-0.03 - 0.03)	(0.04 - 0.1)	(-2.83 - -2.61)	(-2.47 - -2.39)	(-2.53 - -2.44)	(-2.71 - -2.58)
11	Ethofumesat	μ	**0.12**	0.01	-6.11	-5.49	-6.18	-6.1
			(0.06 - 0.17)	(-0.05 - 0.06)	(-6.27 - -5.96)	(-5.56 - -5.42)	(-6.29 - -6.08)	(-6.24 - -5.95)
12	Flufenacet	μ	0.03	**0.05**	-3.71	-3.7	-3.29	-3.63
			(-0.02 - 0.08)	(0.01 - 0.1)	(-3.79 - -3.62)	(-3.81 - -3.59)	(-3.44 - -3.15)	(-3.68 - -3.57)
13	Glyphosate	μ	-0.04	**0.14**	-6.3	-6.08	-5.73	-6.11
			(-0.09 - 0.01)	(0.09 - 0.19)	(-6.46 - -6.13)	(-6.16 - -6)	(-5.8 - -5.66)	(-6.21 - -6.01)
14	Imidacloprid	μ	0	-0.01	0.61	1.15	1.4	1.24
			(-0.08 - 0.09)	(-0.09 - 0.07)	(0.33 - 0.88)	(1.02 - 1.27)	(1.28 - 1.53)	(1.06 - 1.42)
15	Isoproturon	μ	0.02	**0.21**	-3.29	-3.01	-3.43	-2.79
			(-0.02 - 0.05)	(0.17 - 0.24)	(-3.37 - -3.22)	(-3.06 - -2.96)	(-3.5 - -3.35)	(-2.84 - -2.73)
16	MCPA	μ	0.04	**0.09**	-5.07	-4.25	-4.48	-4.7
			(-0.01 - 0.09)	(0.04 - 0.14)	(-5.27 - -4.87)	(-4.32 - -4.19)	(-4.57 - -4.4)	(-4.81 - -4.58)
17	Mecoprop	μ	0.04	**0.05**	-8.36	-7.59	-7.77	-8.07
			(-0.01 - 0.09)	(0.01 - 0.1)	(-8.49 - -8.22)	(-7.65 - -7.52)	(-7.85 - -7.69)	(-8.18 - -7.97)
18	Metazachlor	μ	**-0.07**	**0.09**	-2.97	-2.94	-2.21	-2.77
			(-0.12 - -0.02)	(0.04 - 0.13)	(-3.06 - -2.88)	(-3.04 - -2.85)	(-2.28 - -2.14)	(-2.84 - -2.7)
19	Nicosulfuron	μ	**0.23**	**-0.28**	-0.98	-0.2	-0.07	-0.97
			(0.12 - 0.34)	(-0.39 - -0.18)	(-1.22 - -0.74)	(-0.36 - -0.03)	(-0.25 - 0.11)	(-1.16 - -0.78)
20	Propiconazol	μ	**0.08**	0.01	-3.99	-3.63	-3.82	-3.63
			(0.02 - 0.14)	(-0.05 - 0.07)	(-4.15 - -3.83)	(-3.71 - -3.55)	(-3.91 - -3.72)	(-3.74 - -3.53)
21	Quinmerac	μ	0.02	0.05	-9.08	-9.12	-8.46	-8.64
			(-0.05 - 0.09)	(-0.01 - 0.12)	(-9.19 - -8.96)	(-9.24 - -9)	(-8.59 - -8.33)	(-8.72 - -8.55)
22	Tebuconazol	μ	-0.01	**0.09**	-2.17	-1.93	-2.2	-2.15
			(-0.06 - 0.03)	(0.04 - 0.14)	(-2.28 - -2.06)	(-2 - -1.86)	(-2.28 - -2.11)	(-2.24 - -2.06)
23	Terbuthylazin	μ	**0.09**	**0.11**	-3.65	-2.78	-3.25	-3.52
			(0.06 - 0.13)	(0.08 - 0.15)	(-3.73 - -3.56)	(-2.84 - -2.73)	(-3.3 - -3.19)	(-3.59 - -3.44)
24	Azoxystrobin	ν	0	**0.24**	-3.5	-2.33	-2.14	-3.2
			(-0.13 - 0.13)	(0.11 - 0.37)	(-3.76 - -3.25)	(-2.54 - -2.13)	(-2.36 - -1.92)	(-3.45 - -2.95)
25	Bentazon	ν	0	0.05	-2.26	-1.53	-1.88	-2.25
			(-0.08 - 0.08)	(-0.03 - 0.13)	(-2.44 - -2.09)	(-1.65 - -1.4)	(-2.02 - -1.74)	(-2.4 - -2.11)
26	Boscalid	ν	-0.01	**0.45**	-1.99	-1.22	-1.24	-1.81
			(-0.1 - 0.08)	(0.37 - 0.54)	(-2.16 - -1.82)	(-1.36 - -1.07)	(-1.38 - -1.09)	(-1.96 - -1.65)
27	Carbendazim	ν	0.09	**0.19**	-2.72	-1.49	-1.26	-2.31
			(-0.04 - 0.22)	(0.06 - 0.32)	(-3 - -2.44)	(-1.69 - -1.28)	(-1.48 - -1.04)	(-2.56 - -2.06)
28	Chlorpyrifos	ν	**0.11**	0.1	-3.27	-2.63	-3.22	-3.42
			(0.01 - 0.21)	(0 - 0.19)	(-3.45 - -3.1)	(-2.79 - -2.48)	(-3.39 - -3.05)	(-3.61 - -3.23)
29	Clothianidin	ν	-0.05	0.19	-2.66	-2.58	-3.19	-3.93
			(-0.3 - 0.2)	(-0.07 - 0.44)	(-3.06 - -2.26)	(-2.97 - -2.19)	(-3.69 - -2.69)	(-4.46 - -3.41)
30	Diflufenican	ν	0.06	**0.26**	-1.89	-2.45	-3.14	-2.09
			(-0.02 - 0.14)	(0.17 - 0.34)	(-2.03 - -1.75)	(-2.59 - -2.31)	(-3.3 - -2.98)	(-2.22 - -1.95)
31	Dimethenamid	ν	-0.04	**0.22**	-3.44	-2.7	-2.79	-2.99
			(-0.16 - 0.08)	(0.11 - 0.34)	(-3.69 - -3.2)	(-2.88 - -2.51)	(-2.98 - -2.59)	(-3.19 - -2.78)
32	Dimoxystrobin	ν	0.19	**0.23**	-3.37	-2.25	-3.14	-3.58
			(-0.02 - 0.41)	(0.01 - 0.46)	(-3.78 - -2.96)	(-2.58 - -1.91)	(-3.55 - -2.72)	(-4.02 - -3.15)
33	Diuron	ν	0.05	**0.28**	-3.88	-1.67	-1.74	-2.72
			(-0.01 - 0.12)	(0.22 - 0.35)	(-4.09 - -3.67)	(-1.76 - -1.58)	(-1.84 - -1.63)	(-2.85 - -2.6)
34	Ethofumesat	ν	0.09	**0.21**	-4.39	-2.23	-3.49	-4.23
			(-0.01 - 0.18)	(0.12 - 0.3)	(-4.63 - -4.16)	(-2.35 - -2.11)	(-3.66 - -3.32)	(-4.44 - -4.01)

35	Flufenacet	ν	**0.16** (0.06 - 0.27)	**0.59** (0.49 - 0.69)	-2.57 (-2.75 - -2.39)	-3.8 (-4.01 - -3.58)	-4.17 (-4.44 - -3.89)	-1.76 (-1.88 - -1.64)
36	Glyphosate	ν	0.11 (0 - 0.23)	**0.29** (0.18 - 0.4)	-1.79 (-2.09 - -1.48)	-0.12 (-0.3 - 0.05)	0.34 (0.17 - 0.51)	-0.53 (-0.73 - -0.32)
37	Imidacloprid	ν	-0.01 (-0.26 - 0.25)	-0.1 (-0.34 - 0.15)	-4.68 (-5.35 - -4)	-3.04 (-3.41 - -2.68)	-2.83 (-3.21 - -2.45)	-4.07 (-4.56 - -3.58)
38	Isoproturon	ν	0.04 (-0.02 - 0.09)	**0.31** (0.25 - 0.36)	-1.82 (-1.93 - -1.7)	-1.19 (-1.27 - -1.12)	-2.11 (-2.22 - -2.01)	-0.8 (-0.88 - -0.72)
39	MCPA	ν	-0.06 (-0.13 - 0.02)	**0.35** (0.28 - 0.42)	-3.79 (-4.04 - -3.54)	-1.27 (-1.37 - -1.18)	-1.81 (-1.93 - -1.68)	-2.77 (-2.92 - -2.62)
40	Mecoprop	ν	0.07 (-0.01 - 0.15)	**0.35** (0.27 - 0.42)	-3.04 (-3.23 - -2.84)	-1.56 (-1.67 - -1.45)	-1.89 (-2.02 - -1.76)	-2.71 (-2.86 - -2.56)
41	Metazachlor	ν	0.06 (-0.01 - 0.13)	**0.21** (0.14 - 0.27)	-2.81 (-2.94 - -2.67)	-3.22 (-3.36 - -3.09)	-2.11 (-2.22 - -2.01)	-2.05 (-2.16 - -1.95)
42	Nicosulfuron	ν	**0.2** (0.01 - 0.39)	**0.26** (0.07 - 0.45)	-3.87 (-4.27 - -3.48)	-2.96 (-3.26 - -2.66)	-2.99 (-3.3 - -2.68)	-3.23 (-3.56 - -2.9)
43	Propiconazol	ν	-0.02 (-0.13 - 0.09)	**0.39** (0.29 - 0.5)	-4.05 (-4.32 - -3.78)	-2.72 (-2.88 - -2.57)	-2.88 (-3.06 - -2.7)	-3.43 (-3.63 - -3.24)
44	Quinmerac	ν	-0.03 (-0.13 - 0.08)	**0.32** (0.22 - 0.42)	-2.23 (-2.43 - -2.02)	-2.58 (-2.76 - -2.41)	-2.49 (-2.69 - -2.29)	-1.2 (-1.34 - -1.06)
45	Tebuconazol	ν	**0.1** (0.01 - 0.2)	**0.3** (0.21 - 0.39)	-3.41 (-3.61 - -3.2)	-2.66 (-2.8 - -2.53)	-2.9 (-3.06 - -2.75)	-3.17 (-3.34 - -3)
46	Terbuthylazin	ν	**0.06** (0.01 - 0.12)	**0.28** (0.22 - 0.33)	-2.92 (-3.05 - -2.79)	-1.45 (-1.53 - -1.37)	-1.48 (-1.57 - -1.39)	-2.47 (-2.58 - -2.37)

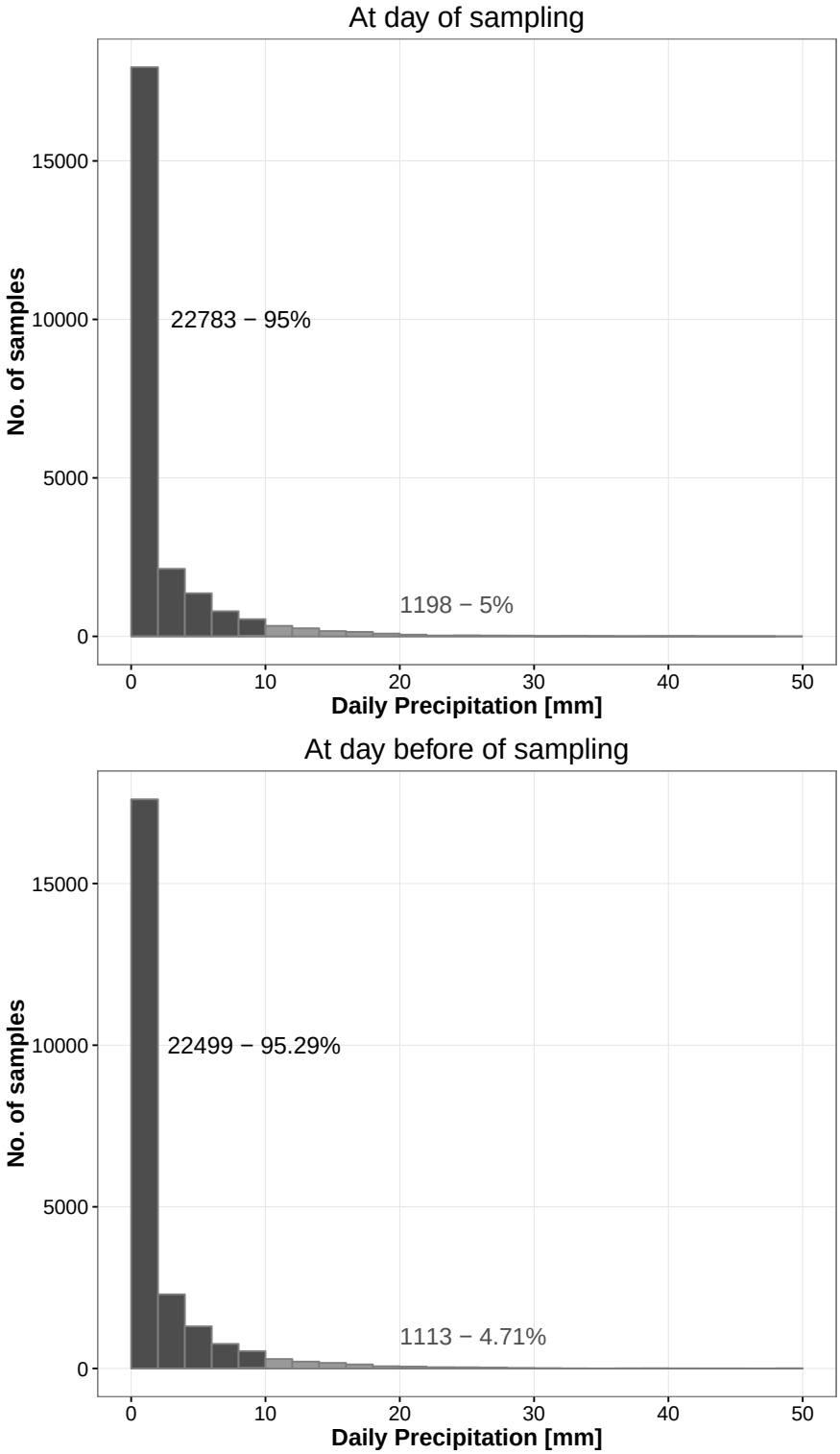

Figure S6: Distribution of precipitation at sampling occasions. top: at sampling date. bottom: at day before sampling.

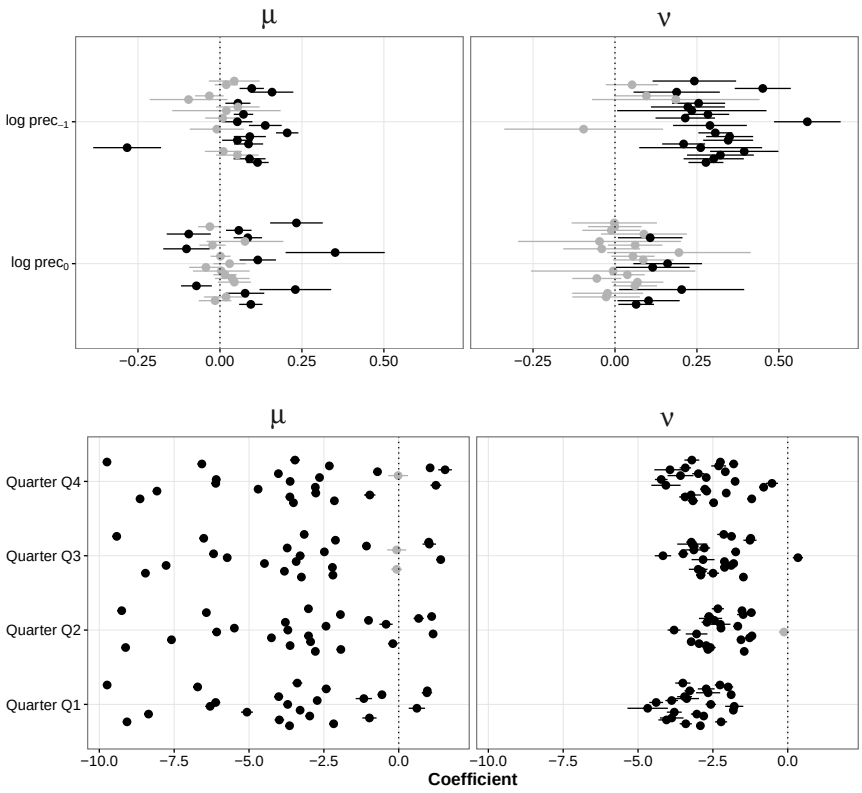

Figure S7: Graphical representation of coefficients from table S4. Top row: Effect of precipitation at day before sampling and at day of sampling. Bottom row: estimates for the four Quarters. Each dot represent one compound (in the order described in table S3). Coefficients where the CI encompasses zero are shown in gray colour. Coefficients are shown on the link scale (log for μ and logit for ν).

5 Pesticides in small streams

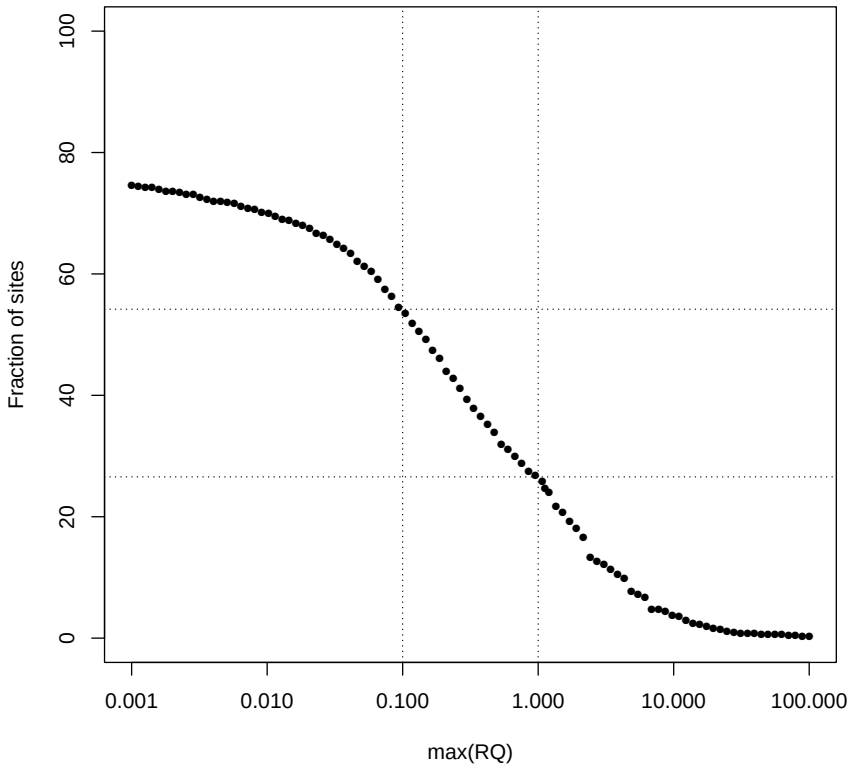

Figure S8: Cumulative distribution of sites exceeding RAC. Dotted lines indicate fraction of sites exceeding a RQ of 1 and 0.1. 23% of sites showed no detection of compounds with RAC and are not shown due to logarithmic x-axis.

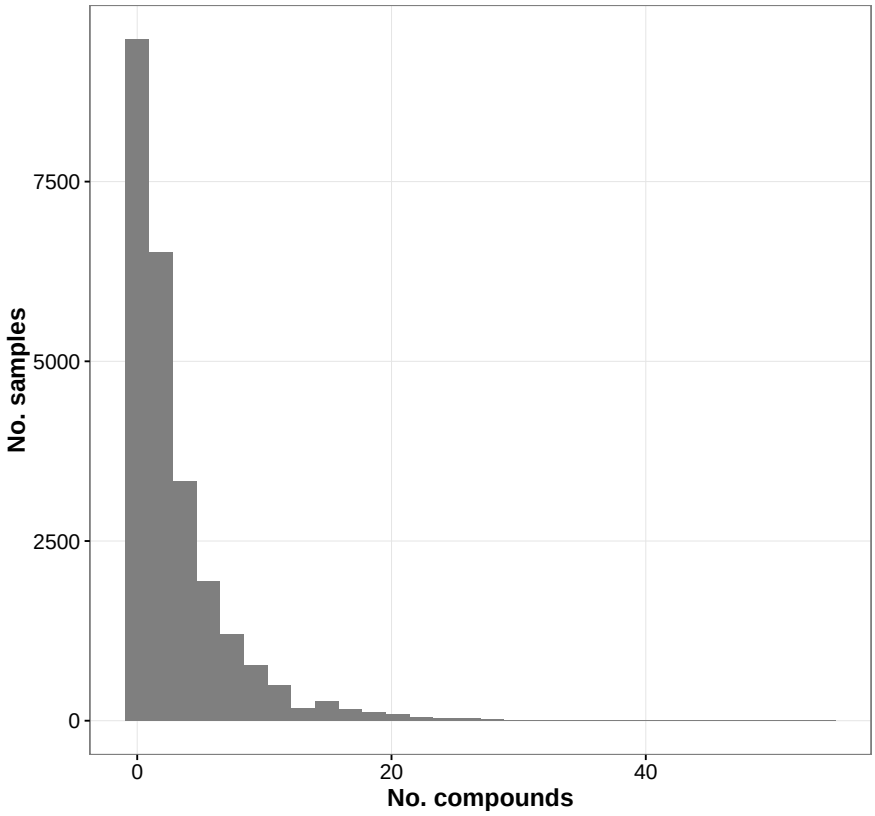

Figure S9: Distribution the number of quantified compounds in the samples from small streams.

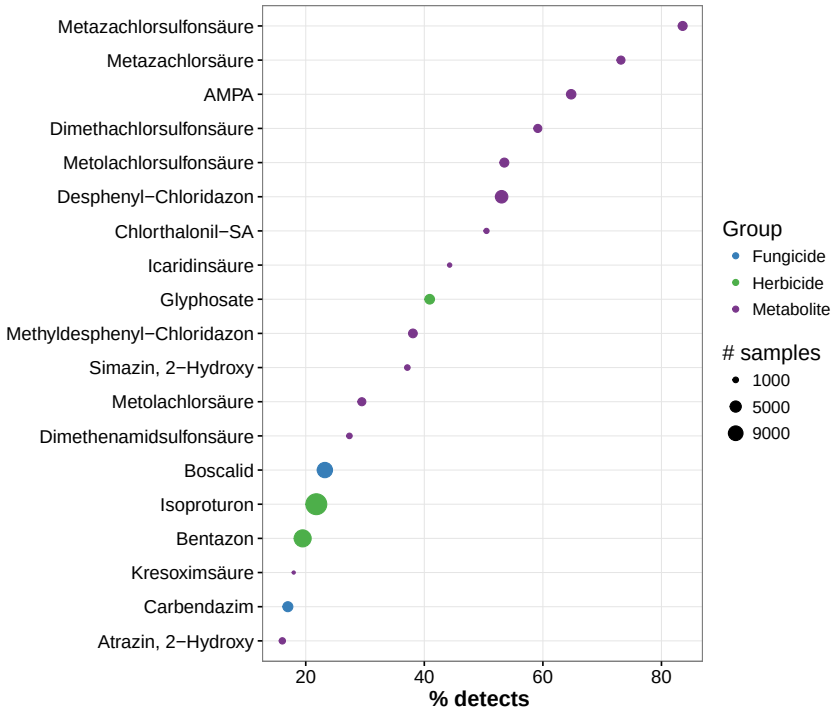

Figure S10: Proportion of samples with detects in small streams. Only Compounds with more than 100 samples and 15% of detects are show.

Bibliography

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