

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

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1 Data Cleaning

Each of more than 30 datasets have been cleaned and homogenized separately, before combining in a common database. Cleaning steps comprised (Figure 1.1 gives a graphical overview).

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

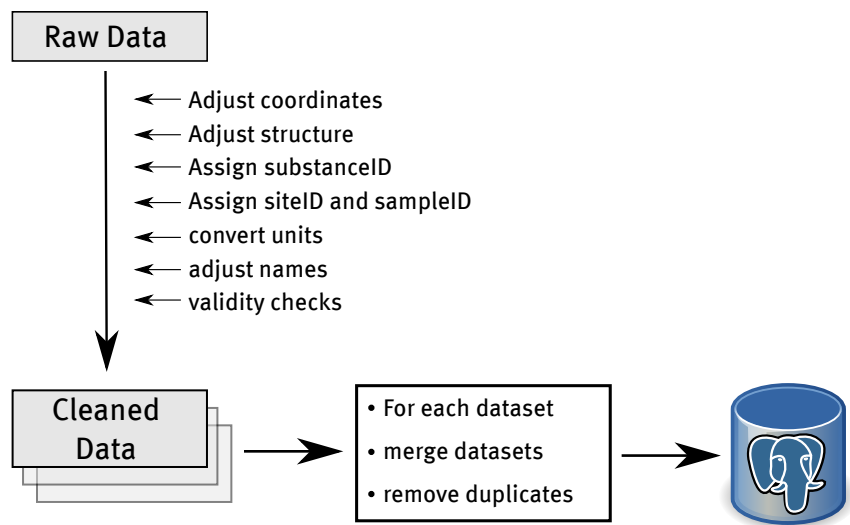


Figure 1.1: Overview on data cleaning steps. After cleaning data has been stored in a relational spatial PostgreSQL database.

2 Overview on compiled data

Table 2.1: Overview on chemical samples. Only data from running waters and grab sampling is shown. ^a: Abbreviations according to IS 3166-2:DE. ^b: Including metabolites

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

Table 2.2: Analysed chemical compounds. ^a Maximum Annual Concentration Environmental Quality Standard [ug/L]. ^b Regulatory Acceptable Concentration [ug/L] (Source: German EPA). ^c Authorized in Germany (Source: BVL, 2015). ^d Authorized in the EU (Source: EU).

	Name	CAS	Group	MAC-EQS ^a	RAC ^b	Auth. GER ^c	Auth. EU ^d
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	1.00	1.10	x	x
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	0.12	1.06	x	x

15	Alachlor	15972-60-8	herbicide	0.70			
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	2.00			
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		0.55	x	x
26	Benalaxyl	71626-11-4	fungicide		20.00	x	x
27	Bensulfuron-methyl	83055-99-6	herbicide				x
28	Bentazon	25057-89-0	herbicide		710.00	x	x
29	Bifenox	42576-02-3	herbicide	0.04		x	x
30	Bifenthrin	82657-04-3	insecticide				x
31	Boscalid	188425-85-6	fungicide		12.50	x	x
32	Bromacil	314-40-9	herbicide				
33	Bromocyclen	1715-40-8	insecticide				
34	Bromoxynil	1689-84-5	herbicide		3.30	x	x
35	Carbendazim	10605-21-7	fungicide	0.70	0.15		
36	Carbofuran	1563-66-2	insecticide				
37	Chlordan	57-74-9	insecticide				
38	Chlorfenvinphos	470-90-6	insecticide	0.30			
39	Chloridazon	1698-60-8	herbicide		56.00	x	x
40	Chloroxuron	1982-47-4	herbicide				
41	Chlorpyrifos	2921-88-2	insecticide	0.10	0.00		x
42	Chlortoluron	15545-48-9	herbicide		2.30	x	x
43	Clomazon	81777-89-1	herbicide		5.70	x	x
44	Clopyralid	1702-17-6	herbicide		1080.00	x	x
45	Clothianidin	210880-92-5	insecticide		0.01	x	x
46	Coumaphos	56-72-4	insecticide				
47	Cyanazin	21725-46-2	herbicide				
48	Cyazofamid	120116-88-3	fungicide			x	x
49	Cypermethrin	52315-07-8	insecticide	0.00	0.00	x	x
50	Cyprodinil	121552-61-2	fungicide		0.75	x	x
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	Desethylterbutylazin	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	0.00			
63	Dicofol	115-32-2	insecticide				
64	Dieldrin	60-57-1	insecticide				
65	Diffufenican	83164-33-4	herbicide		0.03	x	x
66	Dimefuron	34205-21-5	herbicide		0.83		
67	Dimethachlor	50563-36-5	herbicide		3.50	x	x
68	Dimethachlorsäure		metabolite				
69	Dimethachlorsulfonsäure		metabolite				
70	Dimethenamid	87674-68-8	herbicide		1.35		
71	Dimethenamidsulfonsäure		metabolite				
72	Dimethoat	60-51-5	insecticide	1.00	4.00	x	x
73	Dimethomorph	110488-70-5	fungicide		5.60	x	x

74	Dimoxystrobin	149961-52-4	fungicide	2.00	0.03	x	x
75	Disulfoton	298-04-4	insecticide				
76	Diuron	330-54-1	herbicide	1.80	0.79		x
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		0.54	x	x
81	Ethofenprox	80844-07-1	insecticide			x	x
82	Ethofumesat	26225-79-6	herbicide		24.00	x	x
83	Etrifos	38260-54-7	insecticide				
84	Fenhexamid	126833-17-8	fungicide		10.10	x	x
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	20.00	0.20	x	x
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	0.20	2.40	x	x
93	Fluopicolide	239110-15-7	fungicide			x	x
94	Fluoxastrobin	361377-29-9	fungicide			x	x
95	Fluquinconazole	136426-54-5	fungicide		0.80	x	x
96	Fluroxypyr	69377-81-7	herbicide		16.00	x	x
97	Flurtamone	96525-23-4	herbicide	1.00	0.99	x	x
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		100.00	x	x
102	Haloxyfop	69806-34-4	herbicide				
103	HCH, gamma (Lindan)	58-89-9	insecticide				
104	Heptachlor	76-44-8	insecticide	0.00			
105	Heptachlorepoxyd	1024-57-3	metabolite	0.00			
106	Heptenophos	23560-59-0	insecticide				
107	Hexachlorbenzen	118-74-1	fungicide	0.05			
108	Hexazinon	51235-04-2	herbicide				
109	Imidacloprid	138261-41-3	insecticide	0.10	0.01	x	x
110	Ioxynil	1689-83-4	herbicide		2.70	x	
111	Isodrin	465-73-6	insecticide				
112	Isoproturon	34123-59-6	herbicide	1.00	1.30	x	x
113	Isoxaben	82558-50-7	herbicide			x	x
114	Kresoxim-methyl	143390-89-0	fungicide		1.00	x	x
115	Lenacil	2164-08-1	herbicide		0.65	x	x
116	Linuron	330-55-2	herbicide				x
117	Malathion	121-75-5	insecticide				x
118	MCPA	94-74-6	herbicide		9.00	x	x
119	MCPB	94-81-5	herbicide				x
120	Mecoprop	93-65-2	herbicide		160.00		x
121	Metalaxyl	57837-19-1	fungicide		46.00		x
122	Metaldehyd	108-62-3	other			x	x
123	Metamitron	41394-05-2	herbicide		38.00	x	x
124	Metazachlor	67129-08-2	herbicide		0.88	x	x
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		2.00		x
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	0.58	x		x
138	Mevinphos	7786-34-7	insecticide				
139	Mirex	2385-85-5	insecticide				
140	Monolinuron	1746-81-2	herbicide	20.00			
141	Napropamid	15299-99-7	herbicide	6.70	x		x
142	Nicosulfuron	111991-09-4	herbicide	0.09	0.09	x	x
143	o,p-DDE	3424-82-6	metabolite				
144	o,p-DDT	789-02-6	insecticide				
145	Omethoat	1113-02-6	insecticide	2.00			
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	3.20	x		x
154	Pencycuron	66063-05-6	fungicide		x		x
155	Pendimethalin	40487-42-1	herbicide	0.63	x		x
156	Pethoxamid	106700-29-2	herbicide	1.77	x		x
157	Phenmedipham	13684-63-4	herbicide		x		x
158	Phoxim	14816-18-3	insecticide	0.01			
159	Picolinafen	137641-05-5	herbicide	0.04	x		x
160	Picoxystrobin	117428-22-5	fungicide	0.60	x		x
161	Pirimicarb	23103-98-2	insecticide	0.09	x		x
162	Prochloraz	67747-09-5	fungicide	5.00	x		x
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	2.00	x		x
168	Propoxur	114-26-1	insecticide				
169	Propyzamid	23950-58-5	herbicide	34.00	x		x
170	Prosulfocarb	52888-80-9	herbicide	3.80	x		x
171	Pyraclostrobin	175013-18-0	fungicide		x		x
172	Pyrimethanil	53112-28-0	fungicide	8.00	x		x
173	Quinmerac	90717-03-6	herbicide	316.00	x		x
174	Quinoxifen (5,7-dichloro-4-(p-fluorophenoxy)quinoline)	124495-18-7	fungicide	2.70	x		x
175	Sebuthylazin	7286-69-3	herbicide				
176	Simazin	122-34-9	herbicide	4.00			
177	Simazin, 2-Hydroxy	2599-11-3	metabolite				
178	Spiroxamin	118134-30-8	fungicide	0.13	x		x
179	Tebuconazol	107534-96-3	fungicide	0.58	x		x
180	Terbutryn	886-50-0	herbicide	0.34			
181	Terbutylazin	5915-41-3	herbicide	1.20	x		x
182	Thiacloprid	111988-49-9	insecticide	0.00	x		x
183	Thiamethoxam	153719-23-4	insecticide	0.04	x		x
184	Thifensulfuron-methyl	79277-27-3	herbicide				
185	Tolclofos-methyl	57018-04-9	fungicide		x		x
186	Tolyfluanid	731-27-1	fungicide				
187	trans-Chlordan	5103-74-2	insecticide				
188	Triadimenol	55219-65-3	fungicide	3.40	x		x
189	Quintozen	82-68-8	fungicide				
190	Triazophos	24017-47-8	insecticide	0.03			

191	Tribenuron	106040-48-6	herbicide		x	x
192	Trichlorfon	52-68-6	insecticide			
193	Trifloxystrobin	141517-21-7	fungicide	0.09	x	x
194	Trifluralin	1582-09-8	herbicide			
195	Tritosulfuron	142469-14-5	herbicide		x	x
196	Tefluthrin	79538-32-2	insecticide		x	x
197	tau-Fluvalinat	102851-06-9	insecticide	0.03	x	x
198	Sulcotrion	99105-77-8	herbicide	5.00	x	x
199	Methiocarb	2032-65-7	insecticide	0.01	x	x
200	Mesotrion	104206-82-8	herbicide		x	x
201	Fluazifop	69335-91-7	herbicide			
202	Fenoxaprop	95617-09-7	herbicide			
203	Esfenvalerat	66230-04-4	insecticide		x	x
204	Dinoterb	1420-07-1	herbicide			
205	Dicamba	1918-00-9	herbicide	180.00	x	x
206	Deltamethrin	52918-63-5	insecticide		x	x
207	Cyhalothrin (Summe Isomere)	91465-08-6	insecticide		x	x
208	Cyfluthrin (Summe Isomere)	68359-37-5	insecticide			
209	Chlormequat	7003-89-6	other		x	x
210	Thiometon	640-15-3	insecticide			
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	0.50	x	x
221	Anthranilsäureisopropylamid	30391-89-0	metabolite			
222	Diflubenzuron	35367-38-5	insecticide			x
223	Pyrifeno	88283-41-4	fungicide			
224	Difenoconazol	119446-68-3	fungicide	0.36	x	x
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	0.46	x	x
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	0.26	x	x
233	Oxamyl	23135-22-0	insecticide			x
234	Acibenzolar-S-methyl	135158-54-2	fungicide			x
235	Bromuconazol	116255-48-2	fungicide			x
236	Carfentrazon-ethyl	128639-02-1	herbicide	0.31	x	x
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	7.60	x	x
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	189.00	x	x
260	Myclobutanil	88671-89-0	fungicide	2.40	x	x
261	Acetamiprid	135410-20-7	insecticide	0.24	x	x
262	Chlorfluaazuron	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	0.08	x	x
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	0.35	x	x
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	0.95	x	x
311	Imazosulfuron	122548-33-8	herbicide		x	x
312	Mesosulfuron	400852-66-6	herbicide		x	x
313	Prothioconazol-desthio	120983-64-4	metabolite			
314	Quinoclam	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	Thiencarbazone-methyl	317815-83-1	herbicide		x	x
325	Fluopyram	658066-35-4	fungicide	5.12	x	x
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	Cycloxydim	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	Isoprazam	881685-58-1	fungicide		x	x
350	Penflufen	494793-67-8	fungicide			x
351	Pyroxulam	422556-08-9	herbicide		x	x
352	Fipronil	120068-37-3	insecticide	0.00		x
353	Hexachlorophen	70-30-4	other			
354	(E)-7-(Z)-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	9.00	x	x
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	Benzoessäure	65-85-0	fungicide		x	x
365	Bifenazate	149877-41-8	insecticide		x	x
366	Bixafen	581809-46-3	fungicide	0.46	x	x
367	Bromadiolon	28772-56-7	other			x

368	Captan	133-06-2	fungicide	5.00	x	x
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	4.40	x	x
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	1.35	x	x
381	Dithianon	3347-22-6	fungicide	0.78	x	x
382	Dodin	2439-10-3	fungicide	5.33	x	x
383	Fenoxaprop-p-ethyl	71283-80-2	herbicide			
384	Flonicamid	158062-67-0	insecticide	310.00	x	x
385	Fluazifop-P	83066-88-0	herbicide	146.00	x	x
386	Flumioxazin	103361-09-7	herbicide		x	x
387	Fluroxypyr-methylheptyl	81406-37-3	herbicide	0.31		
388	Fosetyl	15845-66-6	fungicide		x	x
389	gamma-Cyhalothrin	76703-62-3	insecticide		x	x
390	Haloxypop-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	0.22	x	x
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	46.00	x	x
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	1.71	x	x
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	0.06	x	x
417	Sulfurylfluorid	2699-79-8	insecticide		x	x
418	Tembotrione	335104-84-2	herbicide		x	x
419	Tepaloxymdim	149979-41-9	herbicide		x	x
420	Thiram	137-26-8	fungicide	0.11	x	x
421	Topramezone	210631-68-8	herbicide	0.90	x	
422	Trinexapac-ethyl	95266-40-3	other		x	x
423	Warfarin	81-81-2	other			
424	Aziprotrryn	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	Desmethyloproton	34123-57-4	metabolite		
437	Metamitron-Desamino	36993-94-9	metabolite		
438	Orysastrobilin	248593-16-0	fungicide		
439	Desethyl-2-hydroxyterbutylazin	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	Chlorpyrifos 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	Thifensulfuron	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	0.01	x
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	Desethylsebutylazin	37019-18-4	metabolite		
480	Prometon	1610-18-0	herbicide		
481	Atraton	1610-17-9	herbicide		
482	Terbutylazin-Metabolit SYN	545666	metabolite		
483	2-Hydroxydesethylazin	19988-24-0	metabolite		

484	Terbutylazin-Metabolit	CGA	309923-18-0	metabolite
	324007			

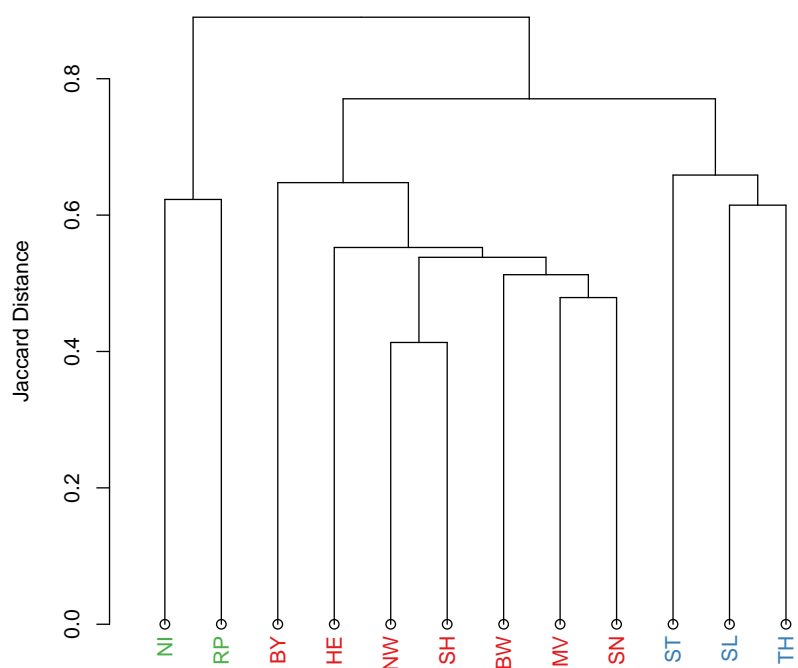


Figure 2.1: Complete Linkage Cluster Dendrogram of Jaccard Similarity of analysed compound spectra between federal states. Abbreviations of state names according to ISO 3166-2:DE.

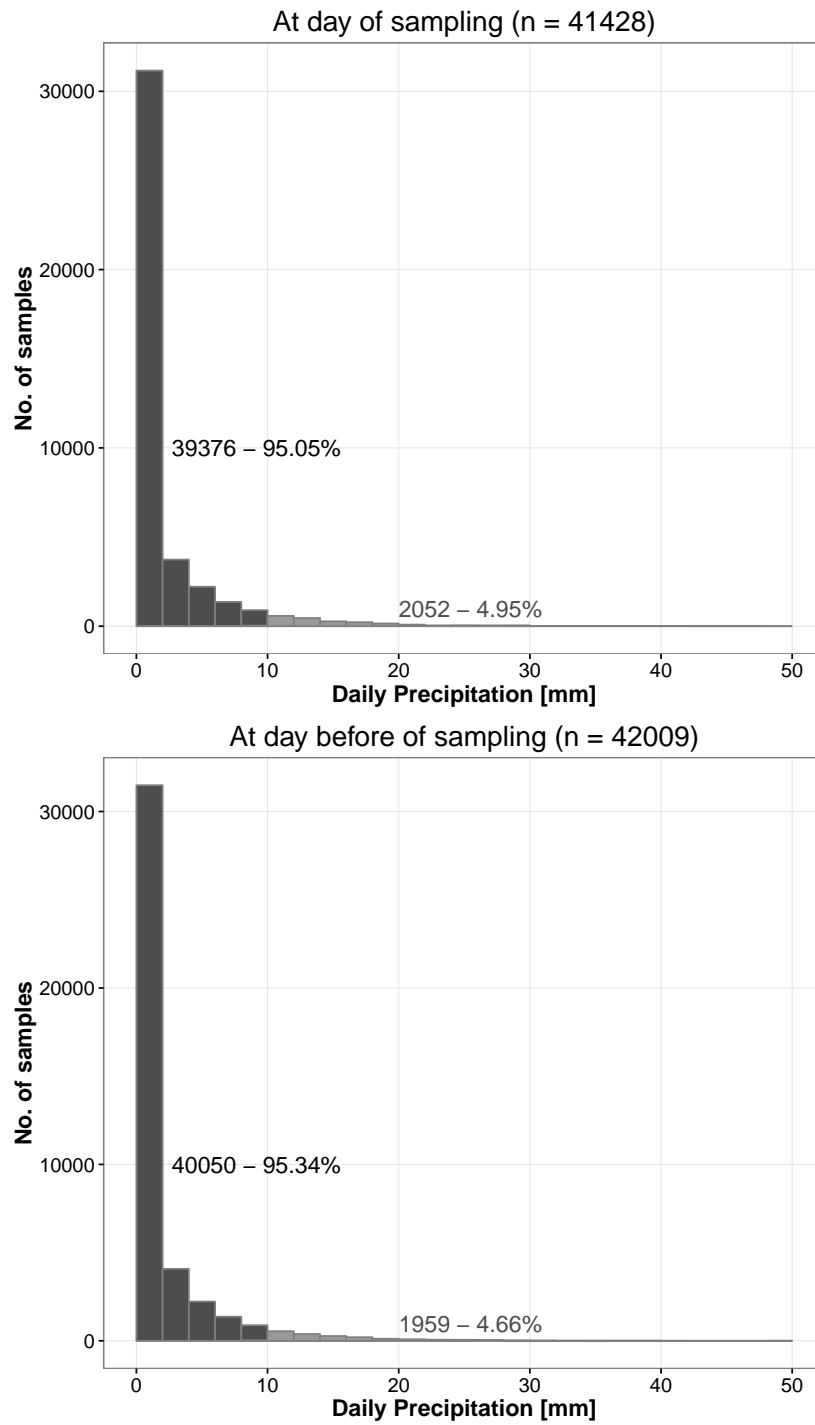


Figure 2.2: Distribution of precipitation at sampling occasions. top: at sampling date. bottom: at day before sampling.

Bibliography

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