

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

Eduard Szöcs, Marvin Brinke, Bilgin Karaoglan, Ralf B. Schäfer

July 29, 2016

Contents

| | | |
|---|---|----|
| 1 | Data Cleaning | 5 |
| 2 | Overview on compiled data | 7 |
| 3 | Are small agricultural waters more polluted compared to bigger streams? | 19 |

List of Figures

| | | |
|-----|---|----|
| 1.1 | Overview on data cleaning steps. After cleaning data has been stored in a relational spatial PostgreSQL database. | 6 |
| 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. | 17 |
| 2.2 | Distribution of precipitation at sampling occasions. top: at sampling date. bottom: at day before sampling. | 18 |
| 3.1 | Raw data used for the model in equation xxx and Figure xxx of the main article. Color codes the number of RAC exceedances (on a log-scale). Grey points are sites without any exceedance. | 20 |

List of Tables

| | | |
|-----|---|---|
| 2.1 | 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 | 7 |
| 2.2 | Analysed chemical compounds. ^a Authorized in Germany (Source: BVL, 2015). ^b Authorized in the EU (Source: EU). ^c [ug/L]. ^d chemprop: Read-Across (Schüürmann et al., 2011); epa: US EPA (U.S. EPA, 2015); malaj:(Malaj et al., 2014); ppdb: Pesticides Properties database (Lewis et al., 2016); none: no LC50 could be found. ^e Maximum Annual Concentration Environmental Quality Standard [ug/L]. ^f Regulatory Acceptable Concentration [ug/L] (Source: German EPA). | 7 |

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).

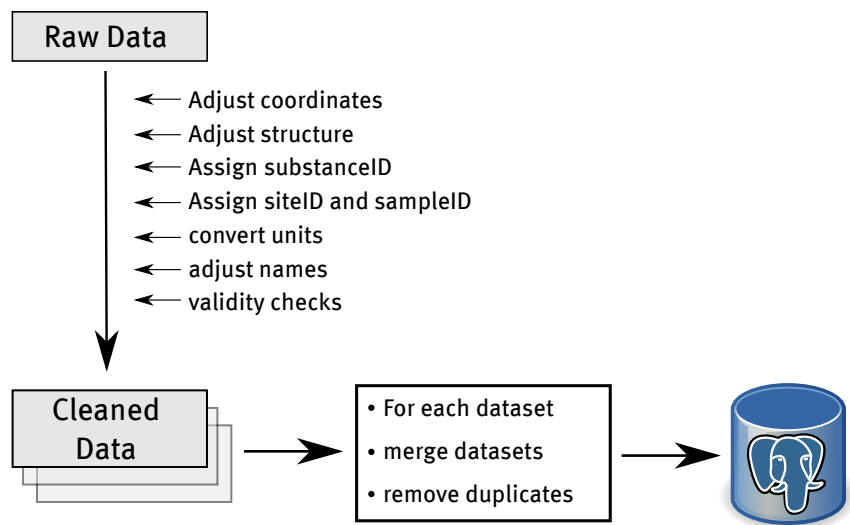


Figure 1.1: Overview on data cleaning steps. After cleaning data has been stored in a relational spatial PostgreSQL database.

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 ISO 3166-2:DE. ^b: Including metabolites

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

Table 2.2: Analysed chemical compounds. ^a Authorized in Germany (Source: BVL, 2015). ^b Authorized in the EU (Source: EU). ^c [ug/L]. ^d chemprop: Read-Across (Schüürmann et al., 2011); epa: US EPA (U.S. EPA, 2015); malaj:(Malaj et al., 2014); ppdb: Pesticides Properties database (Lewis et al., 2016); none: no LC50 could be found. ^e Maximum Annual Concentration Environmental Quality Standard [ug/L]. ^f Regulatory Acceptable Concentration [ug/L] (Source: German EPA).

| | Name | CAS | Group | Auth. GER ^a | Auth. EU ^b | LC50 _{D.magna} ^c | Source LC50 ^d | MAC- EQS ^e | RAC ^f |
|----|-------------------------|------------|-------------|---------------------------|--------------------------|--------------------------------------|-----------------------------|--------------------------|------------------|
| 1 | 1,3-cis-Dichlorpropen | 10061-01-5 | other | | | 6483.44 | chemprop | | |
| 2 | 1,3-trans-Dichlorpropen | 10061-02-6 | other | | | 6483.44 | chemprop | | |
| 3 | 2,4-D | 94-75-7 | herbicide | x | x | 148281.00 | malaj | 1.00 | 1.10 |
| 4 | 2,4-DB | 94-82-6 | herbicide | | x | 25000.00 | malaj | | |
| 5 | 2,4-Dichlorphenol | 120-83-2 | metabolite | | | 2600.00 | malaj | | |
| 6 | 2,4,5-T | 93-76-5 | herbicide | | | 5000.00 | malaj | | |
| 7 | 2,4,6-Trichlorphenol | 88-06-2 | metabolite | | | 1710.00 | malaj | | |
| 8 | 2,6-Dichlorobenzamid | 2008-58-4 | metabolite | | | 180000.00 | malaj | | |
| 9 | 3-Hydroxy Carbofuran | 16655-82-6 | metabolite | | | 293.44 | chemprop | | |
| 10 | 4,6-Dinitro-o-Cresol | 534-52-1 | insecticide | | | 3200.00 | malaj | | |
| 11 | Acetochlor | 34256-82-1 | herbicide | | | 8600.00 | malaj | | |

| | | | | | | | | | |
|----|------------------------|-------------|-------------|---|---|-----------|----------|------|---------|
| 12 | Acetochlorsäure | 194992-44-4 | metabolite | | | | none | | |
| 13 | Acetochlorsulfonsäure | 187022-11-3 | metabolite | | | 139523.68 | chemprop | | |
| 14 | Aclonifen | 74070-46-5 | herbicide | x | x | 1200.00 | ppdb | 0.12 | 1.06 |
| 15 | Alachlor | 15972-60-8 | herbicide | | | 10000.00 | malaj | 0.70 | |
| 16 | Aldicarb | 116-06-3 | insecticide | | | 339.52 | epa | | |
| 17 | Aldrin | 309-00-2 | insecticide | | | 28.00 | malaj | | |
| 18 | Ametryn | 834-12-8 | herbicide | | | 28000.00 | malaj | | |
| 19 | AMPA | 1066-51-9 | metabolite | | | | none | | |
| 20 | Atrazin | 1912-24-9 | herbicide | | | 54000.00 | malaj | 2.00 | |
| 21 | Atrazin, 2-Hydroxy | 2163-68-0 | metabolite | | | 36738.13 | chemprop | | |
| 22 | Avermectin B1a | 71751-41-2 | insecticide | x | x | | none | | |
| 23 | Azinphos-ethyl | 2642-71-9 | insecticide | | | 4.00 | epa | | |
| 24 | Azinphos-methyl | 86-50-0 | insecticide | | | 2.09 | epa | | |
| 25 | Azoxystrobin | 131860-33-8 | fungicide | x | x | 254.47 | epa | | 0.55 |
| 26 | Benalaxyl | 71626-11-4 | fungicide | x | x | 590.00 | ppdb | | 20.00 |
| 27 | Bensulfuron-methyl | 83055-99-6 | herbicide | | x | 130000.00 | ppdb | | |
| 28 | Bentazon | 25057-89-0 | herbicide | x | x | 125000.00 | malaj | | 710.00 |
| 29 | Bifenox | 42576-02-3 | herbicide | x | x | 350.00 | epa | 0.04 | |
| 30 | Bifenthrin | 82657-04-3 | insecticide | | x | 1.53 | epa | | |
| 31 | Boscalid | 188425-85-6 | fungicide | x | x | 5330.00 | ppdb | | 12.50 |
| 32 | Bromacil | 314-40-9 | herbicide | | | 121000.00 | malaj | | |
| 33 | Bromocyclen | 1715-40-8 | insecticide | | | 700.00 | ppdb | | |
| 34 | Bromoxynil | 1689-84-5 | herbicide | x | x | 12500.00 | malaj | | 3.30 |
| 35 | Carbendazim | 10605-21-7 | fungicide | | | 131.52 | epa | 0.70 | 0.15 |
| 36 | Carbofuran | 1563-66-2 | insecticide | | | 9.40 | malaj | | |
| 37 | Chlordan | 57-74-9 | insecticide | | | 98.40 | malaj | | |
| 38 | Chlorfenvinphos | 470-90-6 | insecticide | | | 0.25 | malaj | 0.30 | |
| 39 | Chloridazon | 1698-60-8 | herbicide | x | x | 132000.00 | malaj | | 56.00 |
| 40 | Chloroxuron | 1982-47-4 | herbicide | | | 2950.00 | epa | | |
| 41 | Chlorpyrifos | 2921-88-2 | insecticide | | x | 0.10 | malaj | 0.10 | 0.00 |
| 42 | Chlortoluron | 15545-48-9 | herbicide | x | x | 67000.00 | ppdb | | 2.30 |
| 43 | Clomazon | 81777-89-1 | herbicide | x | x | 5200.00 | epa | | 5.70 |
| 44 | Clopyralid | 1702-17-6 | herbicide | x | x | 225000.00 | malaj | | 1080.00 |
| 45 | Clothianidin | 210880-92-5 | insecticide | x | x | 119000.00 | epa | | 0.01 |
| 46 | Coumaphos | 56-72-4 | insecticide | | | 0.19 | epa | | |
| 47 | Cyanazin | 21725-46-2 | herbicide | | | 49000.00 | malaj | | |
| 48 | Cyazofamid | 120116-88-3 | fungicide | x | x | 429.19 | epa | | |
| 49 | Cypermethrin | 52315-07-8 | insecticide | x | x | 0.57 | epa | 0.00 | 0.00 |
| 50 | Cyprodinil | 121552-61-2 | fungicide | x | x | 32.00 | epa | | 0.75 |
| 51 | Demeton-O | 298-03-3 | insecticide | | | | none | | |
| 52 | Demeton-S | 126-75-0 | insecticide | | | 22.07 | chemprop | | |
| 53 | Demeton-S-methyl | 919-86-8 | insecticide | | | 23.00 | malaj | | |
| 54 | Demeton-S-methylsulfon | 17040-19-6 | insecticide | | | 259.00 | malaj | | |
| 55 | Desethylatrazin | 6190-65-4 | metabolite | | | 76529.00 | malaj | | |
| 56 | Desethylterbutylazin | 30125-63-4 | metabolite | | | 42000.00 | malaj | | |
| 57 | Desisopropylatrazin | 1007-28-9 | metabolite | | | 132340.00 | malaj | | |
| 58 | Desmetryn | 1014-69-3 | herbicide | | | 26000.00 | malaj | | |
| 59 | Desphenyl-Chloridazon | 6339-19-1 | metabolite | | | | none | | |
| 60 | Diazinon | 333-41-5 | insecticide | | | 1.26 | epa | | |
| 61 | Dichlorprop | 120-36-5 | herbicide | | | 100000.00 | malaj | | |
| 62 | Dichlorvos | 62-73-7 | insecticide | | | 0.19 | malaj | 0.00 | |
| 63 | Dicofol | 115-32-2 | insecticide | | | 140.00 | ppdb | | |
| 64 | Dieldrin | 60-57-1 | insecticide | | | 250.00 | malaj | | |
| 65 | Diflufenican | 83164-33-4 | herbicide | x | x | 4937.72 | chemprop | | 0.03 |
| 66 | Dimefuron | 34205-21-5 | herbicide | | | | none | | 0.83 |
| 67 | Dimethachlor | 50563-36-5 | herbicide | x | x | 24000.00 | ppdb | | 3.50 |
| 68 | Dimethachlorsäure | | metabolite | | | | none | | |

| | | | | | | | | | |
|-----|-------------------------|--------------|-------------|---|---|-----------|----------|-------|--------|
| 69 | Dimethachlorsulfonsäure | | metabolite | | | | none | | |
| 70 | Dimethenamid | 87674-68-8 | herbicide | | | 16000.00 | epa | | 1.35 |
| 71 | Dimethenamidsulfonsäure | | metabolite | | | | none | | |
| 72 | Dimethoat | 60-51-5 | insecticide | x | x | 2000.00 | malaj | 1.00 | 4.00 |
| 73 | Dimethomorph | 110488-70-5 | fungicide | x | x | 10600.00 | epa | | 5.60 |
| 74 | Dimoxystrobin | 149961-52-4 | fungicide | x | x | 39.40 | ppdb | 2.00 | 0.03 |
| 75 | Disulfoton | 298-04-4 | insecticide | | | 13.00 | epa | | |
| 76 | Diuron | 330-54-1 | herbicide | | x | 5700.00 | malaj | 1.80 | 0.79 |
| 77 | Endosulfan, alpha | 959-98-8 | insecticide | | | 440.00 | malaj | | |
| 78 | Endosulfan, beta | 33213-65-9 | insecticide | | | 550.00 | epa | | |
| 79 | Endrin | 72-20-8 | insecticide | | | 117.00 | malaj | | |
| 80 | Epoxiconazol | 133855-98-8 | fungicide | x | x | | chemprop | | 0.54 |
| 81 | Ethofenprox | 80844-07-1 | insecticide | x | x | 0.57 | epa | | |
| 82 | Ethofumesat | 26225-79-6 | herbicide | x | x | 14000.00 | malaj | | 24.00 |
| 83 | Etrinfos | 38260-54-7 | insecticide | | | 1.48 | chemprop | | |
| 84 | Fenhexamid | 126833-17-8 | fungicide | x | x | | chemprop | | 10.10 |
| 85 | Fenitrothion | 122-14-5 | insecticide | | | 8.60 | malaj | | |
| 86 | Fenoprop | 93-72-1 | herbicide | | | 4379.00 | malaj | | |
| 87 | Fenpropidin | 67306-00-7 | fungicide | x | x | 540.00 | ppdb | | |
| 88 | Fenpropimorph | 67564-91-4 | fungicide | x | x | 2380.00 | epa | 20.00 | 0.20 |
| 89 | Fenthion | 55-38-9 | insecticide | | | 12.17 | epa | | |
| 90 | Fenuron | 101-42-8 | herbicide | | | 1679.96 | chemprop | | |
| 91 | Fluazifop-P-butyl | 79241-46-6 | herbicide | | | 2995.84 | chemprop | | 7.70 |
| 92 | Flufenacet | 142459-58-3 | herbicide | x | x | 30900.00 | ppdb | 0.20 | 2.40 |
| 93 | Fluopicolide | 239110-15-7 | fungicide | x | x | 1700.00 | epa | | |
| 94 | Fluoxastrobin | 361377-29-9 | fungicide | x | x | 646.22 | epa | | |
| 95 | Fluquinconazole | 136426-54-5 | fungicide | x | x | | chemprop | | 0.80 |
| 96 | Fluroxypyr | 69377-81-7 | herbicide | x | x | 100000.00 | epa | | 16.00 |
| 97 | Flurtamone | 96525-23-4 | herbicide | x | x | 13000.00 | ppdb | 1.00 | 0.99 |
| 98 | Flusilazol | 85509-19-9 | fungicide | | | 3400.00 | ppdb | | 1.10 |
| 99 | Flutriafol | 76674-21-0 | fungicide | | x | 21749.83 | epa | | |
| 100 | Glufosinat | 51276-47-2 | herbicide | x | x | | none | | |
| 101 | Glyphosate | 1071-83-6 | herbicide | x | x | 40000.00 | malaj | | 100.00 |
| 102 | Haloxifop | 69806-34-4 | herbicide | | | 63160.93 | chemprop | | |
| 103 | HCH, gamma (Lindan) | 58-89-9 | insecticide | | | 1600.00 | malaj | | |
| 104 | Heptachlor | 76-44-8 | insecticide | | | 42.00 | malaj | 0.00 | |
| 105 | Heptachlorepoxyd | 1024-57-3 | metabolite | | | 240.00 | malaj | 0.00 | |
| 106 | Heptenophos | 23560-59-0 | insecticide | | | 2.20 | ppdb | | |
| 107 | Hexachlorbenzen | 118-74-1 | fungicide | | | 5.70 | malaj | 0.05 | |
| 108 | Hexazinon | 51235-04-2 | herbicide | | | 85000.00 | malaj | | |
| 109 | Imidacloprid | 138261-41-3 | insecticide | x | x | 30638.85 | epa | 0.10 | 0.01 |
| 110 | Ioxynil | 1689-83-4 | herbicide | x | | 3900.00 | malaj | | 2.70 |
| 111 | Isodrin | 465-73-6 | insecticide | | | 69.00 | malaj | | |
| 112 | Isoproturon | 34123-59-6 | herbicide | x | x | 580.00 | malaj | 1.00 | 1.30 |
| 113 | Isoxaben | 82558-50-7 | herbicide | x | x | 1300.00 | epa | | |
| 114 | Kresoxim-methyl | 143390-89-0 | fungicide | x | x | 332.00 | epa | | 1.00 |
| 115 | Lenacil | 2164-08-1 | herbicide | x | x | 8400.00 | malaj | | 0.65 |
| 116 | Linuron | 330-55-2 | herbicide | | x | 477.00 | malaj | | |
| 117 | Malathion | 121-75-5 | insecticide | | x | 0.70 | malaj | | |
| 118 | MCPA | 94-74-6 | herbicide | x | x | 190000.00 | malaj | | 9.00 |
| 119 | MCPB | 94-81-5 | herbicide | | x | 55000.00 | malaj | | |
| 120 | Mecoprop | 93-65-2 | herbicide | | x | 10000.00 | epa | | 160.00 |
| 121 | Metalaxyl | 57837-19-1 | fungicide | | x | 28000.00 | malaj | | 46.00 |
| 122 | Metaldehyd | 108-62-3 | other | x | x | 77660.00 | epa | | |
| 123 | Metamitron | 41394-05-2 | herbicide | x | x | 97000.00 | malaj | | 38.00 |
| 124 | Metazachlor | 67129-08-2 | herbicide | x | x | 33000.00 | malaj | | 0.88 |
| 125 | Metazachlorsäure | 1231244-60-2 | metabolite | | | | none | | |
| 126 | Metazachlorsulfonsäure | 172960-62-2 | metabolite | | | | none | | |
| 127 | Metconazol | 125116-23-6 | fungicide | x | x | 4200.00 | ppdb | | |

| | | | | | | | | | |
|-----|--|-------------|-------------|---|---|------------|----------|-------|--------|
| 128 | Methabenzthiazuron | 18691-97-9 | herbicide | | | 30600.00 | ppdb | | |
| 129 | Methamidophos | 10265-92-6 | insecticide | | | 270.00 | malaj | | 2.60 |
| 130 | Methobromuron | 3060-89-7 | herbicide | | x | 44100.00 | ppdb | | 2.00 |
| 131 | Methoxychlor | 72-43-5 | insecticide | | | 50.00 | malaj | | |
| 132 | Methyl desphenyl-Chloridazon | 17254-80-7 | metabolite | | | | none | | |
| 133 | Metolachlor | 51218-45-2 | herbicide | | | 15595.00 | malaj | | |
| 134 | Metolachlorsäure | 152019-73-3 | metabolite | | | 87605.85 | chemprop | | |
| 135 | Metolachlorsulfonsäure | 171118-09-5 | metabolite | | | 156909.76 | chemprop | | |
| 136 | Metoxuron | 19937-59-8 | herbicide | | | 160000.00 | epa | | |
| 137 | Metribuzin | 21087-64-9 | herbicide | x | x | 49000.00 | malaj | | 0.58 |
| 138 | Mevinphos | 7786-34-7 | insecticide | | | 12.08 | chemprop | | |
| 139 | Mirex | 2385-85-5 | insecticide | | | 65.00 | malaj | | |
| 140 | Monolinuron | 1746-81-2 | herbicide | | | 32500.00 | ppdb | 20.00 | |
| 141 | Napropamid | 15299-99-7 | herbicide | x | x | 15229.22 | epa | | 6.70 |
| 142 | Nicosulfuron | 111991-09-4 | herbicide | x | x | 1000000.00 | epa | 0.09 | 0.09 |
| 143 | o,p-DDE | 3424-82-6 | metabolite | | | 19.00 | malaj | | |
| 144 | o,p-DDT | 789-02-6 | insecticide | | | 5.00 | malaj | | |
| 145 | Omethoat | 1113-02-6 | insecticide | | | 21.00 | malaj | 2.00 | |
| 146 | Oxadixyl | 77732-09-3 | fungicide | | | 530000.00 | epa | | |
| 147 | Oxydemeton-methyl | 301-12-2 | insecticide | | | 50.23 | epa | | 1.10 |
| 148 | p,p-DDD (p,p TDE) | 72-54-8 | insecticide | | | 9.00 | malaj | | |
| 149 | p,p-DDE | 72-55-9 | metabolite | | | 13.00 | malaj | | |
| 150 | p,p-DDT | 50-29-3 | insecticide | | | 5.00 | malaj | | |
| 151 | Parathion-ethyl | 56-38-2 | insecticide | | | 2.50 | malaj | | |
| 152 | Parathion-methyl | 298-00-0 | insecticide | | | 7.30 | malaj | | |
| 153 | Penconazol | 66246-88-6 | fungicide | x | x | 6750.00 | ppdb | | 3.20 |
| 154 | Pencycuron | 66063-05-6 | fungicide | x | x | 666.50 | chemprop | | |
| 155 | Pendimethalin | 40487-42-1 | herbicide | x | x | 280.00 | malaj | | 0.63 |
| 156 | Pethoxamid | 106700-29-2 | herbicide | x | x | 23000.00 | ppdb | | 1.77 |
| 157 | Phenmedipham | 13684-63-4 | herbicide | x | x | 14000.00 | epa | | |
| 158 | Phoxim | 14816-18-3 | insecticide | | | 0.81 | ppdb | | 0.01 |
| 159 | Picolinafen | 137641-05-5 | herbicide | x | x | 13805.30 | chemprop | | 0.04 |
| 160 | Picoxystrobin | 117428-22-5 | fungicide | x | x | 24.00 | ppdb | | 0.60 |
| 161 | Pirimicarb | 23103-98-2 | insecticide | x | x | 17.00 | malaj | | 0.09 |
| 162 | Prochloraz | 67747-09-5 | fungicide | x | x | 3681.99 | epa | | 5.00 |
| 163 | Prometryn | 7287-19-6 | herbicide | | | 12660.00 | malaj | | |
| 164 | Propamocarb | 24579-73-5 | fungicide | x | x | 106000.00 | epa | | |
| 165 | Propanil | 709-98-8 | herbicide | | | 3008.45 | epa | | |
| 166 | Propazin | 139-40-2 | herbicide | | | 11000.00 | malaj | | |
| 167 | Propiconazol | 60207-90-1 | fungicide | x | x | 10200.00 | malaj | | 2.00 |
| 168 | Propoxur | 114-26-1 | insecticide | | | 134.64 | epa | | |
| 169 | Propyzamid | 23950-58-5 | herbicide | x | x | 5600.00 | malaj | | 34.00 |
| 170 | Prosulfocarb | 52888-80-9 | herbicide | x | x | 510.00 | ppdb | | 3.80 |
| 171 | Pyraclostrobin | 175013-18-0 | fungicide | x | x | 32.67 | epa | | |
| 172 | Pyrimethanil | 53112-28-0 | fungicide | x | x | 3040.00 | epa | | 8.00 |
| 173 | Quinmerac | 90717-03-6 | herbicide | x | x | 86745.74 | chemprop | | 316.00 |
| 174 | Quinoxifen (5,7-dichloro-4-(p-fluorophenoxy)quinoline) | 124495-18-7 | fungicide | x | x | 91.00 | epa | 2.70 | |
| 175 | Sebuthylazin | 7286-69-3 | herbicide | | | 34498.39 | chemprop | | |
| 176 | Simazin | 122-34-9 | herbicide | | | 94000.00 | malaj | 4.00 | |
| 177 | Simazin, 2-Hydroxy | 2599-11-3 | metabolite | | | 165760.00 | malaj | | |
| 178 | Spiroxamin | 118134-30-8 | fungicide | x | x | 4164.13 | epa | | 0.13 |
| 179 | Tebuconazol | 107534-96-3 | fungicide | x | x | 2051.97 | epa | | 0.58 |
| 180 | Terbutryn | 886-50-0 | herbicide | | | 7100.00 | malaj | 0.34 | |
| 181 | Terbutylazin | 5915-41-3 | herbicide | x | x | 5000.00 | epa | | 1.20 |
| 182 | Thiacloprid | 111988-49-9 | insecticide | x | x | 44516.96 | epa | | 0.00 |
| 183 | Thiamethoxam | 153719-23-4 | insecticide | x | x | 106000.00 | epa | | 0.04 |

| | | | | | | | | |
|-----|-----------------------------|-------------|-------------|---|---|------------|----------|--------|
| 184 | Thifensulfuron-methyl | 79277-27-3 | herbicide | | | 470000.00 | ppdb | |
| 185 | Tolclofos-methyl | 57018-04-9 | fungicide | x | x | 48000.00 | ppdb | |
| 186 | Tolyfluanid | 731-27-1 | fungicide | | | 190.00 | epa | |
| 187 | trans-Chlordan | 5103-74-2 | insecticide | | | 153.23 | chemprop | |
| 188 | Triadimenol | 55219-65-3 | fungicide | x | x | 2500.00 | epa | 3.40 |
| 189 | Triazophos | 24017-47-8 | insecticide | | | 12.92 | epa | 0.03 |
| 190 | Tribenuron | 106040-48-6 | herbicide | x | x | 1765007.38 | chemprop | |
| 191 | Trichlorfon | 52-68-6 | insecticide | | | 1.28 | epa | |
| 192 | Trifloxystrobin | 141517-21-7 | fungicide | x | x | 136.83 | epa | 0.09 |
| 193 | Trifluralin | 1582-09-8 | herbicide | | | 245.00 | malaj | |
| 194 | Tritosulfuron | 142469-14-5 | herbicide | x | x | | none | |
| 195 | Tefluthrin | 79538-32-2 | insecticide | x | x | 0.11 | epa | |
| 196 | tau-Fluvalinat | 102851-06-9 | insecticide | x | x | 0.94 | epa | 0.03 |
| 197 | Sulcotrion | 99105-77-8 | herbicide | x | x | 430221.57 | chemprop | 5.00 |
| 198 | Methiocarb | 2032-65-7 | insecticide | x | x | 19.00 | epa | 0.01 |
| 199 | Mesotrion | 104206-82-8 | herbicide | x | x | 840000.00 | epa | |
| 200 | Fluazifop | 69335-91-7 | herbicide | | | 31317.92 | chemprop | |
| 201 | Fenoxaprop | 95617-09-7 | herbicide | | | 1260.00 | ppdb | |
| 202 | Esfenvalerat | 66230-04-4 | insecticide | x | x | 0.27 | epa | |
| 203 | Dinoterb | 1420-07-1 | herbicide | | | 2552.17 | chemprop | |
| 204 | Dicamba | 1918-00-9 | herbicide | x | x | 110300.00 | malaj | 180.00 |
| 205 | Deltamethrin | 52918-63-5 | insecticide | x | x | 0.15 | epa | |
| 206 | Cyhalothrin (Summe Isomere) | 91465-08-6 | insecticide | x | x | 0.24 | epa | |
| 207 | Cyfluthrin (Summe Isomere) | 68359-37-5 | insecticide | | | 0.43 | epa | |
| 208 | Chlormequat | 7003-89-6 | other | x | x | | none | |
| 209 | Thiometon | 640-15-3 | insecticide | | | 70.40 | chemprop | |
| 210 | Quintozen | 82-68-8 | fungicide | | | 770.00 | malaj | |
| 211 | Vinclozolin | 50471-44-8 | fungicide | | | 3650.00 | ppdb | |
| 212 | Dichlofluanid | 1085-98-9 | fungicide | | | 1050.00 | epa | |
| 213 | Iprodion | 36734-19-7 | fungicide | x | x | 1010.05 | epa | |
| 214 | Dinoseb | 88-85-7 | herbicide | | | 240.00 | malaj | |
| 215 | Kresoximsäure | | metabolite | | | | none | |
| 216 | Quizalofop | 76578-12-6 | herbicide | | | 57700.00 | ppdb | |
| 217 | Acifluorfen | 50594-66-6 | herbicide | | | 28000.00 | ppdb | |
| 218 | Diclofop | 40843-25-2 | herbicide | | x | 709.06 | epa | |
| 219 | Flamprop | 58667-63-3 | herbicide | | | | none | |
| 220 | Fludioxonil | 131341-86-1 | fungicide | x | x | 900.00 | epa | 0.50 |
| 221 | Anthranilsäureisopropylamid | 30391-89-0 | metabolite | | | | none | |
| 222 | Diflubenzuron | 35367-38-5 | insecticide | | x | 3.76 | epa | |
| 223 | Pyrifeno | 88283-41-4 | fungicide | | | 3600.00 | ppdb | |
| 224 | Difenoconazol | 119446-68-3 | fungicide | x | x | 15.15 | epa | 0.36 |
| 225 | Amidosulfuron | 120923-37-7 | herbicide | x | x | 36000.00 | ppdb | |
| 226 | Triasulfuron | 82097-50-5 | herbicide | x | x | | chemprop | |
| 227 | Metsulfuron | 79510-48-8 | herbicide | x | x | | chemprop | |
| 228 | Rimsulfuron | 122931-48-0 | herbicide | x | x | | chemprop | 0.46 |
| 229 | Triflusulfuron | 135990-29-3 | herbicide | x | x | | chemprop | |
| 230 | Methidathion | 950-37-8 | insecticide | | | 8.73 | epa | |
| 231 | Triflumuron | 64628-44-0 | insecticide | | x | 1.60 | ppdb | |
| 232 | Fluazinam | 79622-59-6 | fungicide | x | x | 199.90 | epa | 0.26 |
| 233 | Oxamyl | 23135-22-0 | insecticide | | x | 1665.36 | epa | |
| 234 | Acibenzolar-S-methyl | 135158-54-2 | fungicide | | x | 2900.00 | epa | |
| 235 | Bromuconazol | 116255-48-2 | fungicide | | x | 869.77 | epa | |
| 236 | Carfentrazon-ethyl | 128639-02-1 | herbicide | x | x | 9800.00 | epa | 0.31 |
| 237 | Clodinafop-propargyl | 105512-06-9 | herbicide | | | 2000.00 | epa | |
| 238 | Cycloat | 1134-23-2 | herbicide | | | 24000.00 | epa | |
| 239 | Cyflufenamid | 180409-60-3 | fungicide | x | x | | none | |
| 240 | Diniconazol | 83657-24-3 | fungicide | | | 7400.00 | ppdb | |

| | | | | | | | | |
|-----|----------------------|-------------|-------------|---|---|------------|----------|--------|
| 241 | Fenamidon | 161326-34-7 | fungicide | x | x | 96.19 | epa | |
| 242 | Fenbuconazol | 114369-43-6 | fungicide | | x | 2300.00 | epa | |
| 243 | Fosthiazat | 98886-44-3 | other | x | x | 414.25 | epa | |
| 244 | Fuberidazol | 3878-19-1 | fungicide | x | x | 4700.00 | ppdb | |
| 245 | Hexaconazol | 79983-71-4 | fungicide | | | 3549.63 | epa | |
| 246 | Hexythiazox | 78587-05-0 | insecticide | x | x | 7155.49 | chemprop | |
| 247 | Indoxacarb | 173584-44-6 | insecticide | x | x | 45.54 | epa | |
| 248 | Mandipropamid | 374726-62-2 | fungicide | x | x | 7100.00 | ppdb | 7.60 |
| 249 | Metrafenon | 220899-03-6 | fungicide | x | x | | none | |
| 250 | Oxadiazon | 19666-30-9 | herbicide | | x | 1935.29 | epa | |
| 251 | Proquinazid | 189278-12-4 | fungicide | x | x | 287.00 | ppdb | |
| 252 | Tebufenpyrad | 119168-77-3 | insecticide | x | x | 40.20 | epa | |
| 253 | Tetraconazol | 112281-77-3 | fungicide | x | x | 3873.84 | epa | |
| 254 | Zoxamid | 156052-68-5 | fungicide | x | x | 780.00 | epa | |
| 255 | Hexaflumuron | 86479-06-3 | insecticide | | | 0.11 | epa | |
| 256 | Neburon | 555-37-3 | herbicide | | | 557.72 | chemprop | |
| 257 | Cyproconazol | 94361-06-5 | fungicide | x | x | 26000.00 | epa | |
| 258 | Fenarimol | 60168-88-9 | fungicide | | | 6800.00 | epa | |
| 259 | Iprovalicarb | 140923-17-7 | fungicide | x | x | 17891.50 | chemprop | 189.00 |
| 260 | Myclobutanil | 88671-89-0 | fungicide | x | x | 11000.00 | epa | 2.40 |
| 261 | Acetamiprid | 135410-20-7 | insecticide | x | x | 50000.00 | epa | 0.24 |
| 262 | Chlorfluazuron | 71422-67-8 | insecticide | | | 0.91 | ppdb | |
| 263 | Cyromazin | 66215-27-8 | insecticide | | x | 32349.03 | epa | |
| 264 | Etaconazol | 60207-93-4 | fungicide | | | 9276.38 | chemprop | |
| 265 | Ethidimuron | 30043-49-3 | herbicide | | | | none | |
| 266 | Fenpyroximat | 134098-61-6 | insecticide | x | x | 22.00 | ppdb | |
| 267 | Flazasulfuron | 104040-78-0 | herbicide | x | x | 13223.50 | chemprop | |
| 268 | Flufenoxuron | 101463-69-8 | insecticide | | | 0.04 | ppdb | |
| 269 | Mepronil | 55814-41-0 | fungicide | | | 10000.00 | epa | |
| 270 | Methomyl | 16752-77-5 | insecticide | | x | 7.60 | malaj | |
| 271 | Methoxyfenozyd | 161050-58-4 | insecticide | x | x | 3700.00 | epa | |
| 272 | Pirimicarb-desmethyl | 30614-22-3 | metabolite | | | 62.44 | chemprop | |
| 273 | Spirodiclofen | 148477-71-8 | insecticide | x | x | | none | |
| 274 | Spiromesifen | 283594-90-1 | insecticide | | x | 92.30 | epa | |
| 275 | Tebufenozid | 112410-23-8 | insecticide | x | x | 3800.00 | malaj | |
| 276 | Thiabendazol | 148-79-8 | fungicide | x | x | 761.18 | epa | |
| 277 | Triflumizol | 99387-89-0 | fungicide | | x | 2110.00 | ppdb | |
| 278 | Triforin | 26644-46-2 | fungicide | | | 13811.28 | epa | |
| 279 | Triticonazol | 131983-72-7 | fungicide | x | x | 7600.00 | epa | |
| 280 | Teflubenzuron | 83121-18-0 | insecticide | | x | 2.80 | ppdb | |
| 281 | Triadimefon | 43121-43-3 | fungicide | | | 7450.34 | epa | |
| 282 | cis-Chlordan | 5103-71-9 | insecticide | | | 153.23 | chemprop | |
| 283 | Monuron | 150-68-5 | herbicide | | | 14358.54 | chemprop | |
| 284 | Propachlor | 1918-16-7 | herbicide | | | 10097.83 | epa | |
| 285 | Fluazifop-butyl | 69806-50-4 | herbicide | | | 316000.00 | ppdb | |
| 286 | Carbetamid | 16118-49-3 | herbicide | | x | 81000.00 | ppdb | |
| 287 | Propetamphos | 31218-83-4 | insecticide | | | 6.86 | epa | |
| 288 | Triallat | 2303-17-5 | herbicide | | x | 115.58 | epa | |
| 289 | Dichlobenil | 1194-65-6 | herbicide | | | 6200.00 | malaj | |
| 290 | Propham | 122-42-9 | herbicide | | | 23000.00 | ppdb | |
| 291 | Endosulfansulfat | 1031-07-8 | metabolite | | | 1023.68 | epa | |
| 292 | Beflubutamid | 113614-08-7 | herbicide | x | x | 1640.00 | ppdb | |
| 293 | Flurochloridon | 61213-25-0 | herbicide | | x | 5100.00 | ppdb | |
| 294 | Iodosulfuron | 185119-76-0 | herbicide | x | x | | chemprop | 0.08 |
| 295 | Metosulam | 139528-85-1 | herbicide | x | x | 8876593.52 | chemprop | |
| 296 | Triclopyr | 55335-06-3 | herbicide | x | x | 132900.00 | epa | |
| 297 | Florasulam | 145701-23-1 | herbicide | x | x | 40074.93 | epa | |
| 298 | Famoxadone | 131807-57-3 | fungicide | x | x | 11.80 | epa | |
| 299 | Folpet | 133-07-3 | fungicide | x | x | 314.86 | epa | |

| | | | | | | | | |
|-----|--------------------------------|-------------|-------------|---|---|-----------|----------|------|
| 300 | Procymidon | 32809-16-8 | fungicide | | | | none | |
| 301 | Thiophanat-methyl | 23564-05-8 | fungicide | x | x | 10719.28 | epa | |
| 302 | Fluometuron | 2164-17-2 | herbicide | | x | 4626.07 | epa | |
| 303 | Bupirimat | 41483-43-6 | fungicide | | x | 7142.95 | chemprop | |
| 304 | Carboxin | 5234-68-4 | fungicide | | x | 69359.93 | epa | |
| 305 | Chlorantraniliprole | 500008-45-7 | insecticide | x | x | 11.07 | epa | 0.35 |
| 306 | Dinotefuran | 165252-70-0 | insecticide | | | 327252.17 | epa | |
| 307 | Fenazaquin | 120928-09-8 | insecticide | x | x | 4.10 | malaj | |
| 308 | Fenoxycarb | 72490-01-8 | insecticide | | x | 400.00 | epa | |
| 309 | Flupyrsulfuron | 150315-10-9 | herbicide | x | x | | none | |
| 310 | Foramsulfuron | 173159-57-4 | herbicide | x | x | 100000.00 | ppdb | 0.95 |
| 311 | Imazosulfuron | 122548-33-8 | herbicide | x | x | 32000.00 | epa | |
| 312 | Mesosulfuron | 400852-66-6 | herbicide | x | x | | none | |
| 313 | Prothioconazol-desthio | 120983-64-4 | metabolite | | | | none | |
| 314 | Quinoclamín | 2797-51-5 | herbicide | x | x | 2150.00 | ppdb | |
| 315 | Sulfosulfuron | 141776-32-1 | herbicide | | x | | chemprop | |
| 316 | Triazoxid | 72459-58-6 | fungicide | x | x | 7200.00 | ppdb | |
| 317 | Tribenuron-methyl | 101200-48-0 | herbicide | | | 894000.00 | ppdb | |
| 318 | Ametoctradin | 865318-97-4 | fungicide | x | x | | none | |
| 319 | Clodinafop | 114420-56-3 | herbicide | x | x | | none | |
| 320 | Cyclanilide | 113136-77-9 | other | | | 8062.26 | epa | |
| 321 | Mepanipyrim | 110235-47-7 | fungicide | x | x | 630.00 | ppdb | |
| 322 | Profoxydim | 139001-49-3 | herbicide | | x | 18100.00 | ppdb | |
| 323 | Propoxycarbazon | 145026-81-9 | herbicide | x | x | 950866.02 | chemprop | |
| 324 | Thiencazabon-methyl | 317815-83-1 | herbicide | x | x | 99297.53 | epa | |
| 325 | Fluopyram | 658066-35-4 | fungicide | x | x | 25483.33 | epa | 5.12 |
| 326 | Flutolanil | 66332-96-5 | fungicide | x | x | 8246.21 | epa | |
| 327 | Chlorthalonil-SA | | metabolite | | | | none | |
| 328 | Dimethachlor-CA | | metabolite | | | | none | |
| 329 | Dimethenamid-CA | | metabolite | | | | none | |
| 330 | Dimethenamid-SA | | metabolite | | | | none | |
| 331 | Flufenacet-SA | | metabolite | | | | none | |
| 332 | Metaxyl-CA | 75596-99-5 | metabolite | | | 37321.03 | chemprop | |
| 333 | Metazachlordicarbonsäure | | metabolite | | | | none | |
| 334 | Metaxyl-CA2 | 104390-56-9 | metabolite | | | | none | |
| 335 | Azoxystrobin-CA | | metabolite | | | | none | |
| 336 | Thiacloprid-SA | | metabolite | | | | none | |
| 337 | Trifloxystrobin-CA2 | | metabolite | | | | none | |
| 338 | Clethodim | 99129-21-2 | herbicide | x | x | | epa | |
| 339 | Cycloxydim | 101205-02-1 | herbicide | x | x | | none | |
| 340 | Imazamox | 114311-32-9 | herbicide | x | x | 122000.00 | epa | |
| 341 | Imazapic | 104098-48-8 | herbicide | | | | none | |
| 342 | Imazaquin | 81335-37-7 | herbicide | | x | 280000.00 | epa | |
| 343 | Imazethapyr | 81335-77-5 | herbicide | | | 331662.48 | epa | |
| 344 | Meptyldinocap | 131-72-6 | fungicide | | x | | none | |
| 345 | Tralkoxydim | 87820-88-0 | herbicide | | x | 14720.73 | epa | |
| 346 | Saflufenacil | 372137-35-4 | herbicide | | | 98200.00 | epa | |
| 347 | Valifenalate | 283159-90-0 | fungicide | x | x | | none | |
| 348 | Fluxapyroxad | 907204-31-3 | fungicide | x | x | 104000.00 | epa | |
| 349 | Isopyrazam | 881685-58-1 | fungicide | x | x | 44.00 | ppdb | |
| 350 | Penflufen | 494793-67-8 | fungicide | | x | | none | |
| 351 | Pyroxulam | 422556-08-9 | herbicide | x | x | 100000.00 | epa | |
| 352 | Fipronil | 120068-37-3 | insecticide | | x | 118.82 | epa | 0.00 |
| 353 | Hexachlorophen | 70-30-4 | other | | | | none | |
| 354 | (E)-7-(Z)-9-Dodecadienylacetat | 55774-32-8 | other | x | x | | none | |
| 355 | (Z)-9-Dodecadienylacetat | 16974-11-1 | other | x | x | 2600.00 | ppdb | |
| 356 | 1-Decanol | 112-30-1 | other | x | x | 6510.00 | epa | |
| 357 | 1-Methylcyclopropen | 3100-04-7 | other | x | x | | none | |

| | | | | | | | | |
|-----|-----------------------------|-------------|-------------|---|---|-----------|----------|--------|
| 358 | Acequinocyl | 57960-19-7 | insecticide | x | x | 2.70 | epa | 9.00 |
| 359 | alpha-Cypermethrin | 67375-30-8 | insecticide | x | x | 0.30 | ppdb | |
| 360 | Aminopyralid | 150114-71-9 | herbicide | x | x | 98600.00 | epa | |
| 361 | Amisulbrom | 348635-87-0 | fungicide | x | x | 37.00 | ppdb | |
| 362 | Azadirachtin (Neem) | 11141-17-6 | insecticide | x | x | 622.58 | epa | |
| 363 | Benthiavalicarb | 413615-35-7 | fungicide | x | x | | none | |
| 364 | Benzoesaure | 65-85-0 | fungicide | x | x | 293257.57 | epa | |
| 365 | Bifenazate | 149877-41-8 | insecticide | x | x | 500.00 | epa | |
| 366 | Bixafen | 581809-46-3 | fungicide | x | x | 1200.00 | ppdb | 0.46 |
| 367 | Bromadiolon | 28772-56-7 | other | | x | 2000.00 | ppdb | |
| 368 | Captan | 133-06-2 | fungicide | x | x | 7100.00 | malaj | 5.00 |
| 369 | Chlorpropham | 101-21-3 | herbicide | x | x | 3700.00 | epa | |
| 370 | Chlorthalonil | 1897-45-6 | fungicide | x | x | 100.82 | epa | |
| 371 | Cinidon-ethyl | 142891-20-1 | herbicide | | | 59200.00 | ppdb | |
| 372 | Clofentezin | 74115-24-5 | insecticide | | x | 44.56 | epa | |
| 373 | Codlemone (Codlelure) | 33956-49-9 | other | x | x | 2800.00 | epa | |
| 374 | Cymoxanil | 57966-95-7 | fungicide | x | x | 2616.85 | epa | 4.40 |
| 375 | Daminozid | 1596-84-5 | other | x | x | 99742.17 | epa | |
| 376 | Deiquat | 2764-72-9 | herbicide | x | x | 1392.94 | epa | |
| 377 | Desmedipham | 13684-56-5 | herbicide | x | x | 450.00 | malaj | |
| 378 | Dichlorprop-P | 15165-67-0 | herbicide | x | x | 3821.30 | epa | |
| 379 | Difenacoum | 56073-07-5 | other | | x | 520.00 | ppdb | |
| 380 | Dimethenamid-P | 163515-14-8 | herbicide | x | x | 12000.00 | epa | 1.35 |
| 381 | Dithianon | 3347-22-6 | fungicide | x | x | 260.00 | ppdb | 0.78 |
| 382 | Dodin | 2439-10-3 | fungicide | x | x | 48.32 | epa | 5.33 |
| 383 | Fenoxaprop-p-ethyl | 71283-80-2 | herbicide | | | 4134.71 | chemprop | |
| 384 | Flonicamid | 158062-67-0 | insecticide | x | x | 98600.00 | epa | 310.00 |
| 385 | Fluazifop-P | 83066-88-0 | herbicide | x | x | 31317.92 | chemprop | 146.00 |
| 386 | Flumioxazin | 103361-09-7 | herbicide | x | x | 5500.00 | epa | |
| 387 | Fluroxypyr- methylheptyl | 81406-37-3 | herbicide | | | | none | 0.31 |
| 388 | Fosetyl | 15845-66-6 | fungicide | x | x | | none | |
| 389 | gamma-Cyhalothrin | 76703-62-3 | insecticide | x | x | 2.91 | epa | |
| 390 | Haloxifop-P | 95977-29-0 | herbicide | x | x | | none | |
| 391 | Hymexazol | 10004-44-1 | fungicide | x | x | 30800.00 | epa | |
| 392 | Imazalil | 35554-44-0 | fungicide | x | x | 3540.00 | epa | |
| 393 | Isoxaflutole | 141112-29-0 | herbicide | x | x | 1500.00 | epa | |
| 394 | Mancozeb | 8018-01-7 | fungicide | x | x | 910.17 | epa | 0.22 |
| 395 | Maneb | 12427-38-2 | fungicide | x | x | 346.41 | epa | |
| 396 | Mepiquat | 15302-91-7 | other | x | x | | none | |
| 397 | Metaflumizone | 139968-49-3 | insecticide | x | x | 920.52 | epa | |
| 398 | Metalaxyl-M | 70630-17-0 | fungicide | x | x | 84682.67 | epa | 46.00 |
| 399 | Metiram | 9006-42-2 | fungicide | x | x | 573.97 | epa | |
| 400 | Metsulfuron-methyl | 74223-64-6 | herbicide | | | | chemprop | |
| 401 | Milbemectin | 51596-11-3 | insecticide | x | x | 64.81 | epa | |
| 402 | Paclobutrazol | 76738-62-0 | other | x | x | 15839.70 | epa | |
| 403 | Pelargonsaure | 112-05-0 | herbicide | x | x | 96000.00 | epa | |
| 404 | Penoxsulam | 219714-96-2 | herbicide | x | x | 94110.73 | epa | |
| 405 | Picloram | 1918-02-1 | herbicide | x | x | 54852.97 | epa | |
| 406 | Pinoxaden | 243973-20-8 | herbicide | x | | | none | |
| 407 | Pirimiphos-methyl | 29232-93-7 | insecticide | x | x | 0.22 | epa | |
| 408 | Prohexadion | 88805-35-0 | other | x | x | | none | |
| 409 | Propaquizafop | 111479-05-1 | herbicide | x | x | 1252.20 | chemprop | |
| 410 | Prosulfuron | 94125-34-5 | herbicide | x | x | | chemprop | |
| 411 | Prothioconazol | 178928-70-6 | fungicide | x | x | 1200.00 | epa | 1.71 |
| 412 | Pymetrozin | 123312-89-0 | insecticide | x | x | 87000.00 | ppdb | |
| 413 | Pyraflufen | 129630-17-7 | herbicide | x | x | | none | |
| 414 | Pyridat | 55512-33-9 | herbicide | x | x | 1080.00 | epa | |

| | | | | | | | | |
|-----|--------------------------------|-------------|-------------|---|---|-----------|----------|------|
| 415 | Silthiofam | 175217-20-6 | fungicide | x | x | 14000.00 | ppdb | |
| 416 | Spinosad | 168316-95-8 | insecticide | x | x | 6500.00 | epa | 0.06 |
| 417 | Sulfurylfluorid | 2699-79-8 | insecticide | x | x | 620.00 | ppdb | |
| 418 | Tembotrione | 335104-84-2 | herbicide | x | x | 48900.00 | epa | |
| 419 | Tepraloxymid | 149979-41-9 | herbicide | x | x | 7400.00 | epa | |
| 420 | Thiram | 137-26-8 | fungicide | x | x | 11.00 | malaj | 0.11 |
| 421 | Topramezone | 210631-68-8 | herbicide | x | | 99995.00 | epa | 0.90 |
| 422 | Trinexapac-ethyl | 95266-40-3 | other | x | x | 40445.07 | chemprop | |
| 423 | Warfarin | 81-81-2 | other | | | 57770.44 | epa | |
| 424 | Aziprotrryn | 4658-28-0 | herbicide | | | 26000.00 | epa | |
| 425 | Chlorsulfuron | 64902-72-3 | herbicide | | | | chemprop | |
| 426 | Norflurazon | 27314-13-2 | herbicide | | | 15000.00 | epa | |
| 427 | Primisulfuron-methyl | 86209-51-0 | herbicide | | | 260000.00 | ppdb | |
| 428 | Pyrazophos | 13457-18-6 | fungicide | | | 0.36 | ppdb | |
| 429 | Quinalphos | 13593-03-8 | insecticide | | | 0.21 | epa | |
| 430 | Secbumeton | 26259-45-0 | herbicide | | | 3992.00 | malaj | |
| 431 | Tebutam | 35256-85-0 | herbicide | | | | none | |
| 432 | Fluchloralin | 33245-39-5 | herbicide | | | 669.33 | epa | |
| 433 | Furalaxyl | 57646-30-7 | fungicide | | | 39000.00 | ppdb | |
| 434 | Methoprotrryn | 841-06-5 | herbicide | | | 42000.00 | epa | |
| 435 | Furmecyclox | 60568-05-0 | fungicide | | | | none | |
| 436 | Desmethyldisoproturon | 34123-57-4 | metabolite | | | 18407.25 | chemprop | |
| 437 | Metamitron-Desamino | 36993-94-9 | metabolite | | | 61635.23 | chemprop | |
| 438 | Orysastobin | 248593-16-0 | fungicide | | | 1300.00 | ppdb | |
| 439 | Desethyl-2-hydroxyterbutylazin | 66753-06-8 | metabolite | | | 59384.47 | chemprop | |
| 440 | Icaridinsäure | | metabolite | | | | none | |
| 441 | Desaminometribuzin | 35045-02-4 | metabolite | | | | none | |
| 442 | Karbutylat | 4849-32-5 | herbicide | | | | none | |
| 443 | Crimidin | 535-89-7 | other | | | | none | |
| 444 | Buturon | 3766-60-7 | herbicide | | | | none | |
| 445 | Chlorbromuron | 13360-45-7 | herbicide | | | 12342.32 | chemprop | |
| 446 | Fenoxaprop-p | 113158-40-0 | herbicide | x | x | 6247.76 | epa | |
| 447 | Fenamiphos | 22224-92-6 | insecticide | | x | 2.11 | epa | |
| 448 | Isophenphos | 25311-71-1 | insecticide | | | 4.01 | epa | |
| 449 | 4,4-Methoxychlor | 2132-70-9 | insecticide | | | | none | |
| 450 | oxi-Chlordan | 27304-13-8 | metabolite | | | 1300.00 | epa | |
| 451 | 3-Trifluormethylanilin | 98-16-8 | metabolite | | | 2700.00 | epa | |
| 452 | 1-(3,4-Dichlorphenyl)urea | 2327-02-8 | metabolite | | | 8372.59 | chemprop | |
| 453 | 1-(4-Isopropylphenyl)urea | 56046-17-4 | metabolite | | | 22814.20 | chemprop | |
| 454 | Telodrin | 297-78-9 | insecticide | | | 8.00 | malaj | |
| 455 | Terbumeton | 33693-04-8 | herbicide | | | 40000.00 | malaj | |
| 456 | Nitenpyram | 120738-89-8 | insecticide | | | | none | |
| 457 | Permethrin | 52645-53-1 | insecticide | | | 0.60 | malaj | |
| 458 | Quizalofop-ethyl | 76578-14-8 | herbicide | | | 3700.00 | epa | |
| 459 | Mefenpyr-diethyl | 135591-00-3 | other | x | | 5600.00 | epa | |
| 460 | Iodosulfuron-methyl | 144550-06-1 | herbicide | | | | none | |
| 461 | Haloxypop-ethoxyethyl | 87237-48-7 | herbicide | | | | none | |
| 462 | Desmethyldiuron | 3567-62-2 | metabolite | | | 2142.31 | chemprop | |
| 463 | Cloquintocet-mexyl | 99607-70-2 | other | | x | 820.00 | epa | |
| 464 | Chlorpyrifos methyl | 5598-13-0 | insecticide | | x | 0.94 | epa | |
| 465 | Ethirimol | 23947-60-6 | fungicide | | | 53000.00 | ppdb | |
| 466 | Desethylsimazin | 6190-65-4 | metabolite | | | | none | |
| 467 | Nitrofen | 1836-75-5 | herbicide | | | 217.00 | malaj | |
| 468 | Thifenylsulfuron | 79277-67-1 | herbicide | x | x | | none | |
| 469 | Acrinathrin | 101007-06-1 | insecticide | | x | 53000.00 | ppdb | |
| 470 | Betacypermethrin | 65731-84-2 | insecticide | | x | 53000.00 | ppdb | |

| | | | | | | | | |
|-----|-----------------------------------|-------------|-------------|---|---|----------|-------|------|
| 471 | 4-tert. Cyclobutylhex-anon | 98-53-3 | metabolite | | | | none | |
| 472 | Pirimiphos-ethyl | 23505-41-1 | insecticide | | | | none | |
| 473 | Pyrethrum | 8003-34-7 | insecticide | x | x | 17.03 | epa | 0.01 |
| 474 | Pyridaben | 96489-71-3 | insecticide | | x | 0.82 | epa | |
| 475 | Iodosulfuron-methyl-sodium | 144550-36-7 | herbicide | | | | none | |
| 476 | Benazolin | 3813-05-6 | herbicide | | | | none | |
| 477 | Chloramben | 133-90-4 | herbicide | | | 53000.00 | ppdb | |
| 478 | Chlorfenac | 85-34-7 | herbicide | | | | none | |
| 479 | Desethylsebutylazin | 37019-18-4 | metabolite | | | | none | |
| 480 | Prometon | 1610-18-0 | herbicide | | | 41167.00 | malaj | |
| 481 | Atraton | 1610-17-9 | herbicide | | | | none | |
| 482 | Terbutylazin-Metabolit SYN 545666 | | metabolite | | | | none | |
| 483 | 2-Hydroxydesethylatrazin | 19988-24-0 | metabolite | | | | none | |
| 484 | Terbutylazin-Metabolit CGA 324007 | 309923-18-0 | metabolite | | | | none | |

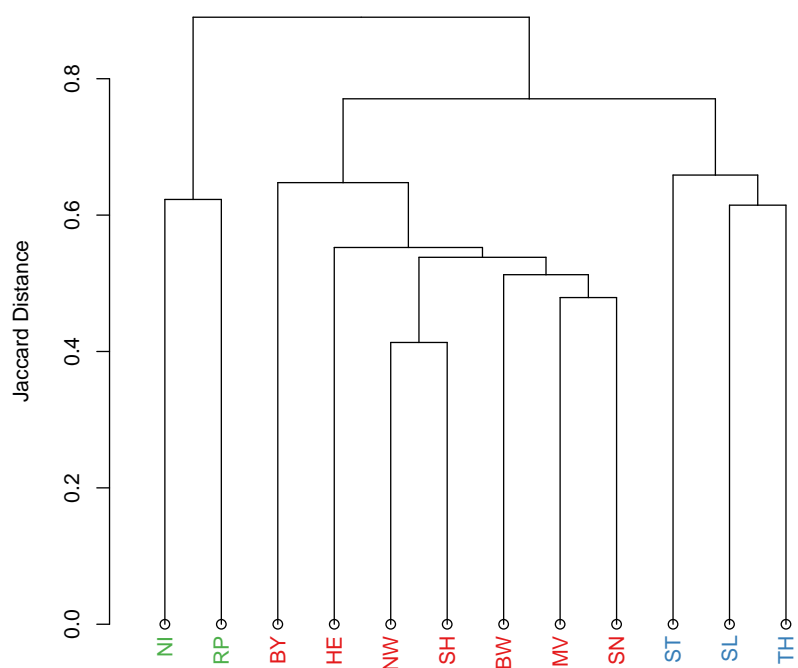


Figure 2.1: Complete Linkage Cluster Dendrogram of Jaccard Similarity of analysed compound spectra between federal states. Abbreviations of state names according to ISO 3166-2:DE.

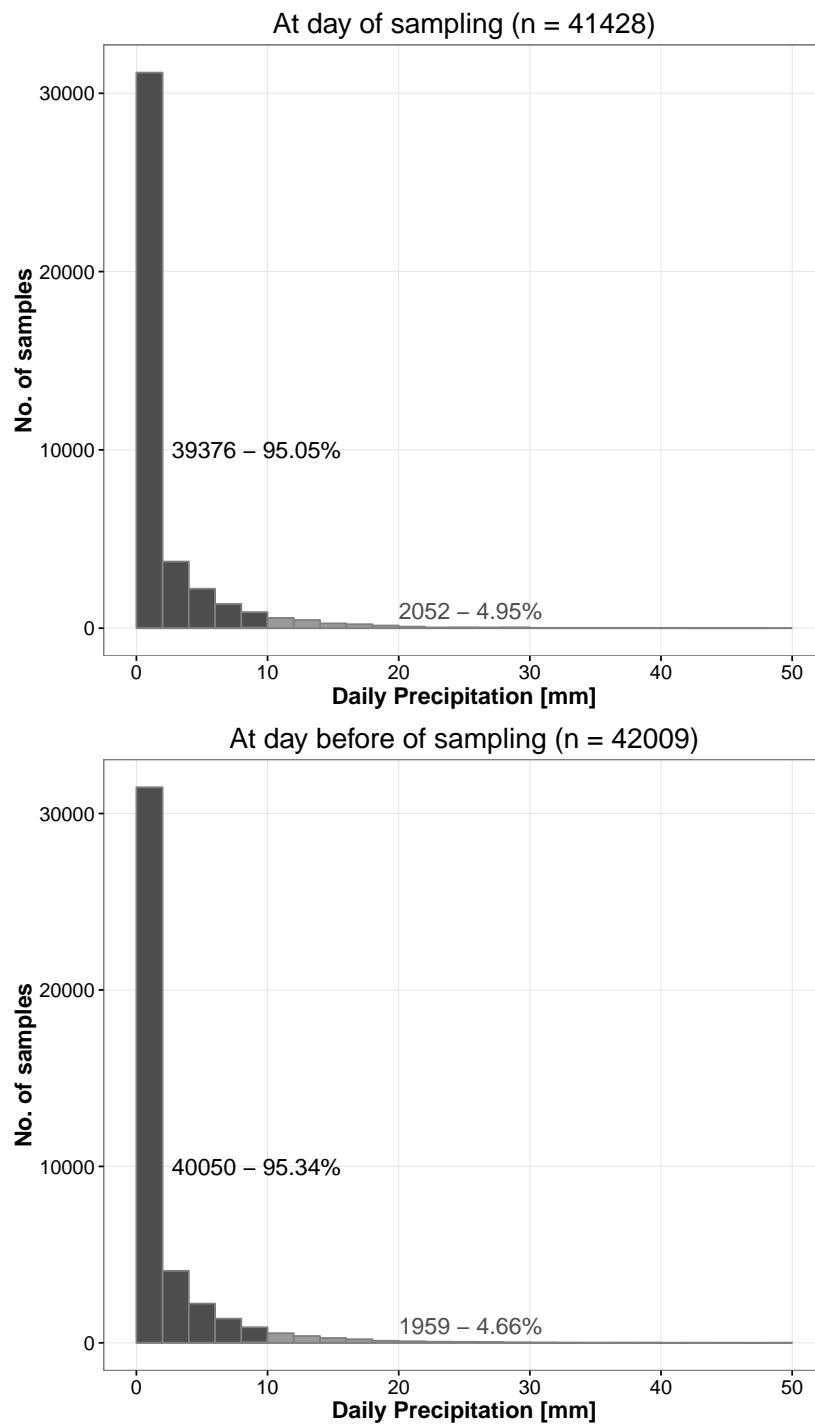


Figure 2.2: Distribution of precipitation at sampling occasions. top: at sampling date. bottom: at day before sampling.

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

update
refs

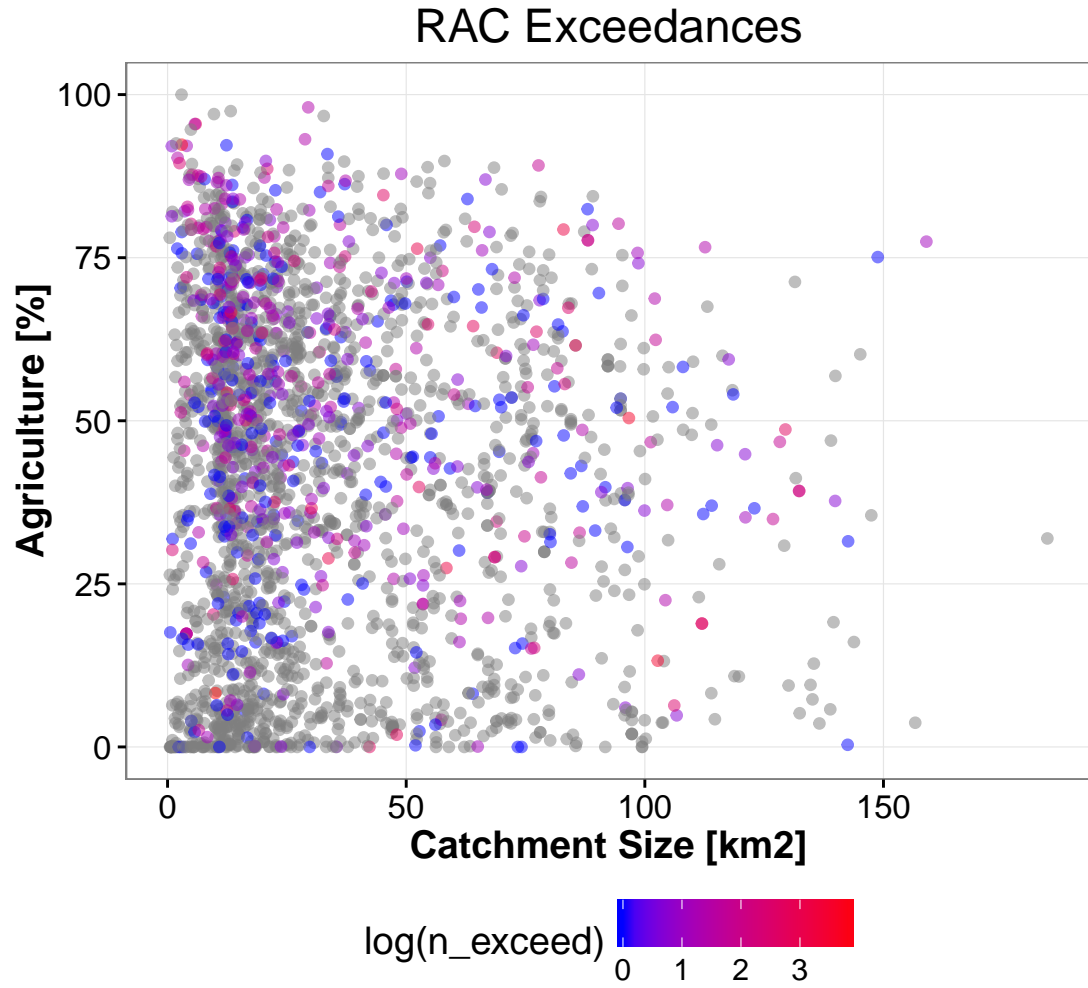


Figure 3.1: Raw data used for the model in equation xxx and Figure xxx of the main article. Color codes the number of RAC exceedances (on a log-scale). Grey points are sites without any exceedance.

Bibliography

- Lewis, K. A., Tzilivakis, J., Warner, D. J., and Green, A. (2016). An international database for pesticide risk assessments and management. *Human and Ecological Risk Assessment: An International Journal*, 22(4):1050–1064.
- Malaj, E., Ohe, P. C. v. d., Grote, M., Kühne, R., Mondy, C. P., Usseglio-Polatera, P., Brack, W., and Schäfer, R. B. (2014). Organic chemicals jeopardize the health of freshwater ecosystems on the continental scale. *Proceedings of the National Academy of Sciences*, 111(26):9549–9554.
- Schüürmann, G., Ebert, R.-U., and Kühne, R. (2011). Quantitative read-across for predicting the acute fish toxicity of organic compounds. *Environmental Science & Technology*, 45(10):4616–4622.
- Szöcs, E. (2016). webchem: webchem v0.1.0. DOI: 10.5281/zenodo.46930.
- U.S. EPA (2015). The ECOTOXicology knowledgebase (ECOTOX).