Research Institute for Chromatography

Application Note 2003/1

# Stir Bar Sorptive Extraction (Twister™) RTL-CGC-MS. A Versatile Method to Monitor more than 400 Pesticides in Different Matrices (Water, Beverages, Fruits, Vegetables, Baby Food)

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**Keywords**
Pesticides, Multi-Residue Analysis, SBSE, TDU, CGC-MS

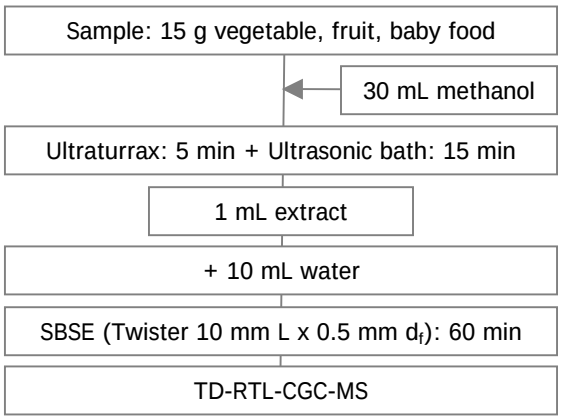
## Introduction

The analysis of pesticides in solid samples (fruits, vegetables, baby food) is discussed in detail because this is much more challenging than aqueous samples (water, beverages). For beverages e.g. wine see Pat Sandra, Bart Tienpont, Joeri Vercammen, Andreas Tredoux, Tom Sandra, Frank David, *J. Chromatogr. A*, 928 (2001) 117. Pesticides from vegetables, fruits and baby food are extracted with methanol and an aliquot is diluted with water for SBSE. Series of 98 stir bars are automatically analyzed by application of a new thermal desorption unit (TDU) developed by Gerstel, in combination with retention time locked

capillary gas chromatography-mass spectrometry (RTL-capillary GC-MS) analysis. Elucidation and identification is finally performed automatically using the Agilent RTL library for pesticides. Accurate quantitation is performed by standard addition or isotope dilution.

**Experimental**

*Sample Preparation*




*Instrumental setup*


**Figure 1.** Sample rack of MPS2-TDU with a capacity of 98 positions; Twisters are put in a clean empty glass liner and capped with a special tube head.


**Figure 2.** MPS-2-TDU-CGC-MS setup; The MPS-2 robot inserts the liners into the TDU for thermal desorption.

*Instrumental*

| | |
|---|---|
| TDU | Gerstel TDU with Gerstel MPS-2 XYZ robot<br>40°C (1 min) – 60°C/min – 280°C (5 min) |
| PTV | Gerstel CIS-4<br>-150°C – 600°C/min – 280°C (2 min) |
| GC | Agilent 6890 (Agilent Technologies) |
| Oven | 70°C (2 min) – 25°C/min – 150°C – 3°C/min – 200°C – 8°C/min – 300°C |
| Column | 30 m L x 250 µm I.D., 0.25 µm $d_f$ HP5-MS (Agilent Technologies) |
| Carrier | Helium, constant pressure eluting p,p'DDT @ 26.98 min |
| MSD | Agilent 5973N (Agilent Technologies)<br>Full scan @ m/z 40-500 |
| RTL library | Agilent RTLpest.L |

**Applications**

*SBSE of pesticides*

The recovery of SBSE for pesticides can be calculated from their log $K_{o/w}$ using the SBSE recovery calculator package (Application Note 2003/2 of this website). Tables 1 to 4 show alphabetical lists of GC amenable pesticides from the Agilent RTL pesticide library that can be analyzed by SBSE. RTLocked retention times (RT), four MSD qualifier ions (Tion, Q1, Q2, Q3), the CAS number, log $K_{o/w}$ and SBSE recoveries for Twisters of 10 mm L x 0.5 mm df (Twister 1) and 20 mm L x 1.0 mm df (Twister 2) are given. The tables comprise four separate lists of pesticides that are grouped in function of SBSE recoveries for Twister 1 between 10-24% (Table 1), 25-49% (Table 2), 50-74% (Table 3) and 75-100% (Table 4). Recoveries are calculated for 10 mL water samples. From all 440 pesticides, 367 compounds are in Table 4 and show very high enrichments in the PDMS coated stir bar. More polar compounds in Table 1 to 3 can also be recovered at minimum 10% and allows their detection at sub-µg/L level.

These recovery values are calculated for water samples and at equilibrium conditions. In the case of solid samples, an extract in methanol is made and diluted with water and SBSE is performed during 60 min. Matrix interferences (10% methanol, sample matrix) and sampling at non-equilibrium conditions decrease the recovery percentages slightly. However, Tables 1 to 4 give a good approximation of the feasibility of SBSE analysis for the listed pesticides.

Thermally sensitive pesticides are annotated with an asterix in the tables and possible partial degradation can occur during TD-CGC-MS analysis. Thermal desorption using the TDU is however equal or better than classical split/splitless injection. However, it was demonstrated that thermal desorption under the prescribed conditions occurs under mild conditions and thermo-sensitive pesticides like captan can be recovered for more than 70%.

*RTL result screener*

The pesticides are automatically identified using the Agilent Result Screener software in combination with the Agilent RTL library for pesticides (RTLPest.l, Agilent Technologies). An example of the detection of permethrin II in grapes is shown in Figure 3 and shows the extracted ion chromatograms at the selective target and qualifier ions of the pesticide (m/z 163, 165, 183, 184) and the mass spectrum at peak apex.

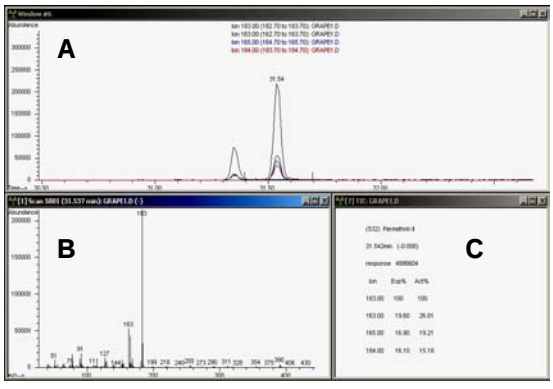



**Figure 3.** Result screener window of the automatic detection of permethrin II in grapes by SBSE-TD-RTL-CGC-MS; **A**: extracted ion chromatograms at m/z 183, 163, 165, 184; **B**: recorded mass spectrum; **C**: identification results.

Besides permethrin II, permethrin I, vinclozolin and procymidone were detected (Figure 4).

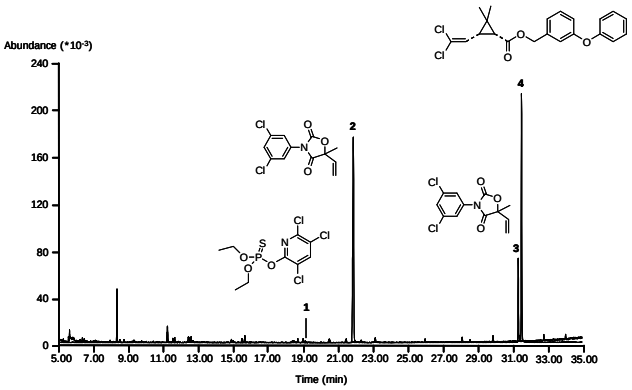



**Figure 4.** Extracted ion chromatograms at m/z 183, 197 and 283 for vinclozolin, procymidone, permethrin I and permethrin II.

An other example is shown for the detection of benalaxyl, vinclozolin, tolylfluanid and procymidone in apple (Figure 5 and 6).

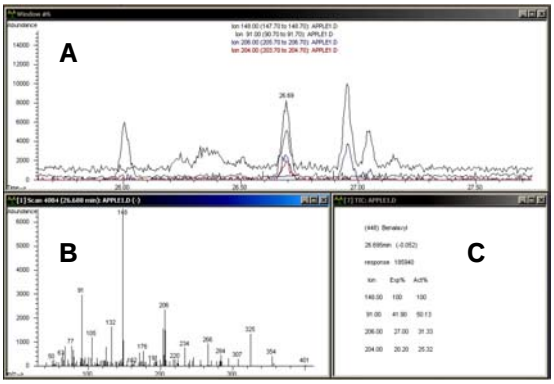



**Figure 5.** Result screener window of the automatic detection of benalaxyl in apple by SBSE-TD-RTL-CGC-MS; **A**: extracted ion chromatograms at m/z 148, 91, 204, 206; **B**: recorded mass spectrum; **C**: identification results.

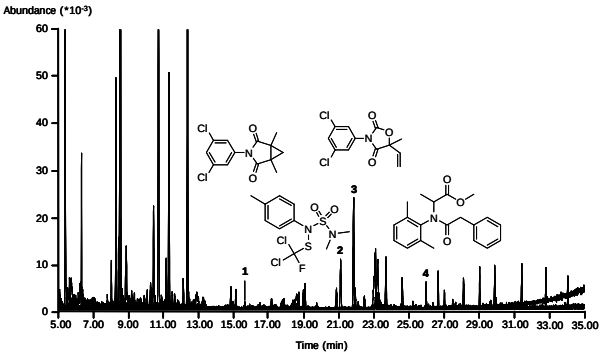



**Figure 6.** Extracted ion chromatograms at m/z 137, 148, 169, 283 for vinclozolin, tolylfluanid, procymidone and benalaxyl.

*Quantitative analysis*

Quantitation of pesticides can be performed into two manners: first, external calibration is performed by spiking a pesticide mixture in an aliquot of methanol (1 mL) before dilution with water and SBSE-TD-CGC-MS analysis. Pat Sandra *et al.* demonstrated negligible matrix effects in the case of vegetable and fruit samples and this permits semi-quantitative measurements of pesticides and differentiation of positives from negatives for in depth quantitation.

Standard addition calibration or isotope dilution are the only solutions for accurate MRM analysis. The paper in reference [1] describes the quantification procedures in detail and illustrates that the required limits of quantitation (LOQ) even for baby food can easily be reached.

**References**

[1] P. Sandra, B. Tienpont, F. David, *accepted for publication in* J. Chromatogr. A.

**Table 1.** Pesticides that result in SBSE recoveries (for 10 mL water) between 10 and 24% for Twister 1 (containing 24 µL PDMS) and 38 and 62% for Twister 2 (containing 116 µL PDMS).

| Compound Name | Cpd | RT | TIon | Q1 | Q2 | Q3 | CAS | log Kow | Twister 1 | Twister 2 |
|---|---|---|---|---|---|---|---|---|---|---|
| 3-Chloroaniline | 16 | 5.45 | 127 | 129 | 65 | 92 | 108-42-9 | 1,72 | 11 | 40 |
| 4-Chloroaniline | 17 | 5.48 | 127 | 129 | 65 | 92 | 106-47-8 | 1,72 | 11 | 40 |
| Allidochlor | 22 | 6.18 | 41 | 56 | 138 | 132 | 93-71-0 | 1,79 | 13 | 44 |
| Aminocarb | 148 | 13.58 | 151 | 150 | 136 | 134 | 2032-59-9 | 1,9 | 16 | 50 |
| Ancymidol | 413 | 25.05 | 228 | 107 | 121 | 215 | 12771-68-5 | 1,99 | 19 | 55 |
| Bentazone | 292 | 19.71 | 198 | 119 | 161 | 92 | 25057-89-0 | 1,67 | 10 | 37 |
| Bromacil | 260 | 18.35 | 205 | 207 | 206 | 42 | 314-40-9 | 1,68 | 10 | 38 |
| Crotoxyphos | 355 | 22.21 | 127 | 105 | 193 | 104 | 7700-17-6 | 1,89 | 16 | 49 |
| Demeton-S | 122 | 12.63 | 88 | 60 | 170 | 89 | 8065-48-3 | 2,09 | 23 | 61 |
| Diethyl dithiobis(thionoformate) (EXD) | 123 | 12.65 | 76 | 89 | 94 | 60 | 502-55-6 | 2,06 | 22 | 59 |
| Ethiofencarb | 196 | 15.61 | 107 | 168 | 77 | 57 | 29973-13-5 | 2,04 | 21 | 58 |
| Ethiolate | 15 | 5.41 | 100 | 72 | 161 | 44 | 2941-55-1 | 2,04 | 21 | 58 |
| Famphur | 447 | 26.64 | 218 | 125 | 217 | 93 | 52-85-7 | 1,99 | 19 | 55 |
| Fenthion sulfoxide | 422 | 25.54 | 278 | 125 | 109 | 279 | - | 1,92 | 17 | 51 |
| Metalaxyl | 238 | 17.34 | 206 | 45 | 160 | 249 | 57837-19-1 | 1,7 | 11 | 39 |
| Metolcarb | 46 | 7.99 | 108 | 107 | 77 | 79 | 1129-41-5 | 1,72 | 11 | 40 |
| N-Methyl-N-1-naphthyl acetamide | 146 | 13.56 | 157 | 156 | 56 | 199 | - | 2,1 | 23 | 61 |
| Paraoxon | 239 | 17.34 | 109 | 149 | 139 | 275 | 311-45-5 | 1,97 | 18 | 54 |
| Propoxur | 76 | 10.35 | 110 | 152 | 57 | 111 | 114-26-1 | 1,9 | 16 | 50 |
| Pyracarbolid | 302 | 20.02 | 125 | 97 | 217 | 55 | 24691-76-7 | 2,08 | 22 | 60 |
| Pyroquilon | 154 | 13.79 | 173 | 130 | 172 | 144 | 57369-32-1 | 1,8 | 13 | 44 |
| Terbacil | 178 | 14.77 | 161 | 160 | 117 | 163 | 5902-51-2 | 1,75 | 12 | 41 |
| Thiabendazole | 320 | 20.94 | 201 | 174 | 202 | 175 | 148-79-8 | 2 | 19 | 56 |
| Thionazin | 74 | 10.26 | 96 | 97 | 107 | 143 | 297-97-2 | 1,86 | 15 | 48 |
| Tycor (SMY 1500) | 245 | 17.58 | 212 | 200 | 213 | 61 | 64529-56-2 | 1,98 | 19 | 55 |

**Table 2.** Pesticides that result in SBSE recoveries (for 10 mL water) between 25 and 49% for Twister 1 (containing 24 µL PDMS) and 63 and 83% for Twister 2 (containing 116 µL PDMS); (*) thermally sensitive pesticides

| Compound Name | Cpd | RT | TIon | Q1 | Q2 | Q3 | CAS | log Kow | Twister 1 | Twister 2 |
|---|---|---|---|---|---|---|---|---|---|---|
| 2,3,5-Trimethacarb | 96 | 11.20 | 136 | 121 | 91 | 135 | 2655-15-4 | 2,56 | 47 | 82 |
| 2,4-Dimethylaniline | 11 | 5.19 | 121 | 120 | 106 | 77 | 1300-73-8 | 2,17 | 26 | 65 |
| 2,6-Dimethylaniline | 12 | 5.20 | 121 | 106 | 120 | 77 | 87-62-7 | 2,17 | 26 | 65 |
| 3,4-Dichloroaniline | 37 | 7.66 | 161 | 163 | 99 | 90 | 95-76-1 | 2,37 | 36 | 75 |
| 3,5-Dichloroaniline | 34 | 7.32 | 161 | 163 | 90 | 99 | 626-43-7 | 2,37 | 36 | 75 |
| 4,6-Dinitro-o-cresol (DNOC) | 78 | 10.36 | 198 | 105 | 121 | 51 | 534-52-1 | 2,27 | 31 | 70 |
| Azinphos-methyl | 514 | 29.65 | 160 | 132 | 77 | 105 | 86-50-0 | 2,53 | 45 | 81 |
| Bendiocarb | 102 | 11.54 | 151 | 126 | 166 | 57 | 22781-23-3 | 2,55 | 46 | 82 |
| Carbaryl | 225 | 16.81 | 144 | 115 | 116 | 145 | 63-25-2 | 2,35 | 35 | 74 |
| Carbofuran | 131 | 13.03 | 164 | 149 | 131 | 123 | 1563-66-2 | 2,3 | 32 | 72 |
| Chlorotoluron* | 261 | 18.37 | 132 | 72 | 167 | 212 | 15545-48-9 | 2,58 | 48 | 83 |
| Chlozolinate | 336 | 21.38 | 188 | 259 | 186 | 187 | 72391-46-9 | 2,22 | 28 | 68 |
| Cyanazine | 282 | 19.35 | 212 | 213 | 214 | 68 | 21725-46-2 | 2,51 | 44 | 80 |
| Cyanophos | 152 | 13.77 | 109 | 243 | 125 | 79 | 2636-26-2 | 2,48 | 42 | 79 |
| Dicamba | 91 | 10.95 | 173 | 175 | 220 | 222 | 1918-00-9 | 2,14 | 25 | 63 |
| Dichlormid | 28 | 6.79 | 41 | 172 | 124 | 56 | 37764-25-3 | 2,28 | 31 | 71 |
| Dicyclopentadiene | 4 | 4.00 | 66 | 132 | 67 | 65 | 542-92-7 | 2,25 | 30 | 69 |
| Dimethachlor | 208 | 16.18 | 134 | 197 | 132 | 210 | 50563-36-5 | 2,33 | 34 | 73 |
| Drazoxolon | 297 | 19.91 | 127 | 125 | 44 | 129 | 5707-69-7 | 2,44 | 40 | 78 |
| Fensulfothion | 421 | 25.56 | 292 | 293 | 156 | 140 | 115-90-2 | 2,35 | 35 | 74 |
| Fluometuron* | 89 | 10.81 | 72 | 187 | 232 | 168 | 2164-17-2 | 2,35 | 35 | 74 |
| Flutriafol | 369 | 23.18 | 123 | 219 | 164 | 83 | 76674-21-0 | 2,52 | 44 | 81 |
| Fuberidazole | 216 | 16.55 | 155 | 156 | 129 | 92 | 3878-19-1 | 2,37 | 36 | 75 |
| Hexazinone | 464 | 27.39 | 171 | 83 | 128 | 71 | 51235-04-2 | 2,15 | 25 | 64 |
| Isoprocarb | 58 | 9.09 | 121 | 136 | 91 | 77 | 2631-40-5 | 2,37 | 36 | 75 |
| Malathion | 270 | 18.80 | 173 | 127 | 125 | 93 | 121-75-5 | 2,29 | 32 | 71 |
| Malathion-o-analog | 229 | 16.87 | 127 | 99 | 109 | 125 | 121-75-5 | 2,29 | 32 | 71 |
| Mecarbam | 344 | 21.74 | 131 | 97 | 159 | 125 | 2595-54-2 | 2,29 | 32 | 71 |
| Metazachlor | 317 | 20.83 | 133 | 81 | 132 | 134 | 67129-08-2 | 2,38 | 37 | 75 |
| Metobromuron* | 192 | 15.51 | 61 | 197 | 199 | 90 | 3060-89-7 | 2,51 | 44 | 80 |
| Monolinuron* | 134 | 13.10 | 61 | 153 | 127 | 125 | 1746-81-2 | 2,26 | 30 | 70 |
| N,N-Diethyl-m-toluamide | 69 | 9.75 | 119 | 190 | 91 | 191 | 134-62-3 | 2,26 | 30 | 70 |
| Norflurazon | 456 | 26.95 | 303 | 145 | 102 | 305 | 27314-13-2 | 2,19 | 27 | 66 |
| Phosmet | 488 | 28.50 | 160 | 161 | 77 | 93 | 732-11-6 | 2,48 | 42 | 79 |
| p-Nitrotoluene | 19 | 5.57 | 91 | 137 | 65 | 107 | 99-99-0 | 2,36 | 35 | 74 |
| Procymidone | 350 | 21.96 | 96 | 283 | 285 | 67 | 32809-16-8 | 2,59 | 48 | 83 |
| Propachlor | 77 | 10.36 | 120 | 176 | 77 | 93 | 1918-16-7 | 2,42 | 39 | 77 |
| Propetamphos | 158 | 13.91 | 138 | 194 | 236 | 222 | 31218-83-4 | 2,51 | 44 | 80 |
| Prothoate | 213 | 16.46 | 286 | 288 | 125 | 109 | 2275-18-5 | 2,17 | 26 | 65 |
| Simazine | 129 | 12.91 | 201 | 186 | 44 | 173 | 122-34-9 | 2,4 | 38 | 76 |
| Thiofanox | 100 | 11.47 | 57 | 68 | 115 | 56 | 39196-18-4 | 2,16 | 26 | 65 |
| Tricyclazole | 379 | 23.61 | 189 | 162 | 161 | 135 | 41814-78-2 | 2,48 | 42 | 79 |

**Table 3.** Pesticides that result in SBSE recoveries (for 10 mL water) between 50 and 74% for Twister 1 (containing 24 µL PDMS) and 84 and 92% for Twister 2 (containing 116 µL PDMS); (*) thermally sensitive pesticides

| Compound Name | Cpd | RT | TIon | Q1 | Q2 | Q3 | CAS | log Kow | Twister 1 | Twister 2 |
|---|---|---|---|---|---|---|---|---|---|---|
| 2,3,5-Trimethylphenyl methyl carbamate | 97 | 11.23 | 136 | 121 | 91 | 135 | 12407-86-2 | 2,81 | 61 | 89 |
| 2,6-Dichlorobenzonitrile | 24 | 6.75 | 171 | 173 | 136 | 100 | 1194-65-6 | 2,83 | 62 | 89 |
| 2-Hydroxyestradiol | 555 | 33.81 | 288 | 289 | 229 | 176 | 50-27-1 | 2,81 | 61 | 89 |
| 3,4,5-Trimethacarb | 127 | 12.78 | 121 | 136 | 135 | 57 | 2686-99-9 | 2,81 | 61 | 89 |
| Atrazine | 136 | 13.16 | 200 | 215 | 202 | 58 | 1912-24-9 | 2,82 | 61 | 89 |
| Azaconazole | 402 | 24.55 | 217 | 219 | 173 | 175 | 60207-31-0 | 2,73 | 56 | 87 |
| Benazolin-ethyl | 321 | 20.96 | 170 | 198 | 271 | 172 | 25059-80-7 | 2,86 | 63 | 90 |
| Benfuresate | 203 | 15.97 | 163 | 256 | 121 | 164 | 68505-69-1 | 2,8 | 60 | 89 |
| Captan* | 330 | 21.23 | 79 | 80 | 151 | 77 | 133-06-2 | 2,74 | 57 | 87 |
| Chlorbufam | 133 | 13.06 | 153 | 127 | 53 | 155 | 1967-16-4 | 3,02 | 72 | 93 |
| Chlordimeform | 94 | 11.20 | 196 | 181 | 117 | 152 | 6164-98-3 | 2,89 | 65 | 91 |
| Chlormefos | 39 | 7.73 | 121 | 97 | 154 | 234 | 24934-91-6 | 3,04 | 72 | 93 |
| Chlorthiamid | 205 | 16.04 | 171 | 173 | 170 | 172 | 1918-13-4 | 2,96 | 69 | 92 |
| Clomazone | 138 | 13.25 | 125 | 204 | 127 | 205 | 81777-89-1 | 2,86 | 63 | 90 |
| Cycluron* | 149 | 13.63 | 72 | 89 | 127 | 45 | 2163-69-1 | 2,84 | 62 | 90 |
| Desmetryn | 204 | 15.99 | 213 | 198 | 171 | 58 | 1014-69-3 | 2,82 | 61 | 89 |
| Dichlofluanid | 262 | 18.41 | 123 | 167 | 224 | 226 | 1085-98-9 | 2,72 | 56 | 87 |
| Dichlone | 166 | 14.29 | 191 | 226 | 228 | 163 | 117-80-6 | 2,65 | 52 | 85 |
| Dichlorprop | 126 | 12.69 | 162 | 164 | 44 | 234 | 120-36-5 | 3,03 | 72 | 93 |
| Dicloran | 120 | 12.56 | 206 | 176 | 178 | 208 | 99-30-9 | 2,76 | 58 | 88 |
| Diphenamid | 307 | 20.20 | 167 | 72 | 165 | 239 | 957-51-7 | 2,86 | 63 | 90 |
| Endosulfan lactone | 309 | 20.56 | 277 | 321 | 239 | 237 | - | 2,91 | 66 | 91 |
| EPTC | 27 | 6.80 | 128 | 43 | 86 | 132 | 759-94-4 | 3,02 | 72 | 93 |
| Ethofumesate | 258 | 18.31 | 207 | 161 | 286 | 137 | 26225-79-6 | 2,89 | 65 | 91 |
| Etrimfos | 184 | 15.16 | 292 | 181 | 153 | 125 | 38260-54-7 | 2,94 | 68 | 92 |
| Fenfuram | 174 | 14.62 | 109 | 201 | 43 | 110 | 24691-80-3 | 2,62 | 50 | 84 |
| Fenobucarb | 75 | 10.28 | 121 | 150 | 91 | 122 | 3766-81-2 | 2,86 | 63 | 90 |
| Folpet | 338 | 21.59 | 104 | 76 | 260 | 147 | 133-07-3 | 2,84 | 62 | 90 |
| Furalaxyl | 349 | 21.92 | 95 | 242 | 152 | 146 | 57646-30-7 | 2,7 | 55 | 86 |
| Iprodione* | 485 | 28.39 | 187 | 314 | 189 | 244 | 36734-19-7 | 2,85 | 63 | 90 |
| Isoprothiolane | 388 | 23.88 | 118 | 162 | 189 | 290 | 50512-35-1 | 2,79 | 60 | 89 |
| Isoproturon* | 231 | 17.09 | 146 | 72 | 206 | 128 | 34123-59-6 | 2,84 | 62 | 90 |
| Linuron* | 254 | 18.19 | 61 | 187 | 189 | 124 | 330-55-2 | 2,91 | 66 | 91 |
| Mefenacet | 518 | 29.97 | 192 | 77 | 120 | 106 | 73250-68-7 | 2,8 | 60 | 89 |
| Mefluidide | 319 | 20.82 | 135 | 268 | 310 | 136 | 53780-34-0 | 2,72 | 56 | 87 |
| Methiocarb | 250 | 18.05 | 168 | 153 | 109 | 57 | 2032-65-7 | 2,87 | 64 | 90 |
| Methoprotryne | 406 | 24.71 | 256 | 213 | 226 | 240 | 841-06-5 | 3,04 | 72 | 93 |
| Methyl parathion | 217 | 16.59 | 263 | 109 | 125 | 79 | 298-00-0 | 2,75 | 57 | 88 |
| Molinate | 57 | 9.11 | 126 | 55 | 187 | 83 | 2212-67-1 | 2,91 | 66 | 91 |
| Nitralin | 480 | 28.18 | 316 | 274 | 300 | 317 | 4726-14-1 | 2,92 | 67 | 91 |
| Oryzalin | 528 | 31.25 | 317 | 275 | 58 | 258 | 19044-88-3 | 2,73 | 56 | 87 |
| Oxabetrinil | 188 | 15.31 | 73 | 103 | 45 | 77 | 74782-23-3 | 2,78 | 59 | 88 |
| Pindone | 165 | 14.28 | 173 | 174 | 146 | 230 | 83-26-1 | 2,87 | 64 | 90 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Probenazole | 259 | 18.33 | 103 | 130 | 76 | 159 | 27605-76-1 | 2,89 | 65 | 91 |
| Propanil | 206 | 16.12 | 161 | 163 | 217 | 219 | 709-98-8 | 2,88 | 65 | 91 |
| Propham | 42 | 7.91 | 93 | 179 | 119 | 137 | 122-42-9 | 2,66 | 52 | 85 |
| Pyridinitril | 340 | 21.64 | 273 | 275 | 237 | 202 | 1086-02-8 | 2,95 | 68 | 92 |
| Quinalphos | 341 | 21.65 | 146 | 157 | 156 | 118 | 13593-03-8 | 3,04 | 72 | 93 |
| Simetryn | 227 | 16.82 | 213 | 170 | 155 | 198 | 1014-70-6 | 2,9 | 66 | 91 |
| Swep | 132 | 13.05 | 187 | 189 | 124 | 219 | 1918-18-9 | 3,04 | 72 | 93 |
| Thiometon | 116 | 12.34 | 88 | 125 | 89 | 93 | 640-15-3 | 2,88 | 65 | 91 |
| Triadimefon | 283 | 19.39 | 57 | 208 | 85 | 210 | 43121-43-3 | 2,94 | 68 | 92 |
| Triadimenol | 342 | 21.67 | 112 | 168 | 128 | 70 | 55219-65-3 | 2,95 | 68 | 92 |
| Triazophos | 442 | 26.46 | 161 | 162 | 172 | 77 | 24017-47-8 | 2,92 | 67 | 91 |
| Vinclozolin | 219 | 16.63 | 212 | 285 | 198 | 187 | 50471-44-8 | 3,03 | 72 | 93 |

**Table 4.** Pesticides that result in SBSE recoveries (for 10 mL water) between 75 and 100 % for Twister 1 (containing 24 µL PDMS) and 93 and 100% for Twister 2 (containing 116 µL PDMS); (*) thermally sensitive pesticides

| Compound Name | Cpd | RT | TIon | Q1 | Q2 | Q3 | CAS | log Kow | Twister 1 | Twister 2 |
|---|---|---|---|---|---|---|---|---|---|---|
| 2-(Octylthio)ethanol | 56 | 8.98 | 145 | 61 | 190 | 159 | 3547-33-9 | 3,38 | 85 | 97 |
| 2,4-D sec-butyl ester | 176 | 14.73 | 57 | 175 | 177 | 162 | - | 4,3 | 98 | 100 |
| 4,4'-Dichlorobenzophenone | 276 | 19.20 | 139 | 111 | 141 | 250 | 90-98-2 | 4,44 | 99 | 100 |
| 5,7-Dihydroxy-4'-methoxyisoflavone | 551 | 33.41 | 284 | 132 | 283 | 285 | 552-59-0 | 3,41 | 86 | 97 |
| Acetochlor | 215 | 16.54 | 146 | 162 | 59 | 223 | 34256-82-1 | 3,37 | 85 | 97 |
| Alachlor | 230 | 17.03 | 160 | 188 | 45 | 146 | 15972-60-8 | 3,37 | 85 | 97 |
| Aldrin* | 265 | 18.53 | 263 | 66 | 265 | 261 | 309-00-2 | 6,75 | 100 | 100 |
| Ametryn | 232 | 17.11 | 227 | 212 | 170 | 185 | 834-12-8 | 3,32 | 83 | 96 |
| Amitraz | 519 | 30.14 | 121 | 162 | 132 | 147 | 33089-61-1 | 5,55 | 100 | 100 |
| Anilazine | 322 | 20.95 | 239 | 241 | 178 | 143 | 101-05-3 | 3,64 | 91 | 98 |
| Atraton | 125 | 12.70 | 196 | 211 | 169 | 58 | 1610-17-9 | 3,15 | 77 | 95 |
| Azinphos-ethyl | 522 | 30.65 | 132 | 160 | 77 | 105 | 2642-71-9 | 3,51 | 89 | 98 |
| Aziprotryne | 173 | 14.58 | 199 | 184 | 139 | 68 | 4658-28-0 | 3,27 | 82 | 96 |
| Azobenzene | 83 | 10.59 | 77 | 182 | 105 | 51 | 103-33-3 | 4,11 | 97 | 99 |
| Barban | 392 | 24.07 | 153 | 127 | 155 | 125 | 101-27-9 | 3,41 | 86 | 97 |
| Benalaxyl | 448 | 26.75 | 148 | 91 | 206 | 204 | 71626-11-4 | 3,69 | 92 | 98 |
| Benfluralin | 104 | 11.73 | 292 | 264 | 276 | 293 | 1861-40-1 | 5,31 | 100 | 100 |
| Benodanil | 434 | 25.95 | 231 | 323 | 203 | 76 | 15310-01-7 | 3,87 | 95 | 99 |
| Benthiocarb | 267 | 18.58 | 100 | 72 | 125 | 257 | 28249-77-6 | 3,9 | 95 | 99 |
| Benzophenone | 84 | 10.67 | 105 | 182 | 77 | 51 | 119-61-9 | 3,15 | 77 | 95 |
| Benzoylprop ethyl | 484 | 28.33 | 105 | 77 | 292 | 106 | 22212-55-1 | 4,27 | 98 | 100 |
| BHC alpha isomer | 113 | 12.08 | 181 | 219 | 183 | 217 | 58-89-9 | 4,26 | 98 | 100 |
| BHC beta isomer | 137 | 13.20 | 219 | 181 | 183 | 217 | 93-72-1 | 3,68 | 92 | 98 |
| BHC delta isomer | 169 | 14.54 | 181 | 219 | 183 | 217 | 93-72-1 | 3,68 | 92 | 98 |
| Bifenox | 506 | 29.18 | 341 | 343 | 311 | 189 | 42576-02-3 | 4,15 | 97 | 99 |
| Bifenthrin | 500 | 28.84 | 181 | 165 | 166 | 182 | 82657-04-3 | 8,15 | 100 | 100 |
| Binapacryl | 416 | 25.18 | 83 | 55 | 82 | 84 | 485-31-4 | 4,49 | 99 | 100 |
| Bioallethrin | 347 | 21.80 | 123 | 136 | 79 | 107 | 584-79-2 | 5,52 | 100 | 100 |
| Bioallethrin S-cyclopentenyl isomer | 345 | 21.75 | 123 | 136 | 79 | 107 | 28434-00-6 | 5,52 | 100 | 100 |
| Bioresmethrin | 477 | 27.98 | 123 | 171 | 128 | 143 | 28434-01-7 | 7,11 | 100 | 100 |
| Bitertanol I | 527 | 31.21 | 170 | 57 | 168 | 171 | 55179-31-2 | 4,07 | 97 | 99 |
| Bitertanol II | 529 | 31.34 | 170 | 57 | 168 | 171 | 55179-31-2 | 4,07 | 97 | 99 |
| Bromobutide | 211 | 16.25 | 119 | 120 | 118 | 232 | 74712-19-9 | 4,33 | 98 | 100 |
| Bromocyclen | 185 | 15.19 | 357 | 359 | 237 | 361 | 1715-40-8 | 6,13 | 100 | 100 |
| Bromophos | 304 | 20.08 | 331 | 329 | 125 | 333 | 2104-96-3 | 5,11 | 100 | 100 |
| Bromophos-ethyl | 360 | 22.53 | 359 | 303 | 357 | 301 | 4824-78-6 | 6,09 | 100 | 100 |
| Bromopropylate | 494 | 28.62 | 341 | 339 | 343 | 183 | 18181-80-1 | 4,9 | 99 | 100 |
| Bromoxynil | 101 | 11.55 | 277 | 275 | 279 | 88 | 1689-84-5 | 3,39 | 85 | 97 |
| Bromoxynil octanoic acid ester | 452 | 26.83 | 127 | 57 | 128 | 88 | 1689-99-2 | 5,86 | 100 | 100 |
| Buprofezin | 404 | 24.58 | 105 | 106 | 104 | 172 | 69327-76-0 | 4,3 | 98 | 100 |
| Butachlor | 371 | 23.22 | 176 | 160 | 188 | 146 | 23184-66-9 | 4,84 | 99 | 100 |
| Butamifos | 378 | 23.59 | 286 | 200 | 96 | 202 | 36335-67-8 | 4,77 | 99 | 100 |
| Butralin | 308 | 20.23 | 266 | 224 | 267 | 220 | 33629-47-9 | 5,15 | 100 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| Butylate | 36 | 7.61 | 57 | 146 | 156 | 174 | 2008-41-5 | 3,85 | 94 | 99 |
| Captafol* | 468 | 27.62 | 79 | 80 | 77 | 151 | 2425-06-1 | 3,42 | 86 | 97 |
| Carbophenothion | 446 | 26.64 | 157 | 121 | 153 | 97 | 786-19-6 | 5,19 | 100 | 100 |
| Carbosulfan | 497 | 28.66 | 164 | 160 | 149 | 118 | 55285-14-8 | 5,57 | 100 | 100 |
| Chinomethionat | 348 | 21.90 | 206 | 234 | 116 | 148 | 2439-01-2 | 3,37 | 85 | 97 |
| Chloranocryl | 222 | 16.74 | 69 | 125 | 229 | 231 | 2164-09-2 | 3,29 | 82 | 96 |
| Chlorbenside | 346 | 21.82 | 125 | 127 | 268 | 270 | 103-17-3 | 5,59 | 100 | 100 |
| Chlorbromuron* | 323 | 20.99 | 61 | 233 | 231 | 124 | 13360-45-7 | 3,15 | 77 | 95 |
| Chlordecone | 436 | 26.02 | 272 | 274 | 270 | 237 | 143-50-0 | 4,91 | 99 | 100 |
| Chlorfenethol | 326 | 21.06 | 251 | 139 | 253 | 178 | 80-06-8 | 4,45 | 99 | 100 |
| Chlorfenprop-methyl | 70 | 9.96 | 125 | 165 | 196 | 197 | 14437-17-3 | 3,4 | 86 | 97 |
| Chlorfenson | 372 | 23.32 | 175 | 111 | 177 | 302 | 80-33-1 | 4,21 | 97 | 100 |
| Chlorfenvinphos | 337 | 21.56 | 267 | 323 | 269 | 325 | 470-90-6 | 4,15 | 97 | 99 |
| Chlorflurecol-methyl ester | 353 | 22.08 | 215 | 152 | 217 | 216 | - | 3,27 | 82 | 96 |
| Chlornitrofen | 444 | 26.53 | 317 | 319 | 287 | 236 | 1836-77-7 | 4,96 | 100 | 100 |
| Chlorobenzilate | 419 | 25.40 | 251 | 139 | 253 | 111 | 510-15-6 | 3,99 | 96 | 99 |
| Chloroneb | 50 | 8.68 | 191 | 193 | 206 | 208 | 2675-77-6 | 3,44 | 87 | 97 |
| Chloropropylate | 420 | 25.42 | 251 | 253 | 139 | 111 | 5836-10-2 | 4,41 | 98 | 100 |
| Chlorothalonil | 179 | 14.78 | 266 | 264 | 268 | 270 | 1897-45-6 | 3,66 | 92 | 98 |
| Chlorpropham | 92 | 11.05 | 127 | 213 | 153 | 154 | 101-21-3 | 3,3 | 83 | 96 |
| Chlorpyrifos | 278 | 19.23 | 197 | 199 | 314 | 97 | 2921-88-2 | 4,66 | 99 | 100 |
| Chlorpyrifos Methyl | 218 | 16.59 | 286 | 288 | 125 | 290 | 2921-88-2 | 4,66 | 99 | 100 |
| Chlorthal-dimethyl | 286 | 19.43 | 301 | 299 | 303 | 332 | 1861-32-1 | 4,24 | 98 | 100 |
| Chlorthion | 293 | 19.75 | 109 | 125 | 297 | 267 | 500-28-7 | 3,39 | 85 | 97 |
| Chlorthiophos | 438 | 26.13 | 269 | 97 | 325 | 271 | 60238-56-4 | 5,8 | 100 | 100 |
| Chlorthiophos sulfone | 508 | 29.37 | 301 | 357 | 97 | 303 | - | 3,77 | 93 | 99 |
| Chlorthiophos sulfoxide | 491 | 28.56 | 97 | 341 | 269 | 285 | - | 3,64 | 91 | 98 |
| cis-Chlordane | 365 | 22.83 | 373 | 375 | 377 | 371 | 57-74-9 | 6,26 | 100 | 100 |
| Coumaphos | 534 | 31.67 | 362 | 226 | 109 | 210 | 56-72-4 | 4,47 | 99 | 100 |
| Crufomate | 298 | 19.90 | 256 | 169 | 182 | 276 | 299-86-5 | 3,3 | 83 | 96 |
| Cyanofenphos | 451 | 26.82 | 157 | 169 | 141 | 185 | 13067-93-1 | 4,2 | 97 | 100 |
| Cycloate | 85 | 10.76 | 83 | 154 | 72 | 84 | 1134-23-2 | 3,81 | 94 | 99 |
| Cyfluthrin I | 539 | 32.22 | 163 | 206 | 165 | 227 | 68359-37-5 | 5,74 | 100 | 100 |
| Cyfluthrin II | 540 | 32.36 | 163 | 206 | 165 | 227 | 68359-37-5 | 5,74 | 100 | 100 |
| Cyfluthrin III | 541 | 32.48 | 163 | 206 | 165 | 227 | 68359-37-5 | 5,74 | 100 | 100 |
| Cyfluthrin IV | 542 | 32.54 | 163 | 206 | 227 | 199 | 68359-37-5 | 5,74 | 100 | 100 |
| Cyhalothrin I (lambda) | 520 | 30.37 | 181 | 197 | 208 | 209 | 68085-85-8 | 6,85 | 100 | 100 |
| Cymoxanil | 80 | 10.45 | 44 | 70 | 111 | 167 | 57966-95-7 | 4,24 | 98 | 100 |
| Cypermethrin I | 543 | 32.69 | 181 | 163 | 165 | 77 | 52315-07-8 | 6,38 | 100 | 100 |
| Cypermethrin II | 544 | 32.84 | 181 | 163 | 165 | 209 | 52315-07-8 | 6,38 | 100 | 100 |
| Cypermethrin III | 546 | 32.97 | 163 | 181 | 165 | 209 | 52315-07-8 | 6,38 | 100 | 100 |
| Cypermethrin IV | 547 | 33.02 | 163 | 181 | 165 | 209 | 52315-07-8 | 6,38 | 100 | 100 |
| Cyprazine | 209 | 16.18 | 212 | 227 | 170 | 214 | 22936-86-3 | 3,12 | 76 | 94 |
| d-(cis-trans)-Phenothrin-I | 510 | 29.45 | 123 | 183 | 81 | 184 | 26002-80-2 | 7,54 | 100 | 100 |
| d-(cis-trans)-Phenothrin-II | 511 | 29.61 | 123 | 183 | 81 | 184 | 26002-80-2 | 7,54 | 100 | 100 |
| Deltamethrin* | 566 | 36.00 | 181 | 253 | 251 | 255 | 52918-63-5 | 6,18 | 100 | 100 |
| Desbromo-bromobutide | 108 | 11.85 | 119 | 120 | 118 | 233 | - | 3,74 | 93 | 99 |
| Desmedipham | 118 | 12.37 | 181 | 135 | 109 | 122 | 13684-56-5 | 3,22 | 80 | 95 |
| Dialifos | 526 | 30.83 | 208 | 173 | 210 | 76 | 10311-84-9 | 4,14 | 97 | 99 |
| Di-allate I | 110 | 11.96 | 86 | 234 | 128 | 236 | 2303-16-4 | 4,08 | 97 | 99 |

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|---|---|---|---|---|---|---|---|---|---|---|
| Di-allate II | 115 | 12.29 | 86 | 234 | 236 | 128 | 2303-16-4 | 4,08 | 97 | 99 |
| Diazinon | 168 | 14.47 | 179 | 137 | 152 | 199 | 333-41-5 | 3,86 | 95 | 99 |
| Dicapthon | 284 | 19.41 | 262 | 125 | 263 | 79 | 2463-84-5 | 3,39 | 85 | 97 |
| Dichlofenthion | 207 | 16.17 | 279 | 223 | 97 | 162 | 97-17-6 | 5,2 | 100 | 100 |
| Dichlorophen | 486 | 28.37 | 128 | 141 | 268 | 270 | 97-23-4 | 4,34 | 98 | 100 |
| Diclobutrazol | 398 | 24.42 | 270 | 272 | 159 | 82 | 75736-33-3 | 4,01 | 96 | 99 |
| Diclofop methyl | 469 | 27.68 | 253 | 340 | 255 | 342 | 51338-27-3 | 4,54 | 99 | 100 |
| Dieldrin | 387 | 23.87 | 79 | 263 | 277 | 279 | 60-57-1 | 5,45 | 100 | 100 |
| Diethatyl ethyl | 381 | 23.60 | 188 | 162 | 238 | 160 | 38727-55-8 | 3,62 | 91 | 98 |
| Diethofencarb | 274 | 19.12 | 151 | 207 | 150 | 267 | 87130-20-9 | 3,29 | 82 | 96 |
| Difenoconazol I | 563 | 35.09 | 323 | 265 | 325 | 267 | 119446-68-3 | 5,2 | 100 | 100 |
| Difenoconazol II | 564 | 35.23 | 323 | 265 | 325 | 267 | 119446-68-3 | 5,2 | 100 | 100 |
| Diflufenican | 472 | 27.79 | 266 | 394 | 267 | 246 | 83164-33-4 | 3,53 | 89 | 98 |
| Dimethametryn | 327 | 21.11 | 212 | 213 | 255 | 71 | 22936-75-0 | 4,22 | 98 | 100 |
| Dimethylvinphos(z) | 275 | 19.15 | 295 | 297 | 109 | 299 | 2274-67-1 | 3,16 | 78 | 95 |
| Diniconazole | 423 | 25.55 | 268 | 270 | 70 | 269 | 83657-24-3 | 3,92 | 95 | 99 |
| Dinitramine | 180 | 14.81 | 305 | 307 | 261 | 216 | 29091-05-2 | 3,96 | 96 | 99 |
| Dinobuton | 351 | 21.98 | 45 | 44 | 211 | 207 | 973-21-7 | 3,94 | 95 | 99 |
| Dinocap I | 474 | 27.85 | 69 | 44 | 41 | 159 | 39300-45-3 | 5,98 | 100 | 100 |
| Dinocap II | 482 | 28.22 | 69 | 44 | 68 | 70 | 39300-45-3 | 5,98 | 100 | 100 |
| Dinocap III | 495 | 28.60 | 69 | 70 | 197 | 77 | 39300-45-3 | 5,98 | 100 | 100 |
| Dinocap IV | 504 | 28.93 | 69 | 44 | 207 | 41 | 39300-45-3 | 5,98 | 100 | 100 |
| Dinoseb | 171 | 14.54 | 211 | 163 | 147 | 117 | 88-85-7 | 3,67 | 92 | 98 |
| Dinoseb acetate | 241 | 17.53 | 60 | 240 | 211 | 205 | 2813-95-8 | 3,17 | 78 | 95 |
| Dinoterb | 163 | 14.07 | 225 | 177 | 131 | 77 | 1420-07-1 | 3,64 | 91 | 98 |
| Dinoterb acetate | 248 | 17.91 | 225 | 77 | 177 | 240 | 3204-27-1 | 3,13 | 76 | 94 |
| Dioxathion | 537 | 31.84 | 97 | 125 | 271 | 153 | 78-34-2 | 3,45 | 87 | 97 |
| Diphacinone | 557 | 34.26 | 173 | 168 | 167 | 165 | 82-66-6 | 4,85 | 99 | 100 |
| Diphenylamine | 82 | 10.52 | 169 | 168 | 170 | 83 | 122-39-4 | 3,29 | 82 | 96 |
| Dipropetryn | 268 | 18.72 | 255 | 240 | 184 | 222 | 4147-51-7 | 4,22 | 98 | 100 |
| Disulfoton | 170 | 14.55 | 88 | 89 | 97 | 142 | 298-04-4 | 3,86 | 95 | 99 |
| Ditalimfos | 370 | 23.17 | 130 | 148 | 299 | 209 | 5131-24-8 | 3,74 | 93 | 99 |
| Dithiopyr | 252 | 18.10 | 354 | 306 | 286 | 237 | 97886-45-8 | 4,46 | 99 | 100 |
| Diuron* | 334 | 21.37 | 72 | 187 | 124 | 189 | 470-90-6 | 4,15 | 97 | 99 |
| Dodemorph I | 299 | 19.92 | 154 | 141 | 155 | 281 | 1593-77-7 | 5,7 | 100 | 100 |
| Dodemorph II | 316 | 20.80 | 154 | 141 | 155 | 238 | 1593-77-7 | 5,7 | 100 | 100 |
| Edifenphos | 449 | 26.79 | 109 | 173 | 110 | 310 | 17109-49-8 | 3,61 | 91 | 98 |
| Endosulfan (alpha isomer) | 362 | 22.64 | 241 | 195 | 239 | 237 | 115-29-7 | 3,5 | 88 | 98 |
| Endosulfan (beta isomer) | 414 | 25.16 | 195 | 237 | 207 | 241 | 115-29-7 | 3,5 | 88 | 98 |
| Endosulfan ether | 189 | 15.35 | 69 | 241 | 239 | 277 | - | 4,15 | 97 | 99 |
| Endosulfan sulfate | 450 | 26.76 | 272 | 274 | 229 | 237 | 1031-07-8 | 3,64 | 91 | 98 |
| Endrin | 408 | 24.76 | 317 | 263 | 315 | 319 | 72-20-8 | 5,45 | 100 | 100 |
| Endrin aldehyde | 431 | 25.91 | 67 | 345 | 250 | 347 | 7421-93-4 | 4,8 | 99 | 100 |
| Endrin ketone | 481 | 28.23 | 317 | 67 | 315 | 319 | 53494-70-5 | 4,99 | 100 | 100 |
| EPN | 496 | 28.66 | 157 | 169 | 141 | 185 | 2104-64-5 | 4,47 | 99 | 100 |
| Epoxiconazole | 478 | 28.02 | 192 | 194 | 138 | 165 | 133855-98-8 | 3,47 | 88 | 97 |
| Erbon | 411 | 24.89 | 169 | 171 | 97 | 135 | 136-25-4 | 5,63 | 100 | 100 |
| Esfenvalerate | 560 | 34.69 | 125 | 167 | 181 | 209 | 51630-58-1 | 6,76 | 100 | 100 |
| Esprocarb | 256 | 18.25 | 91 | 222 | 71 | 162 | 85785-20-2 | 4,58 | 99 | 100 |
| Etaconazole | 427 | 25.76 | 173 | 245 | 55 | 175 | 60207-93-4 | 4,13 | 97 | 99 |

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|---|---|---|---|---|---|---|---|---|---|---|
| Ethalfluralin | 98 | 11.28 | 276 | 316 | 292 | 333 | 55283-68-6 | 5,23 | 100 | 100 |
| Ethion | 435 | 26.00 | 231 | 153 | 97 | 125 | 563-12-2 | 4,75 | 99 | 100 |
| Ethoprophos | 86 | 10.74 | 158 | 97 | 126 | 139 | 13194-48-4 | 3,14 | 77 | 95 |
| Ethoxyquin | 128 | 12.83 | 202 | 174 | 203 | 145 | 91-53-2 | 3,87 | 95 | 99 |
| Etridiazole | 44 | 7.96 | 211 | 183 | 213 | 185 | 2593-15-9 | 3,6 | 91 | 98 |
| Fenarimol | 521 | 30.40 | 139 | 219 | 107 | 251 | 60168-88-9 | 3,62 | 91 | 98 |
| Fenazaflor | 439 | 26.26 | 77 | 374 | 234 | 376 | 14255-88-0 | 4,54 | 99 | 100 |
| Fenbuconazole | 538 | 32.23 | 129 | 198 | 125 | 127 | 114369-43-6 | 4,23 | 98 | 100 |
| Fenchlorphos | 236 | 17.33 | 285 | 287 | 125 | 289 | 299-84-3 | 4,86 | 99 | 100 |
| Fenitrothion | 251 | 18.07 | 277 | 125 | 109 | 260 | 122-14-5 | 3,3 | 83 | 96 |
| Fenoprop | 228 | 16.80 | 196 | 198 | 97 | 200 | 93-72-1 | 3,68 | 92 | 98 |
| Fenoxycarb | 498 | 28.70 | 255 | 186 | 77 | 185 | 72490-01-8 | 4,24 | 98 | 100 |
| Fenpropathrin | 505 | 28.99 | 97 | 181 | 125 | 265 | 39515-41-8 | 5,62 | 100 | 100 |
| Fenpropimorph | 279 | 19.27 | 128 | 129 | 303 | 117 | 67564-91-4 | 5,5 | 100 | 100 |
| Fenson | 290 | 19.66 | 77 | 141 | 268 | 51 | 80-38-6 | 3,57 | 90 | 98 |
| Fenthion | 273 | 19.12 | 278 | 125 | 109 | 169 | 55-38-9 | 4,08 | 97 | 99 |
| Fenvalerate I | 558 | 34.27 | 167 | 125 | 181 | 152 | 51630-58-1 | 6,76 | 100 | 100 |
| Fenvalerate II | 559 | 34.68 | 125 | 167 | 181 | 169 | 51630-58-1 | 6,76 | 100 | 100 |
| Flamprop-isopropyl | 429 | 25.82 | 105 | 77 | 276 | 106 | 52756-22-6 | 4,24 | 98 | 100 |
| Flamprop-methyl | 403 | 24.54 | 105 | 77 | 276 | 106 | 52756-25-9 | 3,33 | 84 | 96 |
| Fluazifop-p-butyl | 417 | 25.32 | 282 | 254 | 383 | 255 | 69806-50-4 | 5,34 | 100 | 100 |
| Flubenzimine | 397 | 24.36 | 135 | 186 | 77 | 416 | 37893-02-0 | 6,66 | 100 | 100 |
| Fluchloralin | 175 | 14.64 | 306 | 326 | 264 | 63 | 33245-39-5 | 5,07 | 100 | 100 |
| Flucythrinate I | 548 | 33.12 | 199 | 157 | 44 | 207 | 70124-77-5 | 6,56 | 100 | 100 |
| Flucythrinate II | 552 | 33.46 | 199 | 157 | 44 | 181 | 70124-77-5 | 6,56 | 100 | 100 |
| Flumetralin | 373 | 23.34 | 143 | 145 | 157 | 404 | 62924-70-3 | 6,09 | 100 | 100 |
| Fluorodifen | 382 | 23.73 | 190 | 126 | 160 | 298 | 15457-05-3 | 3,81 | 94 | 99 |
| Fluotrimazole | 479 | 28.04 | 165 | 311 | 312 | 379 | 31251-03-3 | 5,76 | 100 | 100 |
| Fluridone | 554 | 33.77 | 328 | 329 | 330 | 154 | 2051-24-3 | 10,2 | 100 | 100 |
| Flurochloridone I | 300 | 19.96 | 174 | 311 | 187 | 145 | 61213-25-0 | 3,45 | 87 | 97 |
| Flurochloridone II | 305 | 20.10 | 174 | 311 | 187 | 145 | 31213-25-0 | 3,45 | 87 | 97 |
| Fluroxypyr-1-methylheptyl ester | 470 | 27.73 | 57 | 71 | 209 | 181 | 81406-37-3 | 4,82 | 99 | 100 |
| Flusilazole | 405 | 24.59 | 233 | 206 | 234 | 315 | 85509-19-9 | 4,89 | 99 | 100 |
| Flutolanil | 385 | 23.84 | 173 | 145 | 281 | 323 | 66332-96-5 | 4,65 | 99 | 100 |
| Fluvalinate-tau-I | 561 | 34.72 | 250 | 252 | 209 | 181 | 69409-94-5 | 6,81 | 100 | 100 |
| Fluvalinate-tau-II | 562 | 34.85 | 250 | 252 | 209 | 181 | 69409-94-5 | 6,81 | 100 | 100 |
| Fonofos | 157 | 13.89 | 109 | 246 | 137 | 110 | 944-22-9 | 4,02 | 96 | 99 |
| Furathiocarb | 512 | 29.61 | 163 | 164 | 149 | 76 | 65907-30-4 | 4,43 | 98 | 100 |
| Furmecyclox | 197 | 15.64 | 123 | 124 | 139 | 221 | 60568-05-0 | 4,38 | 98 | 100 |
| Heptachlor | 224 | 16.80 | 272 | 100 | 274 | 270 | 76-44-8 | 5,86 | 100 | 100 |
| Heptachlor epoxide | 313 | 20.72 | 353 | 355 | 351 | 357 | 1024-57-3 | 4,56 | 99 | 100 |
| Heptachlor exo-epoxide isomer B | 312 | 20.72 | 353 | 355 | 351 | 357 | 1024-57-3 | 4,56 | 99 | 100 |
| Hexabromobenzene | 487 | 28.45 | 551 | 549 | 553 | 232 | 87-82-1 | 7,33 | 100 | 100 |
| Hexachlorobenzene | 117 | 12.38 | 284 | 286 | 282 | 288 | 118-74-1 | 5,86 | 100 | 100 |
| Hexachlorophene | 550 | 33.20 | 196 | 198 | 211 | 210 | 70-30-4 | 6,92 | 100 | 100 |
| Hexaconazole | 376 | 23.52 | 83 | 214 | 216 | 82 | 79983-71-4 | 3,66 | 92 | 98 |
| Hexestrol | 457 | 26.98 | 135 | 107 | 134 | 136 | 84-16-2 | 5,6 | 100 | 100 |
| Imazalil | 384 | 23.79 | 41 | 215 | 173 | 217 | 35554-44-0 | 4,1 | 97 | 99 |
| Ioxynil | 247 | 17.86 | 371 | 117 | 88 | 89 | 1689-83-4 | 3,94 | 95 | 99 |
| Iprobenfos | 190 | 15.35 | 91 | 204 | 123 | 122 | 26087-47-8 | 3,57 | 90 | 98 |

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|---|---|---|---|---|---|---|---|---|---|---|
| Isazophos | 182 | 15.05 | 161 | 119 | 162 | 97 | 42509-80-8 | 3,26 | 81 | 96 |
| Isobenzan | 285 | 19.44 | 311 | 103 | 313 | 309 | 297-78-9 | 4,51 | 99 | 100 |
| Isobornyl thiocyanoacetate | 186 | 15.24 | 121 | 93 | 95 | 136 | 115-31-1 | 3,75 | 93 | 99 |
| Isodrin | 303 | 20.03 | 193 | 195 | 263 | 66 | 465-73-6 | 6,75 | 100 | 100 |
| Isofenphos | 339 | 21.62 | 213 | 58 | 121 | 255 | 25311-71-1 | 4,65 | 99 | 100 |
| Isomethiozin | 281 | 19.35 | 225 | 198 | 184 | 199 | 57052-04-7 | 3,99 | 96 | 99 |
| Isopropalin | 314 | 20.70 | 280 | 238 | 281 | 264 | 33820-53-0 | 5,8 | 100 | 100 |
| Isoxaben | 525 | 30.80 | 165 | 68 | 96 | 163 | 82558-50-7 | 3,98 | 96 | 99 |
| Isoxathion | 412 | 24.98 | 105 | 77 | 177 | 313 | 18854-01-8 | 3,9 | 95 | 99 |
| Jodfenphos | 377 | 23.58 | 377 | 379 | 125 | 109 | 18181-70-9 | 5,39 | 100 | 100 |
| Kinoprene | 272 | 19.09 | 149 | 79 | 105 | 71 | 42588-37-4 | 6,45 | 100 | 100 |
| Lenacil | 453 | 26.88 | 153 | 154 | 110 | 136 | 2164-08-1 | 3,09 | 75 | 94 |
| Leptophos | 516 | 29.73 | 171 | 377 | 375 | 155 | 21609-90-5 | 6,34 | 100 | 100 |
| Leptophos oxon | 490 | 28.52 | 155 | 361 | 359 | 77 | 21609-90-5 | 6,34 | 100 | 100 |
| Lindane | 143 | 13.46 | 181 | 183 | 219 | 111 | 58-89-9 | 4,26 | 98 | 100 |
| Mepronil | 440 | 26.29 | 119 | 91 | 269 | 120 | 55814-41-0 | 4,24 | 98 | 100 |
| Methfuroxam | 287 | 19.47 | 137 | 229 | 138 | 67 | 28730-17-8 | 3,71 | 92 | 98 |
| Methoprene I | 318 | 20.90 | 73 | 111 | 81 | 109 | 40596-69-8 | 6,34 | 100 | 100 |
| Methoprene II | 357 | 22.33 | 73 | 111 | 109 | 107 | 40596-69-8 | 6,34 | 100 | 100 |
| Methoxychlor | 502 | 28.86 | 227 | 228 | 152 | 113 | 72-43-5 | 5,67 | 100 | 100 |
| Methyldymron | 333 | 21.37 | 107 | 146 | 106 | 77 | 42609-73-4 | 3,58 | 90 | 98 |
| Metolachlor | 271 | 18.91 | 162 | 238 | 240 | 146 | 51218-45-2 | 3,24 | 81 | 96 |
| Mirex | 517 | 29.84 | 272 | 274 | 270 | 237 | 2385-85-5 | 7,01 | 100 | 100 |
| Monalide | 191 | 15.47 | 85 | 127 | 197 | 239 | 7287-36-7 | 4,09 | 97 | 99 |
| Myclobutanil | 399 | 24.44 | 179 | 150 | 181 | 82 | 88671-89-0 | 3,5 | 88 | 98 |
| Napropamide | 374 | 23.44 | 72 | 128 | 271 | 100 | 15299-99-7 | 3,33 | 84 | 96 |
| Nitrapyrin | 43 | 7.93 | 194 | 196 | 198 | 160 | 1929-82-4 | 3,35 | 84 | 97 |
| Nitrofen | 410 | 24.86 | 283 | 285 | 202 | 253 | 1836-75-5 | 4,32 | 98 | 100 |
| Nitrothal-isopropyl | 296 | 19.87 | 236 | 194 | 212 | 254 | 10552-74-6 | 3,3 | 83 | 96 |
| Nuarimol | 466 | 27.45 | 235 | 107 | 203 | 139 | 63284-71-9 | 3,17 | 78 | 95 |
| o,p'-DDD | 396 | 24.35 | 235 | 237 | 165 | 199 | 53-19-0 | 5,87 | 100 | 100 |
| o,p'-DDE | 359 | 22.50 | 246 | 248 | 318 | 316 | 3424-82-6 | 6 | 100 | 100 |
| o,p'-DDT | 428 | 25.77 | 235 | 237 | 165 | 236 | 50-29-3 | 6,79 | 100 | 100 |
| Octachlorostyrene | 310 | 20.61 | 308 | 380 | 310 | 343 | 29082-74-4 | 7,46 | 100 | 100 |
| o-Phenylphenol | 51 | 8.78 | 170 | 169 | 141 | 115 | 90-43-7 | 3,28 | 82 | 96 |
| Oxadiazon | 400 | 24.42 | 175 | 177 | 258 | 260 | 19666-30-9 | 4,81 | 99 | 100 |
| Oxychlordane | 315 | 20.79 | 115 | 185 | 187 | 149 | 27304-13-8 | 5,48 | 100 | 100 |
| Oxyfluorfen | 407 | 24.73 | 252 | 302 | 331 | 361 | 42874-03-3 | 5,21 | 100 | 100 |
| p,p'-DDD | 425 | 25.69 | 235 | 237 | 165 | 236 | 72-54-8 | 5,87 | 100 | 100 |
| p,p'-DDE | 391 | 24.02 | 246 | 318 | 316 | 248 | 72-55-9 | 6 | 100 | 100 |
| p,p'-DDT | 458 | 26.98 | 235 | 237 | 165 | 236 | 50-29-3 | 6,79 | 100 | 100 |
| Paclobutrazol | 361 | 22.55 | 236 | 125 | 238 | 167 | 76738-62-0 | 3,36 | 85 | 97 |
| Parathion | 280 | 19.27 | 291 | 109 | 97 | 139 | 56-38-2 | 3,73 | 93 | 99 |
| p-Dichlorobenzene | 3 | 3.88 | 146 | 148 | 111 | 75 | 106-46-7 | 3,28 | 82 | 96 |
| Pebulate | 45 | 7.97 | 128 | 57 | 72 | 161 | 1114-71-2 | 3,51 | 89 | 98 |
| Penconazole | 325 | 21.03 | 248 | 159 | 161 | 250 | 66246-88-6 | 4,67 | 99 | 100 |
| Pendimethalin | 324 | 20.99 | 252 | 253 | 281 | 162 | 40487-42-1 | 4,82 | 99 | 100 |
| Pentachloroaniline | 193 | 15.54 | 265 | 267 | 263 | 269 | 527-20-8 | 4,3 | 98 | 100 |
| Pentachloroanisole | 121 | 12.58 | 280 | 265 | 237 | 282 | 1825-21-4 | 5,3 | 100 | 100 |
| Pentachlorobenzene | 55 | 8.95 | 250 | 252 | 248 | 254 | 608-93-5 | 5,22 | 100 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| Pentachloronitrobenzene | 151 | 13.68 | 237 | 249 | 295 | 214 | 82-68-8 | 5,03 | 100 | 100 |
| Pentachlorophenol | 139 | 13.26 | 266 | 268 | 264 | 165 | 87-86-5 | 4,74 | 99 | 100 |
| Pentanochlor | 255 | 18.23 | 141 | 71 | 143 | 239 | 2307-68-8 | 4,18 | 97 | 99 |
| Permethrin I | 530 | 31.37 | 183 | 163 | 165 | 184 | 52645-53-1 | 7,43 | 100 | 100 |
| Permethrin II | 532 | 31.55 | 183 | 163 | 165 | 184 | 52645-53-1 | 7,43 | 100 | 100 |
| Perthane | 415 | 25.15 | 223 | 224 | 165 | 178 | 72-56-0 | 6,66 | 100 | 100 |
| Phenamiphos | 380 | 23.59 | 303 | 154 | 288 | 217 | 22224-92-6 | 3,29 | 82 | 96 |
| Phenkapton | 503 | 28.89 | 121 | 153 | 97 | 191 | 2275-14-1 | 5,84 | 100 | 100 |
| Phenthoate | 343 | 21.71 | 274 | 125 | 121 | 93 | 2597-03-7 | 3,47 | 88 | 97 |
| Phorate | 111 | 11.96 | 75 | 121 | 260 | 97 | 298-02-2 | 3,37 | 85 | 97 |
| Phosalone | 515 | 29.68 | 182 | 121 | 184 | 367 | 2310-17-0 | 4,29 | 98 | 100 |
| Piperalin | 463 | 27.24 | 112 | 314 | 316 | 173 | 3478-94-2 | 5,08 | 100 | 100 |
| Piperonyl butoxide | 475 | 27.90 | 176 | 177 | 149 | 178 | 51-03-6 | 4,29 | 98 | 100 |
| Piperophos | 501 | 28.88 | 122 | 140 | 320 | 97 | 24151-93-7 | 4,23 | 98 | 100 |
| Pirimiphos-ethyl | 311 | 20.65 | 333 | 318 | 304 | 168 | 23505-41-1 | 4,42 | 98 | 100 |
| Pirimiphos-methyl | 257 | 18.31 | 290 | 276 | 305 | 233 | 29232-93-7 | 3,44 | 87 | 97 |
| Plifenat | 220 | 16.64 | 43 | 217 | 175 | 219 | 21757-82-4 | 5,14 | 100 | 100 |
| Pretilachlor | 394 | 24.14 | 162 | 238 | 176 | 202 | 51218-49-6 | 4,29 | 98 | 100 |
| Prochloraz | 535 | 31.73 | 180 | 70 | 308 | 310 | 67747-09-5 | 4,13 | 97 | 99 |
| Profenofos | 389 | 23.90 | 208 | 139 | 206 | 339 | 41198-08-7 | 4,82 | 99 | 100 |
| Profluralin | 162 | 14.04 | 55 | 318 | 330 | 264 | 26399-36-0 | 5,62 | 100 | 100 |
| Promecarb | 109 | 11.92 | 135 | 150 | 91 | 136 | 2631-37-0 | 3,18 | 78 | 95 |
| Prometon | 130 | 12.99 | 210 | 225 | 168 | 183 | 1610-18-0 | 3,57 | 90 | 98 |
| Prometryn | 240 | 17.34 | 241 | 184 | 226 | 105 | 7287-19-6 | 3,73 | 93 | 99 |
| Propargite | 471 | 27.73 | 135 | 150 | 231 | 64 | 2312-35-8 | 5,57 | 100 | 100 |
| Propazine | 141 | 13.36 | 214 | 229 | 172 | 58 | 139-40-2 | 3,24 | 81 | 96 |
| Propiconazole-I | 454 | 26.94 | 173 | 69 | 259 | 175 | 60207-90-1 | 4,13 | 97 | 99 |
| Propiconazole-II | 462 | 27.15 | 173 | 69 | 259 | 175 | 60207-90-1 | 4,13 | 97 | 99 |
| Propyzamide | 159 | 13.95 | 173 | 175 | 145 | 255 | 23950-58-5 | 3,57 | 90 | 98 |
| Prothiofos | 383 | 23.75 | 309 | 267 | 162 | 113 | 34643-46-4 | 5,69 | 100 | 100 |
| Pyrazophos | 523 | 30.72 | 221 | 232 | 237 | 373 | 13457-18-6 | 3,53 | 89 | 98 |
| Pyrazoxyfen | 565 | 35.52 | 105 | 77 | 173 | 51 | 71561-11-0 | 4,97 | 100 | 100 |
| Pyributicarb | 483 | 28.35 | 165 | 108 | 181 | 93 | 88678-67-5 | 5,34 | 100 | 100 |
| Pyridaben | 531 | 31.52 | 147 | 117 | 148 | 132 | 96489-71-3 | 5,47 | 100 | 100 |
| Pyridaphenthion | 489 | 28.52 | 340 | 77 | 199 | 97 | 119-12-0 | 3,66 | 92 | 98 |
| Pyridate | 556 | 33.97 | 207 | 205 | 71 | 206 | 55512-33-9 | 5,73 | 100 | 100 |
| Pyrifenox I | 332 | 21.21 | 171 | 173 | 262 | 100 | 88283-41-4 | 4,2 | 97 | 100 |
| Pyrifenox II | 363 | 22.62 | 171 | 173 | 262 | 92 | 88283-41-4 | 4,2 | 97 | 100 |
| Pyrimethanil | 164 | 14.13 | 198 | 199 | 200 | 77 | 53112-28-0 | 3,19 | 79 | 95 |
| Quizalofop-ethyl | 545 | 32.91 | 299 | 372 | 163 | 301 | 76578-14-8 | 4,35 | 98 | 100 |
| Resmethrin | 476 | 27.98 | 123 | 171 | 128 | 143 | 10453-86-8 | 7,11 | 100 | 100 |
| S,S,S-Tributylphosphorotrithioate (tribufos) | 393 | 24.10 | 169 | 202 | 170 | 147 | 78-48-8 | 5,75 | 100 | 100 |
| Sebuthylazine | 187 | 15.26 | 200 | 202 | 214 | 229 | 7286-69-3 | 3,31 | 83 | 96 |
| Secbumeton | 177 | 14.74 | 196 | 169 | 210 | 225 | 26259-45-0 | 3,64 | 91 | 98 |
| Sulfotep | 106 | 11.83 | 322 | 202 | 97 | 238 | 3689-24-5 | 3,98 | 96 | 99 |
| Sulprofos | 441 | 26.34 | 322 | 156 | 140 | 139 | 35400-43-2 | 5,65 | 100 | 100 |
| Tamoxifen | 536 | 31.75 | 58 | 72 | 371 | 253 | 10540-29-1 | 6,3 | 100 | 100 |
| TCMTB | 368 | 23.10 | 180 | 181 | 136 | 238 | 21564-17-0 | 3,12 | 76 | 94 |
| Tebuconazole | 465 | 27.43 | 125 | 250 | 70 | 83 | 107534-96-3 | 3,89 | 95 | 99 |

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|---|---|---|---|---|---|---|---|---|---|---|
| Tebutam | 107 | 11.83 | 91 | 57 | 190 | 233 | 35256-85-0 | 3,49 | 88 | 97 |
| Tecnazene | 73 | 10.24 | 203 | 215 | 261 | 201 | 117-18-0 | 4,39 | 98 | 100 |
| Temephos | 567 | 40.74 | 466 | 125 | 93 | 109 | 3383-96-8 | 6,17 | 100 | 100 |
| Terbucarb | 221 | 16.69 | 205 | 220 | 206 | 57 | 1918-11-2 | 5,28 | 100 | 100 |
| Terbufos | 153 | 13.80 | 231 | 57 | 103 | 153 | 13071-79-9 | 4,24 | 98 | 100 |
| Terbumeton | 144 | 13.44 | 210 | 169 | 225 | 154 | 33693-04-8 | 3,6 | 91 | 98 |
| Terbuthylazine | 155 | 13.81 | 214 | 173 | 216 | 229 | 5915-41-3 | 3,27 | 82 | 96 |
| Terbutryne | 249 | 17.97 | 226 | 185 | 241 | 170 | 886-50-0 | 3,77 | 93 | 99 |
| Tetrachlorvinphos | 366 | 22.95 | 329 | 331 | 109 | 333 | 22248-79-9 | 3,81 | 94 | 99 |
| Tetradifon | 509 | 29.38 | 159 | 111 | 229 | 227 | 116-29-0 | 5,18 | 100 | 100 |
| Tetramethrin I | 493 | 28.63 | 164 | 123 | 79 | 107 | 7696-12-0 | 5,54 | 100 | 100 |
| Tetramethrin II | 499 | 28.86 | 164 | 123 | 165 | 79 | 7696-12-0 | 5,54 | 100 | 100 |
| Tetrapropyl thiodiphosphate | 277 | 19.21 | 211 | 210 | 253 | 115 | 3244-90-4 | 5,94 | 100 | 100 |
| Tetrasul | 437 | 26.07 | 252 | 254 | 324 | 322 | 2227-13-6 | 6,87 | 100 | 100 |
| Thenylchlor | 467 | 27.49 | 127 | 288 | 141 | 287 | 96491-05-3 | 4,21 | 97 | 100 |
| Tolclofos-methyl | 226 | 16.81 | 265 | 267 | 125 | 266 | 57018-04-9 | 4,77 | 99 | 100 |
| Tolylfluanid | 331 | 21.25 | 137 | 238 | 106 | 63 | 731-27-1 | 3,27 | 82 | 96 |
| Tri-allate | 181 | 14.97 | 86 | 268 | 270 | 128 | 2303-17-5 | 4,57 | 99 | 100 |
| Tributyl phosphorotrithioite | 328 | 21.18 | 209 | 153 | 298 | 97 | 150-50-5 | 7,67 | 100 | 100 |
| Trichloronate | 295 | 19.84 | 109 | 297 | 299 | 271 | 327-98-0 | 5,86 | 100 | 100 |
| Tridiphane | 235 | 17.25 | 173 | 187 | 189 | 175 | 58138-08-2 | 5,18 | 100 | 100 |
| Trietazine | 156 | 13.86 | 200 | 229 | 214 | 186 | 1912-26-1 | 3,44 | 87 | 97 |
| Trifluralin | 103 | 11.64 | 306 | 264 | 307 | 290 | 1582-09-8 | 5,31 | 100 | 100 |
| Tryclopyrbutoxyethyl | 409 | 24.82 | 57 | 56 | 85 | 210 | - | 3,94 | 95 | 99 |
| Vernolate | 40 | 7.81 | 128 | 43 | 86 | 146 | 1929-77-7 | 3,51 | 89 | 98 |
| Uniconizole-P | 390 | 24.02 | 234 | 236 | 70 | 235 | 83657-22-1 | 3,28 | 82 | 96 |