

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

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1 Data Cleaning

Before combining into a common database, more than 30 datasets have been cleaned and homogenized separately. Cleaning steps comprised the following steps (Figure S1 gives a graphical overview):

1. Structure: Datasets have 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 (<https://github.com/ropensci/webchem>).
4. Identifiers: Unique identifiers have been assigned.
5. Units: All concentrations have been converted to $\mu\text{g}/\text{L}$. Values below limit of quantification were set to zero (and can be used to identify non-detects).
6. Other meta-data: meta-data has been standardised.
7. Temporal resolution: The temporal resolution of the database is 1 day. Samplings below this resolution have been aggregated by the maximum daily value.
8. Validity Checks: Simple rules for validity checks have been implemented.

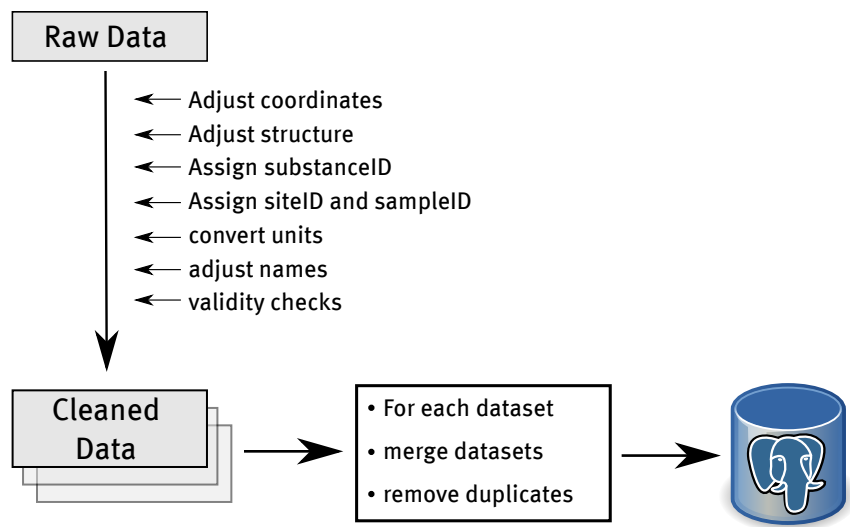


Figure S1: Overview on data cleaning steps. After cleaning, data has been stored in a relational spatial PostgreSQL database.

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

name	abbrv. ^a	Begin	End	No. sites	No.samples	No. pesticides ^b
Baden-Württemberg	BW	2005-03-10	2014-10-02	7	172	98
Bavaria	BY	2006-04-19	2013-12-17	13	218	155
Hesse	HE	2007-01-15	2014-12-18	65	2411	144
Mecklenburg-Western Pomerania	MV	2005-03-08	2014-12-17	130	1503	227
Lower Saxony	NI	2014-03-24	2014-10-13	1	7	226
North Rhine-Westphalia	NW	2005-01-18	2015-01-22	1139	8536	198
Rhineland-Palatinate	RP	2008-01-02	2013-12-18	7	341	236
Schleswig-Holstein	SH	2005-04-26	2014-11-26	269	1380	180
Saarland	SL	2005-01-03	2013-11-25	2	104	57
Saxony	SN	2005-01-02	2013-12-18	606	9141	173
Saxony-Anhalt	ST	2005-01-24	2015-03-19	30	416	88
Thuringia	TH	2005-06-16	2014-12-08	32	514	63
Total		2005-01-02	2015-03-19	2301	24743	478

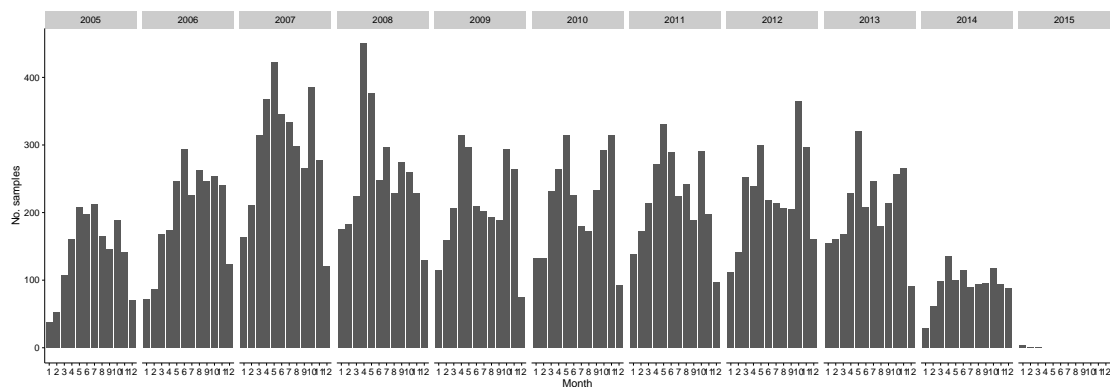


Figure S2: Number of sampling occasions per year and month.

Table S2: Overview on pesticides (and metabolites) in the database. ^a Authorized in Germany (Source: German Federal Office of Consumer Protection and Food Safety (BVL) as at March 2015). ^b Authorized in the European union (Source: EU Pesticides database as at March 2015). ^c Regulatory Acceptable Concentration [ug/L] (Source: German Federal Environment Agency (UBA) as at November 2015).

	Name	CAS	Group	Auth. GER ^a	Auth. EU ^b	RAC ^c
1	(E)7-(Z)9-Dodecadienylacetat	55774-32-8	other	x	x	
2	(Z)-9-Dodecenylacetat	16974-11-1	other	x	x	
3	1,3-cis-Dichlorpropen	10061-01-5	other			
4	1,3-trans-Dichlorpropen	10061-02-6	other			
5	1-(3,4-Dichlorphenyl)urea	2327-02-8	metabolite			
6	1-(4-Isopropylphenyl)urea	56046-17-4	metabolite			
7	1-Decanol	112-30-1	other	x	x	
8	1-Methylcyclopropen	3100-04-7	other	x	x	
9	2,4,5-T	93-76-5	herbicide			
10	2,4,6-Trichlorphenol	88-06-2	metabolite			
11	2,4-D	94-75-7	herbicide	x	x	1.1000
12	2,4-DB	94-82-6	herbicide		x	
13	2,4-Dichlorphenol	120-83-2	metabolite			
14	2,6-Dichlorobenzamid	2008-58-4	metabolite			
15	2-Hydroxydesethylatrazin	19988-24-0	metabolite			
16	3-Hydroxy Carbofuran	16655-82-6	metabolite			
17	4,6-Dinitro-o-Cresol	534-52-1	insecticide			

18	4-tert. Cyclobutylhex-anon	98-53-3	metabolite			
19	AMPA	1066-51-9	metabolite			
20	Acequinocyl	57960-19-7	insecticide	x	x	9.0000
21	Acetamiprid	135410-20-7	insecticide	x	x	0.2400
22	Acetochlor	34256-82-1	herbicide			
23	Acetochlorsulfonsäure	187022-11-3	metabolite			
24	Acetochlorsäure	194992-44-4	metabolite			
25	Acifluorfen	50594-66-6	herbicide			
26	Aclonifen	74070-46-5	herbicide	x	x	1.0600
27	Acrinathrin	101007-06-1	insecticide		x	
28	Alachlor	15972-60-8	herbicide			
29	Aldicarb	116-06-3	insecticide			
30	Aldrin	309-00-2	insecticide			
31	Ametoctradin	865318-97-4	fungicide	x	x	
32	Ametryn	834-12-8	herbicide			
33	Amidosulfuron	120923-37-7	herbicide	x	x	
34	Aminopyralid	150114-71-9	herbicide	x	x	
35	Amisulbrom	348635-87-0	fungicide	x	x	
36	Anthranilsäureisopropylamid	30391-89-0	metabolite			
37	Atraton	1610-17-9	herbicide			
38	Atrazin	1912-24-9	herbicide			
39	Atrazin, 2-Hydroxy	2163-68-0	metabolite			
40	Avermectin B1a	71751-41-2	insecticide	x	x	
41	Azadirachtin (Neem)	11141-17-6	insecticide	x	x	
42	Azinphos-ethyl	2642-71-9	insecticide			
43	Azinphos-methyl	86-50-0	insecticide			
44	Aziprotryn	4658-28-0	herbicide			
45	Azoxystrobin	131860-33-8	fungicide	x	x	0.5500
46	Azoxystrobin-CA		metabolite			
47	Beflubutamid	113614-08-7	herbicide	x	x	
48	Benalaxyl	71626-11-4	fungicide	x	x	20.0000
49	Benazolin	3813-05-6	herbicide			
50	Bensulfuron-methyl	83055-99-6	herbicide		x	
51	Bentazon	25057-89-0	herbicide	x	x	710.0000
52	Benthiavalicarb	413615-35-7	fungicide	x	x	
53	Benzoessäure	65-85-0	fungicide	x	x	
54	Betacypermethrin	65731-84-2	insecticide		x	
55	Bifenazate	149877-41-8	insecticide	x	x	
56	Bifenox	42576-02-3	herbicide	x	x	
57	Bifenthrin	82657-04-3	insecticide		x	
58	Bixafen	581809-46-3	fungicide	x	x	0.4600
59	Boscalid	188425-85-6	fungicide	x	x	12.5000
60	Bromacil	314-40-9	herbicide			

61	Bromadiolon	28772-56-7	other		x	
62	Bromocyclen	1715-40-8	insecticide			
63	Bromoxynil	1689-84-5	herbicide	x	x	3.3000
64	Bupirimat	41483-43-6	fungicide		x	
65	Buturon	3766-60-7	herbicide			
66	Captan	133-06-2	fungicide	x	x	5.0000
67	Carbendazim	10605-21-7	fungicide			0.1500
68	Carbetamid	16118-49-3	herbicide		x	
69	Carbofuran	1563-66-2	insecticide			
70	Carboxin	5234-68-4	fungicide		x	
71	Carfentrazone-ethyl	128639-02-1	herbicide	x	x	0.3100
72	Chloramben	133-90-4	herbicide			
73	Chlorantraniliprole	500008-45-7	insecticide	x	x	0.3550
74	Chlorbromuron	13360-45-7	herbicide			
75	Chlordan	57-74-9	insecticide			
76	Chlorfenac	85-34-7	herbicide			
77	Chlorfenvinphos	470-90-6	insecticide			
78	Chlorfluazuron	71422-67-8	insecticide			
79	Chloridazon	1698-60-8	herbicide	x	x	56.0000
80	Chlormequat	7003-89-6	other	x	x	
81	Chloroxuron	1982-47-4	herbicide			
82	Chlorpropham	101-21-3	herbicide	x	x	
83	Chlorpyrifos	2921-88-2	insecticide		x	0.0004
84	Chlorpyriphos methyl	5598-13-0	insecticide		x	
85	Chlorsulfuron	64902-72-3	herbicide			
86	Chlorthalonil	1897-45-6	fungicide	x	x	
87	Chlorthalonil-SA		metabolite			
88	Chlortoluron	15545-48-9	herbicide	x	x	2.3000
89	Cinidon-ethyl	142891-20-1	herbicide			
90	Clethodim	99129-21-2	herbicide	x	x	
91	Clodinafop	114420-56-3	herbicide	x	x	
92	Clodinafop-propargyl	105512-06-9	herbicide			
93	Clofentezin	74115-24-5	insecticide		x	
94	Clomazon	81777-89-1	herbicide	x	x	5.7000
95	Clopyralid	1702-17-6	herbicide	x	x	1080.0000
96	Cloquintocet-mexyl	99607-70-2	other		x	
97	Clothianidin	210880-92-5	insecticide	x	x	0.0070
98	Codlemone (Codlelure)	33956-49-9	other	x	x	
99	Coumaphos	56-72-4	insecticide			
100	Crimidin	535-89-7	other			
101	Cyanazin	21725-46-2	herbicide			
102	Cyazofamid	120116-88-3	fungicide	x	x	
103	Cyclanilide	113136-77-9	other			
104	Cycloat	1134-23-2	herbicide			

105	Cycloxidim	101205-02-1	herbicide	x	x	
106	Cyflufenamid	180409-60-3	fungicide	x	x	
107	Cyfluthrin (Summe Isomere)	68359-37-5	insecticide			
108	Cyhalothrin (Summe Isomere)	91465-08-6	insecticide	x	x	
109	Cymoxanil	57966-95-7	fungicide	x	x	4.4000
110	Cypermethryn	52315-07-8	insecticide	x	x	0.0010
111	Cyproconazol	94361-06-5	fungicide	x	x	
112	Cyprodinil	121552-61-2	fungicide	x	x	0.7500
113	Cyromazin	66215-27-8	insecticide		x	
114	Daminozid	1596-84-5	other	x	x	
115	Deiquat	2764-72-9	herbicide	x	x	
116	Deltamethrin	52918-63-5	insecticide	x	x	
117	Demeton-O	298-03-3	insecticide			
118	Demeton-S	126-75-0	insecticide			
119	Demeton-S-methyl	919-86-8	insecticide			
120	Demeton-S-methylsulfon	17040-19-6	insecticide			
121	Desaminometribuzin	35045-02-4	metabolite			
122	Desethyl-2-hydroxyterbuthylazin	66753-06-8	metabolite			
123	Desethylatrazin	6190-65-4	metabolite			
124	Desethylsebuthylazin	37019-18-4	metabolite			
125	Desethylsimazin	6190-65-4	metabolite			
126	Desethylterbuthylazin	30125-63-4	metabolite			
127	Desisopropylatrazin	1007-28-9	metabolite			
128	Desmedipham	13684-56-5	herbicide	x	x	
129	Desmethyldiuron	3567-62-2	metabolite			
130	Desmethydisoproturon	34123-57-4	metabolite			
131	Desmetryn	1014-69-3	herbicide			
132	Desphenyl-Chloridazon	6339-19-1	metabolite			
133	Diazinon	333-41-5	insecticide			
134	Dicamba	1918-00-9	herbicide	x	x	180.0000
135	Dichlobenil	1194-65-6	herbicide			
136	Dichlofluanid	1085-98-9	fungicide			
137	Dichlorprop	120-36-5	herbicide			
138	Dichlorprop-P	15165-67-0	herbicide	x	x	
139	Dichlorvos	62-73-7	insecticide			
140	Diclofop	40843-25-2	herbicide		x	
141	Dicofol	115-32-2	insecticide			
142	Dieldrin	60-57-1	insecticide			
143	Difenacoum	56073-07-5	other		x	
144	Difenoconazol	119446-68-3	fungicide	x	x	0.3600

145	Diflubenzuron	35367-38-5	insecticide		x	
146	Diflufenican	83164-33-4	herbicide	x	x	0.0250
147	Dimefuron	34205-21-5	herbicide			0.8300
148	Dimethachlor	50563-36-5	herbicide	x	x	3.5000
149	Dimethachlor-CA		metabolite			
150	Dimethachlorsulfonsäure		metabolite			
151	Dimethachlorsäure		metabolite			
152	Dimethenamid	87674-68-8	herbicide			1.3500
153	Dimethenamid-CA		metabolite			
154	Dimethenamid-P	163515-14-8	herbicide	x	x	1.3500
155	Dimethenamid-SA		metabolite			
156	Dimethenamidsulfonsäure		metabolite			
157	Dimethoat	60-51-5	insecticide	x	x	4.0000
158	Dimethomorph	110488-70-5	fungicide	x	x	5.6000
159	Dimoxystrobin	149961-52-4	fungicide	x	x	0.0316
160	Diniconazol	83657-24-3	fungicide			
161	Dinoseb	88-85-7	herbicide			
162	Dinotefuran	165252-70-0	insecticide			
163	Dinoterb	1420-07-1	herbicide			
164	Disulfoton	298-04-4	insecticide			
165	Dithianon	3347-22-6	fungicide	x	x	0.7800
166	Diuron	330-54-1	herbicide		x	0.7900
167	Dodin	2439-10-3	fungicide	x	x	5.3300
168	Endosulfan, alpha	959-98-8	insecticide			
169	Endosulfan, beta	33213-65-9	insecticide			
170	Endosulfansulfat	1031-07-8	metabolite			
171	Endrin	72-20-8	insecticide			
172	Epoxiconazol	133855-98-8	fungicide	x	x	0.5375
173	Esfenvalerat	66230-04-4	insecticide	x	x	
174	Etaconazol	60207-93-4	fungicide			
175	Ethidimuron	30043-49-3	herbicide			
176	Ethirimol	23947-60-6	fungicide			
177	Ethofenprox	80844-07-1	insecticide	x	x	
178	Ethofumesat	26225-79-6	herbicide	x	x	24.0000
179	Etrimfos	38260-54-7	insecticide			
180	Famoxadone	131807-57-3	fungicide	x	x	
181	Fenamidon	161326-34-7	fungicide	x	x	
182	Fenamiphos	22224-92-6	insecticide		x	
183	Fenarimol	60168-88-9	fungicide			
184	Fenazaquin	120928-09-8	insecticide	x	x	
185	Fenhexamid	126833-17-8	fungicide	x	x	10.1000
186	Fenitrothion	122-14-5	insecticide			
187	Fenoprop	93-72-1	herbicide			
188	Fenoxaprop	95617-09-7	herbicide			

189	Fenoxaprop-p	113158-40-0	herbicide	x	x	
190	Fenoxaprop-p-ethyl	71283-80-2	herbicide			
191	Fenoxycarb	72490-01-8	insecticide		x	
192	Fenpropidin	67306-00-7	fungicide	x	x	
193	Fenpropimorph	67564-91-4	fungicide	x	x	0.1950
194	Fenpyroximat	134098-61-6	insecticide	x	x	
195	Fenthion	55-38-9	insecticide			
196	Fenuron	101-42-8	herbicide			
197	Fipronil	120068-37-3	insecticide		x	0.0008
198	Flamprop	58667-63-3	herbicide			
199	Flazasulfuron	104040-78-0	herbicide	x	x	
200	Flonicamid	158062-67-0	insecticide	x	x	310.0000
201	Florasulam	145701-23-1	herbicide	x	x	
202	Fluazifop	69335-91-7	herbicide			
203	Fluazifop-P	83066-88-0	herbicide	x	x	146.0000
204	Fluazifop-P-butyl	79241-46-6	herbicide			7.7000
205	Fluazifop-butyl	69806-50-4	herbicide			
206	Fluazinam	79622-59-6	fungicide	x	x	0.2600
207	Fluchloralin	33245-39-5	herbicide			
208	Fludioxonil	131341-86-1	fungicide	x	x	0.5000
209	Flufenacet	142459-58-3	herbicide	x	x	2.4000
210	Flufenacet-SA		metabolite			
211	Flufenoxuron	101463-69-8	insecticide			
212	Flumioxazin	103361-09-7	herbicide	x	x	
213	Fluometuron	2164-17-2	herbicide		x	
214	Fluopicolide	239110-15-7	fungicide	x	x	
215	Fluopyram	658066-35-4	fungicide	x	x	5.1200
216	Fluoxastrobin	361377-29-9	fungicide	x	x	
217	Flupyr-sulfuron	150315-10-9	herbicide	x	x	
218	Fluquinconazole	136426-54-5	fungicide	x	x	0.8000
219	Flurochloridon	61213-25-0	herbicide		x	
220	Fluroxypyr	69377-81-7	herbicide	x	x	16.0000
221	Fluroxypyr-methylheptyl	81406-37-3	herbicide			
222	Flurtamone	96525-23-4	herbicide	x	x	0.9900
223	Flusilazol	85509-19-9	fungicide			1.1000
224	Flutolanil	66332-96-5	fungicide	x	x	
225	Flutriafol	76674-21-0	fungicide		x	
226	Fluxapyroxad	907204-31-3	fungicide	x	x	
227	Folpet	133-07-3	fungicide	x	x	
228	Foramsulfuron	173159-57-4	herbicide	x	x	0.9500
229	Fosetyl	15845-66-6	fungicide	x	x	
230	Fosthiazat	98886-44-3	other	x	x	
231	Fuberidazol	3878-19-1	fungicide	x	x	

232	Furalaxyl	57646-30-7	fungicide			
233	Furmecyclox	60568-05-0	fungicide			
234	Glufosinat	51276-47-2	herbicide	x	x	
235	Glyphosate	1071-83-6	herbicide	x	x	100.0000
236	HCH, gamma (Lindan)	58-89-9	insecticide			
237	Haloxypop	69806-34-4	herbicide			
238	Haloxypop-P	95977-29-0	herbicide	x	x	
239	Haloxypop-ethoxyethyl	87237-48-7	herbicide			
240	Heptachlor	76-44-8	insecticide			
241	Heptachlorepoxyd	1024-57-3	metabolite			
242	Heptenophos	23560-59-0	insecticide			
243	Hexachlorbenzen	118-74-1	fungicide			
244	Hexachlorophen	70-30-4	other			
245	Hexaconazol	79983-71-4	fungicide			
246	Hexaflumuron	86479-06-3	insecticide			
247	Hexazinon	51235-04-2	herbicide			
248	Hexythiazox	78587-05-0	insecticide	x	x	
249	Hymexazol	10004-44-1	fungicide	x	x	
250	Icaridinsäure		metabolite			
251	Imazalil	35554-44-0	fungicide	x	x	
252	Imazamox	114311-32-9	herbicide	x	x	
253	Imazapic	104098-48-8	herbicide			
254	Imazaquin	81335-37-7	herbicide		x	
255	Imazethapyr	81335-77-5	herbicide			
256	Imazosulfuron	122548-33-8	herbicide	x	x	
257	Imidacloprid	138261-41-3	insecticide	x	x	0.0090
258	Indoxacarb	173584-44-6	insecticide	x	x	
259	Iodosulfuron	185119-76-0	herbicide	x	x	0.0790
260	Iodosulfuron-methyl	144550-06-1	herbicide			
261	Iodosulfuron-methyl- sodium	144550-36-7	herbicide			
262	Ioxynil	1689-83-4	herbicide	x		2.7000
263	Iprodion	36734-19-7	fungicide	x	x	
264	Iprovalicarb	140923-17-7	fungicide	x	x	189.0000
265	Isodrin	465-73-6	insecticide			
266	Isophenphos	25311-71-1	insecticide			
267	Isoproturon	34123-59-6	herbicide	x	x	1.3000
268	Isopyrazam	881685-58-1	fungicide	x	x	
269	Isoxaben	82558-50-7	herbicide	x	x	
270	Isoxaflutole	141112-29-0	herbicide	x	x	
271	Karbutylat	4849-32-5	herbicide			
272	Kresoxim-methyl	143390-89-0	fungicide	x	x	1.0000
273	Kresoximsäure		metabolite			
274	Lenacil	2164-08-1	herbicide	x	x	0.6500

275	Linuron	330-55-2	herbicide		x	
276	MCPA	94-74-6	herbicide	x	x	9.0000
277	MCPB	94-81-5	herbicide		x	
278	Malathion	121-75-5	insecticide		x	
279	Mancozeb	8018-01-7	fungicide	x	x	0.2190
280	Mandipropamid	374726-62-2	fungicide	x	x	7.6000
281	Maneb	12427-38-2	fungicide	x	x	
282	Mecoprop	93-65-2	herbicide		x	160.0000
283	Mefenpyr-diethyl	135591-00-3	other	x		
284	Mepanipyrim	110235-47-7	fungicide	x	x	
285	Mepiquat	15302-91-7	other	x	x	
286	Mepronil	55814-41-0	fungicide			
287	Meptyldinocap	131-72-6	fungicide		x	
288	Mesosulfuron	400852-66-6	herbicide	x	x	
289	Mesotrion	104206-82-8	herbicide	x	x	
290	Metaflumizone	139968-49-3	insecticide	x	x	
291	Metalaxyl	57837-19-1	fungicide		x	46.0000
292	Metalaxyl-CA	75596-99-5	metabolite			
293	Metalaxyl-CA2	104390-56-9	metabolite			
294	Metalaxyl-M	70630-17-0	fungicide	x	x	46.0000
295	Metaldehyd	108-62-3	other	x	x	
296	Metamitron	41394-05-2	herbicide	x	x	38.0000
297	Metamitron-Desamino	36993-94-9	metabolite			
298	Metazachlor	67129-08-2	herbicide	x	x	0.8800
299	Metazachlordicarbonsäure		metabolite			
300	Metazachlorsulfonsäure	172960-62-2	metabolite			
301	Metazachlorsäure	1231244-60-2	metabolite			
302	Metconazol	125116-23-6	fungicide	x	x	
303	Methabenzthiazuron	18691-97-9	herbicide			
304	Methamidophos	10265-92-6	insecticide			2.6000
305	Methidathion	950-37-8	insecticide			
306	Methiocarb	2032-65-7	insecticide	x	x	0.0100
307	Methobromuron	3060-89-7	herbicide		x	2.0000
308	Methomyl	16752-77-5	insecticide		x	
309	Methoprotryn	841-06-5	herbicide			
310	Methoxychlor	72-43-5	insecticide			
311	Methoxyfenozid	161050-58-4	insecticide	x	x	
312	Methyl-desphenyl- Chloridazon	17254-80-7	metabolite			
313	Metiram	9006-42-2	fungicide	x	x	
314	Metolachlor	51218-45-2	herbicide			
315	Metolachlorsulfonsäure	171118-09-5	metabolite			
316	Metolachlorsäure	152019-73-3	metabolite			
317	Metosulam	139528-85-1	herbicide	x	x	

318	Metoxuron	19937-59-8	herbicide			
319	Metrafenon	220899-03-6	fungicide	x	x	
320	Metribuzin	21087-64-9	herbicide	x	x	0.5840
321	Metsulfuron	79510-48-8	herbicide	x	x	
322	Metsulfuron-methyl	74223-64-6	herbicide			
323	Mevinphos	7786-34-7	insecticide			
324	Milbemectin	51596-11-3	insecticide	x	x	
325	Mirex	2385-85-5	insecticide			
326	Monolinuron	1746-81-2	herbicide			
327	Monuron	150-68-5	herbicide			
328	Myclobutanil	88671-89-0	fungicide	x	x	2.4000
329	Napropamid	15299-99-7	herbicide	x	x	6.7000
330	Neburon	555-37-3	herbicide			
331	Nicosulfuron	111991-09-4	herbicide	x	x	0.0850
332	Nitenpyram	120738-89-8	insecticide			
333	Nitrofen	1836-75-5	herbicide			
334	Norflurazon	27314-13-2	herbicide			
335	Omethoat	1113-02-6	insecticide			
336	Orysastrobin	248593-16-0	fungicide			
337	Oxadiazon	19666-30-9	herbicide		x	
338	Oxadixyl	77732-09-3	fungicide			
339	Oxamyl	23135-22-0	insecticide		x	
340	Oxydemeton-methyl	301-12-2	insecticide			1.1000
341	Paclobutrazol	76738-62-0	other	x	x	
342	Parathion-ethyl	56-38-2	insecticide			
343	Parathion-methyl	298-00-0	insecticide			
344	Pelargonsäure	112-05-0	herbicide	x	x	
345	Penconazol	66246-88-6	fungicide	x	x	3.2000
346	Pencycuron	66063-05-6	fungicide	x	x	
347	Pendimethalin	40487-42-1	herbicide	x	x	0.6300
348	Penflufen	494793-67-8	fungicide		x	
349	Penoxsulam	219714-96-2	herbicide	x	x	
350	Permethrin	52645-53-1	insecticide			
351	Pethoxamid	106700-29-2	herbicide	x	x	1.7720
352	Phenmedipham	13684-63-4	herbicide	x	x	
353	Phoxim	14816-18-3	insecticide			0.0070
354	Picloram	1918-02-1	herbicide	x	x	
355	Picolinafen	137641-05-5	herbicide	x	x	0.0360
356	Picoxystrobin	117428-22-5	fungicide	x	x	0.6000
357	Pinoxaden	243973-20-8	herbicide	x		
358	Pirimicarb	23103-98-2	insecticide	x	x	0.0900
359	Pirimicarb-desmethyl	30614-22-3	metabolite			
360	Pirimiphos-ethyl	23505-41-1	insecticide			
361	Pirimiphos-methyl	29232-93-7	insecticide	x	x	

362	Primisulfuron-methyl	86209-51-0	herbicide			
363	Prochloraz	67747-09-5	fungicide	x	x	5.0000
364	Procymidon	32809-16-8	fungicide			
365	Profoxydim	139001-49-3	herbicide		x	
366	Prohexadion	88805-35-0	other	x	x	
367	Prometryn	7287-19-6	herbicide			
368	Propachlor	1918-16-7	herbicide			
369	Propamocarb	24579-73-5	fungicide	x	x	
370	Propanil	709-98-8	herbicide			
371	Propaquizafop	111479-05-1	herbicide	x	x	
372	Propazin	139-40-2	herbicide			
373	Propetamphos	31218-83-4	insecticide			
374	Propham	122-42-9	herbicide			
375	Propiconazol	60207-90-1	fungicide	x	x	2.0000
376	Propoxur	114-26-1	insecticide			
377	Propoxycarbazone	145026-81-9	herbicide	x	x	
378	Propyzamid	23950-58-5	herbicide	x	x	34.0000
379	Proquinazid	189278-12-4	fungicide	x	x	
380	Prosulfocarb	52888-80-9	herbicide	x	x	3.8000
381	Prosulfuron	94125-34-5	herbicide	x	x	
382	Prothioconazol	178928-70-6	fungicide	x	x	1.7100
383	Prothioconazol-desthio	120983-64-4	metabolite			
384	Pymetrozin	123312-89-0	insecticide	x	x	
385	Pyraclostrobin	175013-18-0	fungicide	x	x	
386	Pyraflufen	129630-17-7	herbicide	x	x	
387	Pyrazophos	13457-18-6	fungicide			
388	Pyrethrum	8003-34-7	insecticide	x	x	0.0140
389	Pyridaben	96489-71-3	insecticide		x	
390	Pyridat	55512-33-9	herbicide	x	x	
391	Pyrifenox	88283-41-4	fungicide			
392	Pyrimethanil	53112-28-0	fungicide	x	x	8.0000
393	Pyroxsulam	422556-08-9	herbicide	x	x	
394	Quinalphos	13593-03-8	insecticide			
395	Quinmerac	90717-03-6	herbicide	x	x	316.0000
396	Quinoclamín	2797-51-5	herbicide	x	x	
397	Quinoxifen (5,7-dichloro-4-(p-fluorophenoxy)quinoline)	124495-18-7	fungicide	x	x	
398	Quintozen	82-68-8	fungicide			
399	Quizalofop	76578-12-6	herbicide			
400	Quizalofop-ethyl	76578-14-8	herbicide			
401	Rimsulfuron	122931-48-0	herbicide	x	x	0.4600
402	Saflufenacil	372137-35-4	herbicide			
403	Sebuthylazin	7286-69-3	herbicide			

404	Seebumeton	26259-45-0	herbicide			
405	Silthiofam	175217-20-6	fungicide	x	x	
406	Simazin	122-34-9	herbicide			
407	Simazin, 2-Hydroxy	2599-11-3	metabolite			
408	Spinosad	168316-95-8	insecticide	x	x	0.0620
409	Spirodiclofen	148477-71-8	insecticide	x	x	
410	Spiromesifen	283594-90-1	insecticide		x	
411	Spiroxamin	118134-30-8	fungicide	x	x	0.1300
412	Sulcotrion	99105-77-8	herbicide	x	x	
413	Sulfosulfuron	141776-32-1	herbicide		x	
414	Sulfurylfluorid	2699-79-8	insecticide	x	x	
415	Tebuconazol	107534-96-3	fungicide	x	x	0.5780
416	Tebufenozid	112410-23-8	insecticide	x	x	
417	Tebufenpyrad	119168-77-3	insecticide	x	x	
418	Tebutam	35256-85-0	herbicide			
419	Teflubenzuron	83121-18-0	insecticide		x	
420	Tefluthrin	79538-32-2	insecticide	x	x	
421	Telodrin	297-78-9	insecticide			
422	Tembotrione	335104-84-2	herbicide	x	x	
423	Tepraloxymid	149979-41-9	herbicide	x	x	
424	Terbumeton	33693-04-8	herbicide			
425	Terbuthylazin	5915-41-3	herbicide	x	x	1.2000
426	Terbutryn	886-50-0	herbicide			
427	Terbutylazin-Metabolit CGA 324007	309923-18-0	metabolite			
428	Terbutylazin-Metabolit SYN 545666		metabolite			
429	Tetraconazol	112281-77-3	fungicide	x	x	
430	Thiabendazol	148-79-8	fungicide	x	x	
431	Thiacloprid	111988-49-9	insecticide	x	x	0.0040
432	Thiacloprid-SA		metabolite			
433	Thiamethoxam	153719-23-4	insecticide	x	x	0.0430
434	Thiencarbazon-methyl	317815-83-1	herbicide	x	x	
435	Thifensulfuron-methyl	79277-27-3	herbicide			
436	Thifenylsulfuron	79277-67-1	herbicide	x	x	
437	Thiometon	640-15-3	insecticide			
438	Thiophanat-methyl	23564-05-8	fungicide	x	x	
439	Thiram	137-26-8	fungicide	x	x	0.1100
440	Tolclofos-methyl	57018-04-9	fungicide	x	x	
441	Tolylfluorid	731-27-1	fungicide			
442	Topramezone	210631-68-8	herbicide	x		0.9000
443	Tralkoxydim	87820-88-0	herbicide		x	
444	Triadimefon	43121-43-3	fungicide			
445	Triadimenol	55219-65-3	fungicide	x	x	3.4000

446	Triallat	2303-17-5	herbicide		x	
447	Triasulfuron	82097-50-5	herbicide	x	x	
448	Triazophos	24017-47-8	insecticide			0.0300
449	Triazoxid	72459-58-6	fungicide	x	x	
450	Tribenuron	106040-48-6	herbicide	x	x	
451	Tribenuron-methyl	101200-48-0	herbicide			
452	Trichlorfon	52-68-6	insecticide			
453	Triclopyr	55335-06-3	herbicide	x	x	
454	Trifloxystrobin	141517-21-7	fungicide	x	x	0.0862
455	Trifloxystrobin-CA2		metabolite			
456	Triflumizol	99387-89-0	fungicide		x	
457	Triflumuron	64628-44-0	insecticide		x	
458	Trifluralin	1582-09-8	herbicide			
459	Triflusulfuron	135990-29-3	herbicide	x	x	
460	Triforin	26644-46-2	fungicide			
461	Trinexapac-ethyl	95266-40-3	other	x	x	
462	Triticonazol	131983-72-7	fungicide	x	x	
463	Tritosulfuron	142469-14-5	herbicide	x	x	
464	Valifenalate	283159-90-0	fungicide	x	x	
465	Vinclozolin	50471-44-8	fungicide			
466	Warfarin	81-81-2	other			
467	Zoxamid	156052-68-5	fungicide	x	x	
468	alpha-Cypermethrin	67375-30-8	insecticide	x	x	
469	cis-Chlordan	5103-71-9	insecticide			
470	gamma-Cyhalothrin	76703-62-3	insecticide	x	x	
471	o,p-DDE	3424-82-6	metabolite			
472	o,p-DDT	789-02-6	insecticide			
473	oxi-Chlordan	27304-13-8	metabolite			
474	p,p-DDD (p,p TDE)	72-54-8	insecticide			
475	p,p-DDE	72-55-9	metabolite			
476	p,p-DDT	50-29-3	insecticide			
477	tau-Fluvalinat	102851-06-9	insecticide	x	x	0.0330
478	trans-Chlordan	5103-74-2	insecticide			

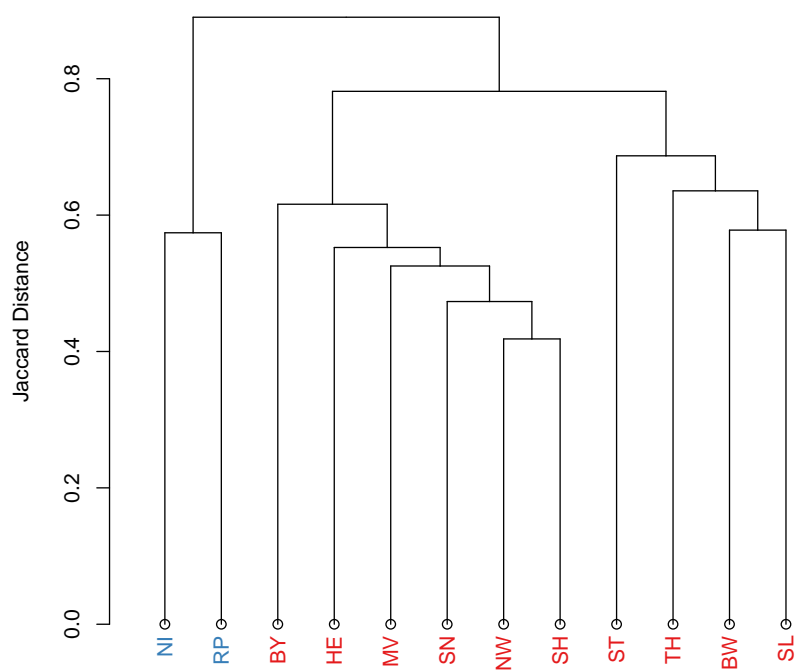


Figure S3: Complete Linkage Cluster Dendrogram of Jaccard Similarity of analysed compound spectra between federal states. Abbreviations of state names according to ISO 3166-2:DE (see also Table S1).

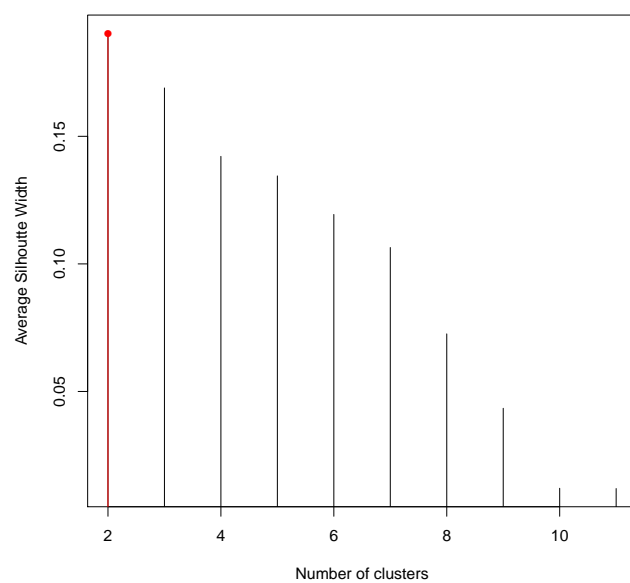


Figure S4: Average silhouette width for different cluster sizes of complete linkage clustering of jaccard similarity of analysed compound spectra between federal states. Two clusters showed maximum silhouette width.

3 Thresholds for agricultural land use and catchment size

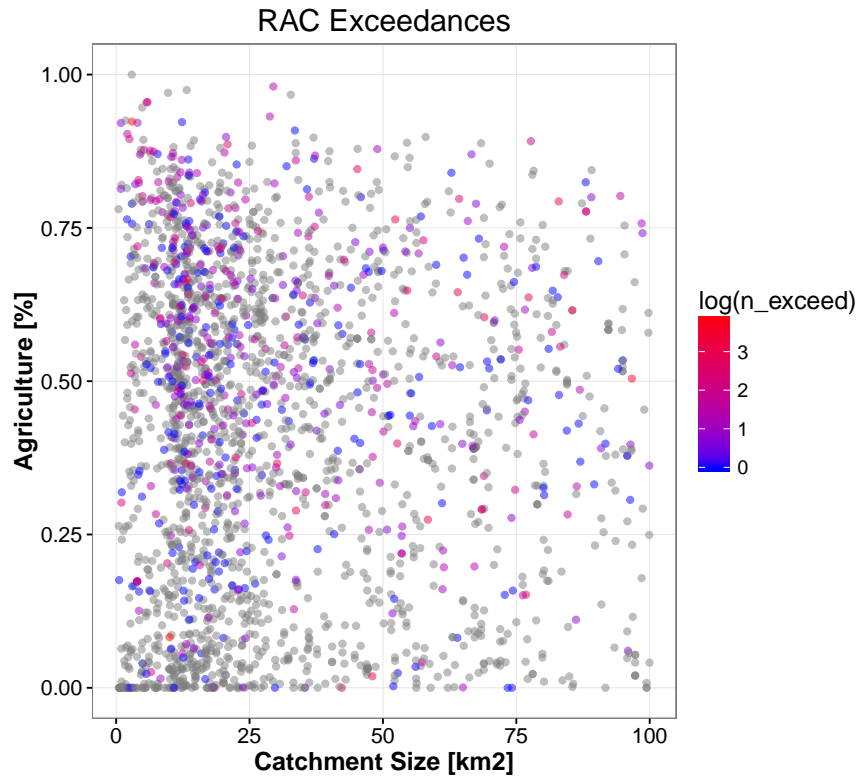


Figure S5: Raw data used for the model in equation 2 and Figure 3 of the main article. Color codes the number of RAC exceedances (on a log-scale). Grey points denote sites without any exceedance.

4 Effect of precipitation and season on RQ

Table S3: 23 pesticides for which we modelled the relationship between RQ and precipitation and seasonality, respectively. Order is the same as in Figure 5 of the main text. See Table S4 for model coefficients.

	Name	CAS	Group	%>LOQ	no. > LOQ	total no.
1	Azoxystrobin	131860-33-8	fungicide	9.76	669	6854
2	Bentazon	25057-89-0	herbicide	19.53	2362	12095
3	Boscalid	188425-85-6	fungicide	23.26	2231	9593
4	Carbendazim	10605-21-7	fungicide	16.28	603	3704
5	Chlorpyrifos	2921-88-2	insecticide	6.21	885	14252
6	Clothianidin	210880-92-5	insecticide	6.42	148	2306
7	Diffufenican	83164-33-4	herbicide	12.61	1891	14997
8	Dimethenamid	87674-68-8	herbicide	6.22	577	9281
9	Dimoxystrobin	149961-52-4	fungicide	7.05	229	3250
10	Diuron	330-54-1	herbicide	12.26	2202	17967
11	Ethofumesat	26225-79-6	herbicide	5.24	1039	19841
12	Flufenacet	142459-58-3	herbicide	5.92	778	13134
13	Glyphosate	1071-83-6	herbicide	40.68	1410	3466
14	Imidacloprid	138261-41-3	insecticide	5.89	180	3057
15	Isoproturon	34123-59-6	herbicide	21.86	4045	18507
16	MCPA	94-74-6	herbicide	12.98	1613	12428
17	Mecoprop	93-65-2	herbicide	12.27	1494	12179
18	Metazachlor	67129-08-2	herbicide	9.25	1964	21222
19	Nicosulfuron	111991-09-4	herbicide	5.38	270	5017
20	Propiconazol	60207-90-1	fungicide	5.74	794	13831
21	Quinmerac	90717-03-6	herbicide	13.50	957	7088
22	Tebuconazol	107534-96-3	fungicide	6.15	993	16144
23	Terbuthylazin	5915-41-3	herbicide	14.80	3236	21863

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
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1	Azoxystrobin	μ	0.23 (0.15 - 0.31)	0.04 (-0.03 - 0.12)	-3.39 (-3.56 - -3.22)	-3.02 (-3.14 - -2.89)	-3.16 (-3.29 - -3.03)	-3.47 (-3.63 - -3.3)
2	Bentazon	μ	-0.03 (-0.07 - 0)	0.02 (-0.02 - 0.05)	-9.74 (-9.81 - -9.67)	-9.25 (-9.31 - -9.2)	-9.42 (-9.48 - -9.36)	-9.74 (-9.81 - -9.68)
3	Boscalid	μ	0.06 (0.02 - 0.1)	0.1 (0.06 - 0.13)	-6.72 (-6.79 - -6.64)	-6.42 (-6.49 - -6.36)	-6.51 (-6.58 - -6.45)	-6.58 (-6.65 - -6.5)
4	Carbendazim	μ	-0.1 (-0.16 - -0.03)	0.16 (0.09 - 0.22)	-2.42 (-2.58 - -2.27)	-1.95 (-2.05 - -1.84)	-2.11 (-2.22 - -2)	-2.32 (-2.46 - -2.18)
5	Chlorpyrifos	μ	0.08 (0.04 - 0.13)	-0.03 (-0.08 - 0.01)	0.95 (0.88 - 1.03)	1.1 (1.03 - 1.17)	1 (0.93 - 1.08)	1.05 (0.96 - 1.14)
6	Clothianidin	μ	0.08 (-0.04 - 0.19)	-0.1 (-0.21 - 0.02)	0.94 (0.77 - 1.12)	0.67 (0.49 - 0.84)	1.02 (0.8 - 1.25)	1.55 (1.32 - 1.78)
7	Diflufenican	μ	-0.02 (-0.06 - 0.02)	0.05 (0.02 - 0.09)	-0.56 (-0.62 - -0.5)	-1.01 (-1.07 - -0.94)	-1.08 (-1.16 - -1)	-0.71 (-0.77 - -0.65)
8	Dimethenamid	μ	-0.1 (-0.17 - -0.03)	0.05 (-0.01 - 0.12)	-4.01 (-4.16 - -3.86)	-3.79 (-3.89 - -3.68)	-3.72 (-3.84 - -3.61)	-4.02 (-4.14 - -3.9)
9	Dimoxystrobin	μ	0.35 (0.2 - 0.5)	0.02 (-0.15 - 0.19)	-1.17 (-1.44 - -0.89)	-0.42 (-0.64 - -0.2)	-0.07 (-0.39 - 0.25)	-0.02 (-0.35 - 0.31)
10	Diuron	μ	0 (-0.03 - 0.03)	0.07 (0.04 - 0.1)	-2.72 (-2.83 - -2.61)	-2.43 (-2.47 - -2.39)	-2.48 (-2.53 - -2.44)	-2.64 (-2.71 - -2.58)
11	Ethofumesat	μ	0.12 (0.06 - 0.17)	0.01 (-0.05 - 0.06)	-6.11 (-6.27 - -5.96)	-5.49 (-5.56 - -5.42)	-6.18 (-6.29 - -6.08)	-6.1 (-6.24 - -5.95)
12	Flufenacet	μ	0.03 (-0.02 - 0.08)	0.05 (0.01 - 0.1)	-3.71 (-3.79 - -3.62)	-3.7 (-3.81 - -3.59)	-3.29 (-3.44 - -3.15)	-3.63 (-3.68 - -3.57)
13	Glyphosate	μ	-0.04 (-0.09 - 0.01)	0.14 (0.09 - 0.19)	-6.3 (-6.46 - -6.13)	-6.08 (-6.16 - -6)	-5.73 (-5.8 - -5.66)	-6.11 (-6.21 - -6.01)
14	Imidacloprid	μ	0 (-0.08 - 0.09)	-0.01 (-0.09 - 0.07)	0.61 (0.33 - 0.88)	1.15 (1.02 - 1.27)	1.4 (1.28 - 1.53)	1.24 (1.06 - 1.42)
15	Isoproturon	μ	0.02 (-0.02 - 0.05)	0.21 (0.17 - 0.24)	-3.29 (-3.37 - -3.22)	-3.01 (-3.06 - -2.96)	-3.43 (-3.5 - -3.35)	-2.79 (-2.84 - -2.73)
16	MCPA	μ	0.04 (-0.01 - 0.09)	0.09 (0.04 - 0.14)	-5.07 (-5.27 - -4.87)	-4.25 (-4.32 - -4.19)	-4.48 (-4.57 - -4.4)	-4.7 (-4.81 - -4.58)
17	Mecoprop	μ	0.04 (-0.01 - 0.09)	0.05 (0.01 - 0.1)	-8.36 (-8.49 - -8.22)	-7.59 (-7.65 - -7.52)	-7.77 (-7.85 - -7.69)	-8.07 (-8.18 - -7.97)
18	Metazachlor	μ	-0.07 (-0.12 - -0.02)	0.09 (0.04 - 0.13)	-2.97 (-3.06 - -2.88)	-2.94 (-3.04 - -2.85)	-2.21 (-2.28 - -2.14)	-2.77 (-2.84 - -2.7)
19	Nicosulfuron	μ	0.23 (0.12 - 0.34)	-0.28 (-0.39 - -0.18)	-0.98 (-1.22 - -0.74)	-0.2 (-0.36 - -0.03)	-0.07 (-0.25 - 0.11)	-0.97 (-1.16 - -0.78)
20	Propiconazol	μ	0.08 (0.02 - 0.14)	0.01 (-0.05 - 0.07)	-3.99 (-4.15 - -3.83)	-3.63 (-3.71 - -3.55)	-3.82 (-3.91 - -3.72)	-3.63 (-3.74 - -3.53)
21	Quinmerac	μ	0.02 (-0.05 - 0.09)	0.05 (-0.01 - 0.12)	-9.08 (-9.19 - -8.96)	-9.12 (-9.24 - -9)	-8.46 (-8.59 - -8.33)	-8.64 (-8.72 - -8.55)
22	Tebuconazol	μ	-0.01 (-0.06 - 0.03)	0.09 (0.04 - 0.14)	-2.17 (-2.28 - -2.06)	-1.93 (-2 - -1.86)	-2.2 (-2.28 - -2.11)	-2.15 (-2.24 - -2.06)
23	Terbuthylazin	μ	0.09 (0.06 - 0.13)	0.11 (0.08 - 0.15)	-3.65 (-3.73 - -3.56)	-2.78 (-2.84 - -2.73)	-3.25 (-3.3 - -3.19)	-3.52 (-3.59 - -3.44)
24	Azoxystrobin	ν	0 (-0.13 - 0.13)	0.24 (0.11 - 0.37)	-3.5 (-3.76 - -3.25)	-2.33 (-2.54 - -2.13)	-2.14 (-2.36 - -1.92)	-3.2 (-3.45 - -2.95)
25	Bentazon	ν	0 (-0.08 - 0.08)	0.05 (-0.03 - 0.13)	-2.26 (-2.44 - -2.09)	-1.53 (-1.65 - -1.4)	-1.88 (-2.02 - -1.74)	-2.25 (-2.4 - -2.11)
26	Boscalid	ν	-0.01 (-0.1 - 0.08)	0.45 (0.37 - 0.54)	-1.99 (-2.16 - -1.82)	-1.22 (-1.36 - -1.07)	-1.24 (-1.38 - -1.09)	-1.81 (-1.96 - -1.65)
27	Carbendazim	ν	0.09 (-0.04 - 0.22)	0.19 (0.06 - 0.32)	-2.72 (-3 - -2.44)	-1.49 (-1.69 - -1.28)	-1.26 (-1.48 - -1.04)	-2.31 (-2.56 - -2.06)
28	Chlorpyrifos	ν	0.11 (0.01 - 0.21)	0.1 (0 - 0.19)	-3.27 (-3.45 - -3.1)	-2.63 (-2.79 - -2.48)	-3.22 (-3.39 - -3.05)	-3.42 (-3.61 - -3.23)
29	Clothianidin	ν	-0.05 (-0.3 - 0.2)	0.19 (-0.07 - 0.44)	-2.66 (-3.06 - -2.26)	-2.58 (-2.97 - -2.19)	-3.19 (-3.69 - -2.69)	-3.93 (-4.46 - -3.41)

30	Diflufenican	ν	0.06 (-0.02 - 0.14)	0.26 (0.17 - 0.34)	-1.89 (-2.03 - -1.75)	-2.45 (-2.59 - -2.31)	-3.14 (-3.3 - -2.98)	-2.09 (-2.22 - -1.95)
31	Dimethenamid	ν	-0.04 (-0.16 - 0.08)	0.22 (0.11 - 0.34)	-3.44 (-3.69 - -3.2)	-2.7 (-2.88 - -2.51)	-2.79 (-2.98 - -2.59)	-2.99 (-3.19 - -2.78)
32	Dimoxystrobin	ν	0.19 (-0.02 - 0.41)	0.23 (0.01 - 0.46)	-3.37 (-3.78 - -2.96)	-2.25 (-2.58 - -1.91)	-3.14 (-3.55 - -2.72)	-3.58 (-4.02 - -3.15)
33	Diuron	ν	0.05 (-0.01 - 0.12)	0.28 (0.22 - 0.35)	-3.88 (-4.09 - -3.67)	-1.67 (-1.76 - -1.58)	-1.74 (-1.84 - -1.63)	-2.72 (-2.85 - -2.6)
34	Ethofumesat	ν	0.09 (-0.01 - 0.18)	0.21 (0.12 - 0.3)	-4.39 (-4.63 - -4.16)	-2.23 (-2.35 - -2.11)	-3.49 (-3.66 - -3.32)	-4.23 (-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	Terbutylazin	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)

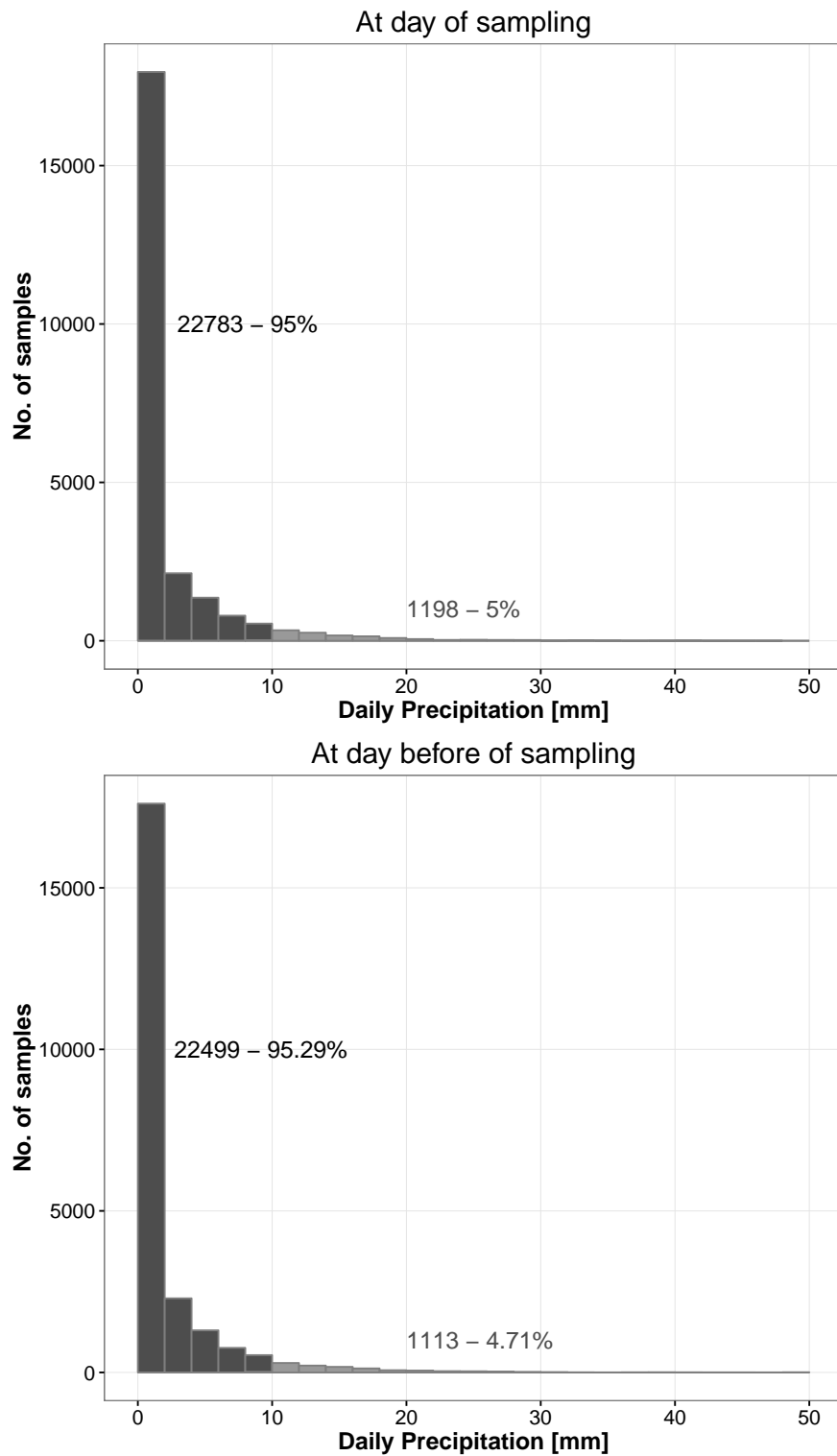


Figure S6: Distribution of precipitation at sampling occasions. top: at sampling date.
bottom: at day before sampling.

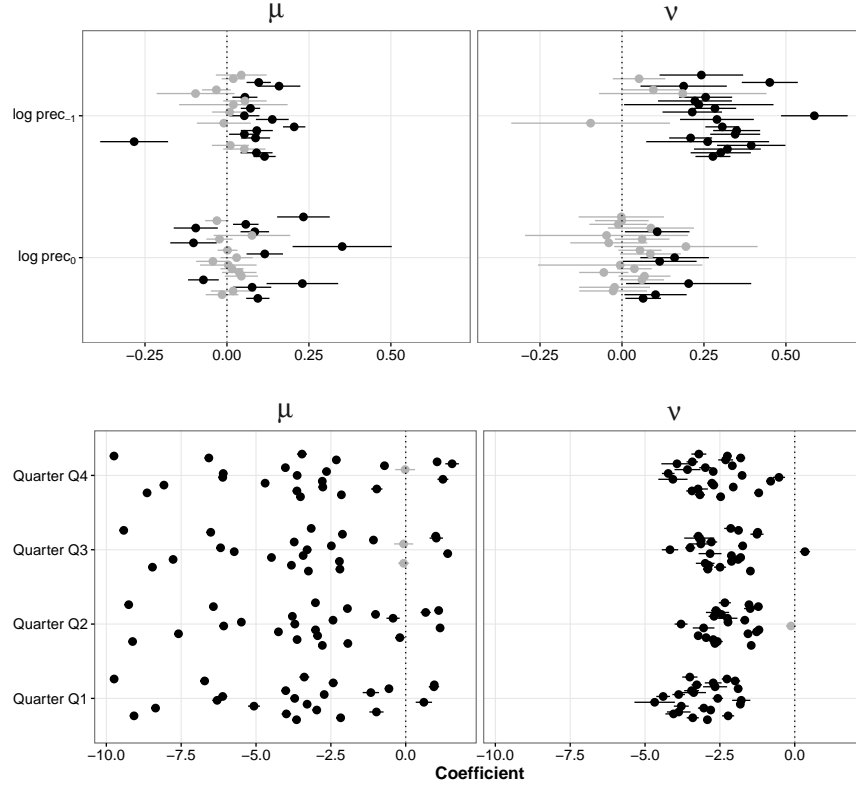


Figure S7: Graphical representation of coefficients from table S4. Top row: Effect of precipitation at day before sampling and at day of sampling. Bottom row: estimates for the four Quarters. Each dot represents one compound (in the order described in table S3). Coefficients where the CI encompasses 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

Table S5: Overview on RAC exceedances of the 76 compounds with more than 1000 measurements. No. = number of measurements; % RQ >1 = RAC exceedances; % RQ >1 | >LOQ= RAC exceedances as fraction of detects.

Name	No.	No. >LOQ	% >LOQ	No. RQ >1	% RQ >1	% RQ >1 >LOQ
2,4-D	12290	284	2.3	10	0.1	3.5
Aclonifen	9861	67	0.7	4	0.0	6.0
Azoxystrobin	7059	690	9.8	6	0.1	0.9
Benalaxyl	6964	10	0.1	0	0.0	0.0
Bentazon	12429	2421	19.5	0	0.0	0.0
Boscalid	9886	2296	23.2	0	0.0	0.0
Bromoxynil	9451	78	0.8	0	0.0	0.0
Carbendazim	3851	654	17.0	12	0.3	1.8
Chloridazon	15724	511	3.2	0	0.0	0.0
Chlorpyrifos	14704	954	6.5	954	6.5	100.0
Chlortoluron	18286	371	2.0	2	0.0	0.5
Clomazon	9268	440	4.7	0	0.0	0.0
Clopyralid	5520	107	1.9	0	0.0	0.0
Clothianidin	2409	154	6.4	123	5.1	79.9
Cypermethrin	1428	5	0.4	1	0.1	20.0
Cyprodinil	9779	118	1.2	0	0.0	0.0
Dicamba	7641	76	1.0	0	0.0	0.0
Difenoconazol	1644	11	0.7	2	0.1	18.2
Diffufenican	15457	1932	12.5	273	1.8	14.1
Dimefuron	7833	5	0.1	0	0.0	0.0
Dimethachlor	8858	344	3.9	0	0.0	0.0
Dimethenamid	9568	594	6.2	5	0.1	0.8
Dimethoat	14423	185	1.3	1	0.0	0.5
Dimethomorph	2316	91	3.9	0	0.0	0.0
Dimoxystrobin	3370	232	6.9	49	1.5	21.1
Diuron	18560	2336	12.6	40	0.2	1.7
Epoxiconazol	16454	621	3.8	7	0.0	1.1
Ethofumesat	20430	1078	5.3	0	0.0	0.0
Fenhexamid	2690	42	1.6	0	0.0	0.0

Fenpropimorph	12850	199	1.5	5	0.0	2.5
Fluazifop-P	4033	14	0.3	0	0.0	0.0
Fluazifop-P-butyl	1728	0	0.0	0	0.0	
Fludioxonil	3203	42	1.3	1	0.0	2.4
Flufenacet	13509	798	5.9	1	0.0	0.1
Fluquinconazole	6762	117	1.7	0	0.0	0.0
Fluroxypyr	8096	378	4.7	0	0.0	0.0
Flurtamone	16958	638	3.8	2	0.0	0.3
Flusilazol	5257	53	1.0	1	0.0	1.9
Glyphosate	3557	1455	40.9	1	0.0	0.1
Imidacloprid	3169	192	6.1	169	5.3	88.0
Ioxynil	8114	20	0.2	0	0.0	0.0
Isoproturon	19112	4164	21.8	92	0.5	2.2
Kresoxim-methyl	6929	14	0.2	0	0.0	0.0
Lenacil	13837	183	1.3	0	0.0	0.0
MCPA	12773	1687	13.2	2	0.0	0.1
Mecoprop	12521	1552	12.4	0	0.0	0.0
Metalaxyl	14460	299	2.1	0	0.0	0.0
Metamitron	15390	613	4.0	0	0.0	0.0
Metazachlor	21906	2015	9.2	55	0.3	2.7
Methamidophos	1303	0	0.0	0	0.0	
Methobromuron	14968	24	0.2	1	0.0	4.2
Metribuzin	15411	192	1.2	15	0.1	7.8
Napropamid	9914	269	2.7	1	0.0	0.4
Nicosulfuron	5172	288	5.6	77	1.5	26.7
Penconazol	4846	159	3.3	0	0.0	0.0
Pendimethalin	16997	328	1.9	4	0.0	1.2
Pethoxamid	3102	37	1.2	0	0.0	0.0
Phoxim	1492	0	0.0	0	0.0	
Picolinafen	8901	11	0.1	2	0.0	18.2
Picoxystrobin	3620	7	0.2	0	0.0	0.0
Pirimicarb	11330	232	2.0	27	0.2	11.6
Prochloraz	5795	33	0.6	0	0.0	0.0
Propiconazol	14250	818	5.7	7	0.0	0.9
Propyzamid	11937	453	3.8	0	0.0	0.0
Prosulfocarb	5001	126	2.5	0	0.0	0.0
Pyrimethanil	8136	122	1.5	0	0.0	0.0
Quinmerac	7291	989	13.6	0	0.0	0.0
Rimsulfuron	1240	2	0.2	0	0.0	0.0
Spiroxamin	2469	109	4.4	1	0.0	0.9
Tebuconazol	16584	1024	6.2	26	0.2	2.5
Terbuthylazin	22568	3370	14.9	35	0.2	1.0
Thiacloprid	3540	85	2.4	85	2.4	100.0
Thiamethoxam	1853	39	2.1	7	0.4	17.9

Triadimenol	3067	51	1.7	0	0.0	0.0
Triazophos	3588	2	0.1	1	0.0	50.0
Trifloxystrobin	3674	10	0.3	1	0.0	10.0

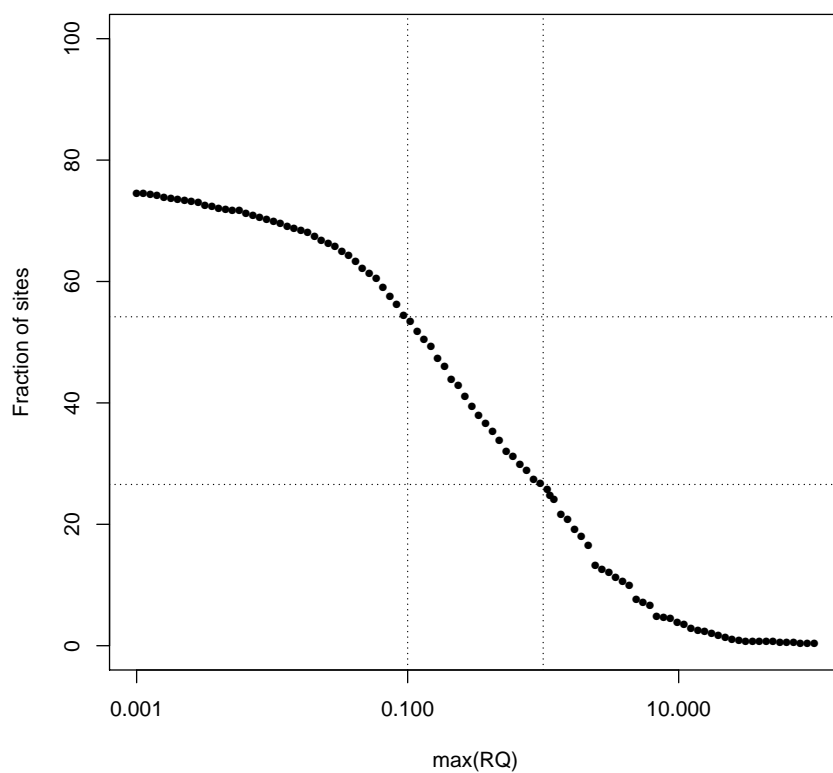


Figure S8: Cumulative distribution of sites exceeding RAC. Dotted lines indicate fraction of sites exceeding a RQ of 1 and 0.1. 23% of the sites showed no detection of compounds with available RAC values and are not shown due to logarithmic x-axis.

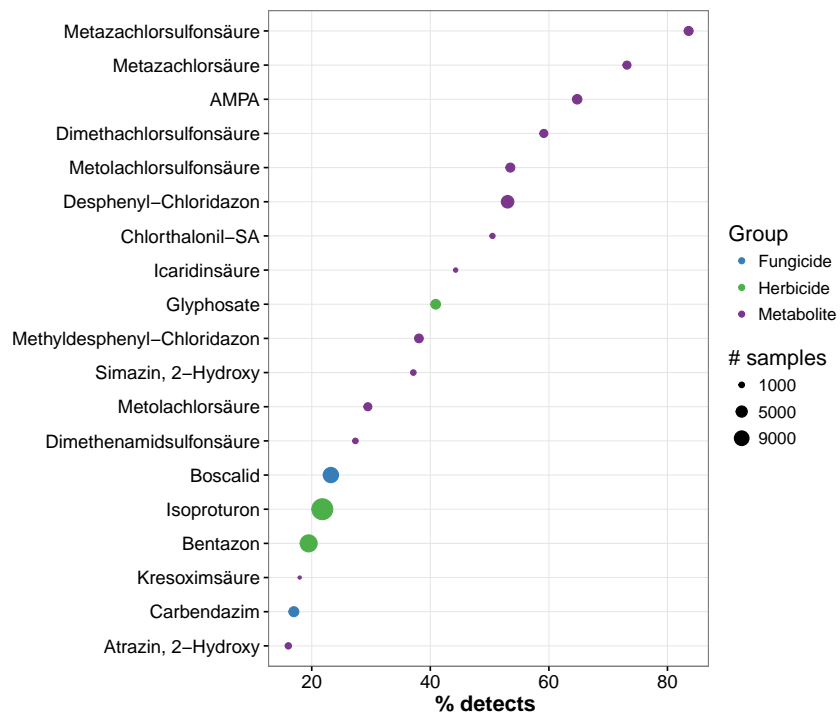


Figure S9: Proportion of samples with detects in small streams. Only Compounds with more than 100 samples and 15% of detects are shown.

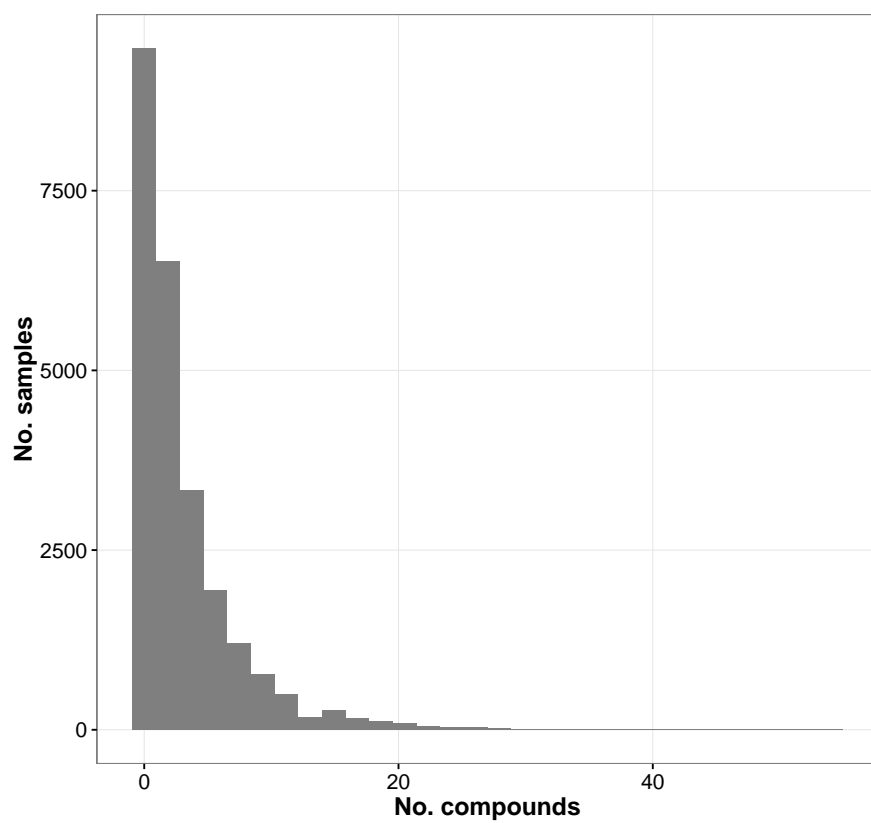


Figure S10: Distribution of the number of quantified compounds in the samples.