

Appendix II

The Eight Peak Index of EI+ MS Data

Pesticide and related compound EI+ MS data ordered by most intense ion

In this section, the EI+ mass spectrometric data are compiled in eight peak index format, to facilitate the identification of unidentified spectra. As these will generally be obtained following gas chromatographic separation, those compounds that are not readily amenable to GC are distinguished by an asterisk. Molecular ion m/z data are underlined. Data for GC contaminants and artefacts are given in *italics*.

For spectra in which the base peak is at low mass, and which therefore may be difficult to observe (either because it is below the acquired mass range or because it is obscured by solvent/co-extractive interference), a second entry has been made under the most intense ion in the spectrum observed at high mass. In this instance $m/z100$ has been chosen as the (arbitrary) threshold between high and low mass. Such entries are readily distinguished by the appearance in the relative intensity list of the 100% value in the second column rather than the first. Of course, some spectra have no ions of any significant intensity greater than $m/z100$ (particularly those whose molecular weight is less than 100), but the only pesticides in this category in this collection are: 2-aminobutane, aminotriazole, binapacryl, dinocap, metaldehyde, methyl bromide, methyl isothiocyanate and thiodicarb.

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|--------------------------|-----------------------------|-------------------|-------------------------|
| 27 107 109 26 28 79 81 93 | 100 80 80 15 10 5 5 5 | 1,2-Dibromoethane | C2H4Br2 | M:186,188,190(1,2,1%) |
| 29 44 43 45 42 26 89 27 | 100 85 55 45 15 10 10 5 | *Metaldehyde | C8H16O4 | M:176(0%) |
| 30 101 127 44 <u>142</u> 99 70 56 | 100 80 80 50 45 45 40 30 | Iprodione related v) | C6H10N2O2 | M:142(45%) |
| 36 38 56 270 272 243 142 29 | 100 35 25 15 15 10 10 10 | *Triforine | C10H14Cl6N4O2 | M:432,434,436(0,0,0%) |
| 39 54 187 213 <u>285</u> 212 53 198 | 100 90 85 80 80 80 73 65 | Vinclozolin | C12H9Cl2NO3 | M:285,287(80,50%) |
| 41 44 47 40 45 61 88 30 | 100 85 55 45 45 45 35 30 | *Thiodicarb | C10H18N4O4S3 | M:354(1%) |
| 41 55 60 83 115 <u>161</u> 40 57 | 100 95 90 90 85 50 40 35 | Thiofanox oxime | C7H15NOS | M:161(50%) |
| 41 68 64 47 63 42 39 131 | 100 80 75 20 10 10 10 5 | *Aldicarb sulphoxide | C7H14N2O3S | M:206(0%) |
| 41 68 64 47 63 42 39 <u>131</u> | 100 80 75 20 10 10 10 5 | Aldicarb sulphoxide related | C5H9NOS | M:131(5%) |
| 41 215 173 217 175 81 159 54 | 100 25 15 15 10 10 5 5 | Imazalil | C14H14Cl2N2O | M:296,298(2,1%) |
| 43 29 259 188 <u>331</u> 187 261 186 | 100 70 30 30 25 25 20 20 | Chlozolinat | C13H11Cl2NO5 | M:331,333,335(25,15,5%) |
| 43 41 27 56 28 30 39 98 | 100 90 75 50 40 30 20 20 | Benomyl related, n-BuNCO | C5H9NO | M:99(3%) |
| 43 41 56 27 159 30 98 191 | 100 85 45 40 35 30 20 15 | *Benomyl | C14H18N4O3 | M:290(0%) |
| 43 70 44 133 <u>162</u> 106 117 147 | 100 85 55 45 30 20 15 10 | Tabun nerve agent (CW) | C5H11N2O2P | M:162(30%) |
| 43 70 180 308 310 266 268 312 | 100 80 55 20 20 15 15 10 | *Prochloraz | C15H16Cl3N3O2 | M:375(0%) |
| 43 86 268 128 270 143 145 84 | 100 85 20 20 15 10 10 5 | Tri-allate | C10H16Cl3NOS | M:303,305,307(0,0,0%) |
| 43 91 128 86 41 65 <u>251</u> 162 | 100 65 60 35 20 15 15 10 | *Prosulfocarb | C14H21NOS | M:251(15%) |
| 43 113 267 162 309 155 164 41 | 100 85 65 65 55 55 45 40 | Prothiofos | C11H15Cl2O2PS2 | M:344,346(1,1%) |
| 43 127 <u>213</u> 171 129 154 41 27 | 100 50 15 15 15 15 15 10 | Chlorpropham | C10H12ClNO2 | M:213,215(15,5%) |
| 43 158 97 41 139 126 74 93 | 100 90 70 60 50 50 40 40 | Ethoprophos | C8H19O2PS2 | M:242(25%) |
| 43 211 41 163 240 205 147 212 | 100 45 15 10 10 10 10 5 | Dinobuton | C14H18N2O7 | M:326(0%) |
| 43 211 240 44 163 147 117 205 | 100 10 10 10 5 5 5 5 | Dinoseb acetate | C12H14N2O6 | M:282(1%) |
| 43 <u>225</u> 139 68 182 58 210 47 | 100 80 75 65 55 45 40 40 | *Aziprotryne | C7H11N7S | M:225(80%) |
| 44 30 29 70 111 167 128 183 | 100 90 40 30 30 20 15 10 | Cymoxanil | C7H10N4O3 | M:198(1%) |
| 44 58 41 30 42 43 29 27 | 100 10 10 5 5 5 5 5 | 2-Aminobutane | C4H11N | M:73(1%) |
| 44 135 153 92 199 243 <u>286</u> 200 | 100 65 45 45 40 20 20 20 | Schradan | C8H24N4O3P2 | M:286(20%) |
| 44 <u>196</u> 181 117 152 42 154 <u>198</u> | 100 85 50 50 40 30 30 25 | Chlordimeform | C10H13ClN2 | M:196,198(85,25%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|--------------------------|----------------------|-------------------|-------------------------|
| 44 <u>201</u> 186 173 43 68 <u>203</u> 158 | 100 90 55 45 35 30 30 25 | Simazine | C7H12ClN5 | M:201,203(90,30%) |
| 45 33 <u>78</u> 61 31 29 42 49 | 100 85 45 40 30 20 10 5 | * Fluoroacetic acid | C2H3FO2 | M:78(45%) |
| 45 105 163 132 120 77 133 91 | 100 60 55 35 25 20 15 15 | Oxadixyl | C14H18N2O4 | M:278(10%) |
| 45 160 188 237 224 146 202 132 | 100 45 40 15 15 10 10 10 | Alachlor | C14H20ClNO2 | M:269(5%) |
| 45 206 192 220 249 234 146 160 | 100 35 25 20 20 15 15 15 | Metalaxyl | C15H21NO4 | M:279(10%) |
| 54 43 39 53 27 118 76 59 | 100 70 50 35 35 25 20 15 | Dimethipin | C6H10O4S2 | M:210(5%) |
| 57 29 41 <u>310</u> <u>312</u> 219 196 211 | 100 40 40 15 15 15 10 10 | 2,4,5-T n-butyl | C12H13Cl3O3 | M:310,312,314(15,15,5%) |
| 57 41 29 <u>310</u> <u>312</u> 196 198 211 | 100 35 30 10 10 10 10 10 | 2,4,5-T i-butyl | C12H13Cl3O3 | M:310,312,314(10,10,3%) |
| 57 43 71 41 70 256 254 55 | 100 70 50 40 40 25 25 25 | 2,4,5-T i-octyl | C16H21Cl3O3 | M:366,368,370(12,12,4%) |
| 57 56 41 220 29 85 175 222 | 100 40 25 20 20 15 15 15 | 2,4-D butoxyethyl | C14H18Cl2O4 | M:320,322(8,5%) |
| 57 71 43 181 209 210 211 254 | 100 85 65 25 25 20 20 15 | Fluroxypyr-meptyl | C15H21Cl2FN2O3 | M:366,368,370(10,7,2%) |
| 57 71 43 220 70 41 222 <u>332</u> | 100 65 65 50 40 35 25 20 | 2,4-D i-octyl | C16H22Cl2O3 | M:332,334(20,15%) |
| 57 97 153 29 125 41 199 186 | 100 85 55 50 50 40 35 30 | *Terbufos sulphoxide | C9H21O3PS3 | M:304(0%) |
| 57 185 41 29 <u>276</u> 175 162 <u>278</u> | 100 50 45 40 30 25 25 20 | 2,4-D n-butyl | C12H14Cl2O3 | M:276,278(30,20%) |
| 57 208 41 85 29 128 110 181 | 100 50 40 35 30 20 20 20 | Triadimefon | C14H16ClN3O2 | M:293,295(2,1%) |
| 57 231 29 103 153 41 65 186 | 100 40 25 20 15 15 15 10 | Terbufos | C9H21O2PS3 | M:288(5%) |
| 57 <u>268</u> 152 170 153 184 76 269 | 100 35 15 15 15 10 5 5 | Bitertanol related | C18H20O2 | M:268(35%) |
| 57 288 204 41 29 184 232 290 | 100 50 30 30 25 20 15 15 | Diniconazole ketone | C15H15Cl2N3O | M:323(0%) |
| 58 31 42 59 129 <u>188</u> 72 84 | 100 20 10 10 5 5 5 5 | *Propamocarb | C9H20N2O2 | M:188(5%) |
| 58 105 42 88 47 45 57 59 | 100 80 35 30 30 25 15 15 | *Methomyl | C5H10N2O2S | M:162(1%) |
| 58 <u>105</u> 47 45 42 88 31 59 | 100 55 45 45 45 35 35 20 | *Methomyl oxime | C3H7NOS | M:105(55%) |
| 58 213 121 185 255 96 43 138 | 100 60 55 40 40 40 30 20 | Isofenphos | C15H24NO4PS | M:345(5%) |
| 58 <u>241</u> 184 226 43 106 68 69 | 100 90 65 60 55 45 40 35 | Prometryn | C10H19N5S | M:241(90%) |
| 59 43 60 42 100 44 118 142 | 100 50 45 20 20 15 10 10 | *Daminozide | C6H12N2O3 | M:160(5%) |
| 59 72 55 41 67 83 126 98 | 100 45 35 25 15 15 10 10 | <i>oleamide</i> | <i>C18H35NO</i> | <i>M:281(5%)</i> |
| 61 <u>214</u> 46 153 127 126 99 90 | 100 15 15 15 15 15 10 5 | *Monolinuron | C9H11ClN2O2 | M:214,216(15,5%) |
| 61 <u>248</u> 46 250 187 200 189 202 | 100 10 10 5 5 5 2 2 | Linuron | C9H10Cl2N2O2 | M:248,250(10,6%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|--------------------------|---------------------------------------|--------------------|------------------------|
| 63 69 156 42 140 65 110 92 | 100 90 85 85 65 50 50 50 | *Triasulfuron | C14H16ClN5O5S | M:401,403(0,0%) |
| 63 249 251 27 143 205 65 223 | 100 85 45 45 40 40 35 25 | <i>tris-(2-chloroethyl) phosphate</i> | <i>C6H12Cl3O4P</i> | <i>M:284,286(0,0%)</i> |
| 64 <u>256</u> 160 128 192 <u>258</u> 96 162 | 100 95 75 70 40 35 25 20 | Sulphur | S8 | M:256,258(95,35%) |
| 66 91 263 261 265 79 101 293 | 100 40 40 30 30 30 25 20 | Aldrin | C12H8Cl6 | M:362,364,366(1,2,1%) |
| 67 82 97 41 54 56 69 <u>125</u> | 100 90 75 70 50 50 30 20 | Hexythiazox related i) | C7H11NO | M:125(20%) |
| 67 317 315 319 345 281 79 147 | 100 55 35 35 30 30 25 25 | Endrin | C12H8Cl6O | M378,380,382(1,2,1%) |
| 68 41 80 69 65 39 79 52 | 100 85 20 10 10 5 5 5 | Aldoxycarb related | C5H9NO2S | M:147(0%) |
| 68 41 115 100 41 47 69 73 | 100 80 70 70 70 20 10 10 | Aldicarb related | C5H9NS | M:115(70%) |
| 69 41 70 - - - - - | 100 5 5 - - - - - | Dinocap | C18H24N2O6 | M:364(0%) |
| 69 <u>140</u> 110 42 58 139 43 68 | 100 75 70 55 25 20 20 15 | Chlorsulfuron related i) | C5H8N4O | M:140(75%) |
| 69 149 151 41 55 70 121 123 | 100 85 85 40 15 10 5 5 | <i>dibromopentane</i> | <i>C5H10Br2</i> | <i>M:228(0%)</i> |
| 69 173 259 41 175 261 191 128 | 100 50 40 40 30 25 20 15 | Propiconazole | C15H17Cl2N3O2 | M:341(0%) |
| 72 44 47 98 48 162 115 145 | 100 80 50 50 35 20 20 20 | Oxamyl oxime | C5H10N2O2S | M:162(20%) |
| 72 44 162 115 57 145 47 98 | 100 95 55 35 35 25 25 20 | *Oxamyl | C7H13N3O3S | M:219(0%) |
| 72 44 <u>212</u> 45 77 132 167 104 | 100 20 10 10 10 5 5 5 | *Chlorotoluron | C10H13ClN2O | M:212,214(10,3%) |
| 72 146 <u>206</u> 191 161 128 91 57 | 100 50 30 20 15 15 10 10 | *Isoproturon | C12H18N2O | M:206(30%) |
| 72 167 165 <u>239</u> 152 166 168 240 | 100 60 25 20 20 15 5 5 | Diphenamid | C16H17NO | M:239(5%) |
| 72 <u>198</u> 153 45 200 44 125 155 | 100 50 20 15 15 10 5 5 | *Monuron | C9H11ClN2O | M:198,200(50,15%) |
| 72 <u>232</u> <u>234</u> 44 73 187 189 45 | 100 15 10 5 5 5 5 5 | *Diuron | C9H10Cl2N2O | M:232,234(15,10%) |
| <u>73</u> 72 45 35 44 70 74 75 | 100 50 25 10 10 5 5 5 | Methyl isothiocyanate | C2H3NS | M:73(100%) |
| 73 163 237 89 341 59 253 429 | 100 65 60 35 30 25 20 20 | <i>silicones, linear (e.g. Si6)</i> | <i>C14H42O7Si6</i> | <i>M:490(0%)</i> |
| 73 429 147 221 355 281 430 431 | 100 45 35 25 25 15 15 15 | <i>silicones, cyclic (e.g. Si9)</i> | <i>C18H54O9Si9</i> | <i>M:666(0%)</i> |
| 74 75 171 111 138 109 47 <u>244</u> | 100 70 45 30 15 15 15 15 | Phorate oxon | C7H17O3PS2 | M:244(15%) |
| 74 75 143 41 76 125 47 109 | 100 33 9 7 6 5 4 3 | Demephion-O | C5H13O3PS2 | M:216(0.5%) |
| 74 142 112 75 109 41 76 79 | 100 15 13 12 10 9 8 7 | Demephion-S | C5H13O3PS2 | M:216(3%) |
| 75 121 97 93 47 <u>260</u> 65 29 | 100 25 10 10 10 10 10 5 | Phorate | C7H17O2PS3 | M:260(10%) |
| 77 51 50 279 277 78 - - | 100 35 15 5 5 5 - - | *Phenylmercury acetate | C8H8HgO2 | M:338(0%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | | | | | | | | | | | | | Relative abundances (%) | | | | Name | Empirical Formula | Molecular ion, m/z (%) |
|--------------------------------|------------|-----|------------|-----|------------|-----|------------|-----|----|----|----|----|-------------------------|----|---------------------------|------------------------------|-----------------------------|-------------------|------------------------|
| 77 | 78 | 79 | - | - | - | - | - | 100 | 6 | 4 | - | - | - | - | <i>dimethylsilanediol</i> | <i>C2H8O2Si</i> | <i>M:92(0%)</i> | | |
| 79 | 80 | 78 | 77 | 107 | 183 | 149 | 150 | 100 | 35 | 15 | 15 | 10 | 10 | 10 | Captafol | C10H9Cl4NO2S | M:347,349,351(2,3,1%) | | |
| 79 | 82 | 81 | 108 | 263 | 277 | 279 | 77 | 100 | 30 | 25 | 15 | 15 | 10 | 10 | Dieldrin | C12H8Cl6O | M:378,380,382,384(3,6,5,2%) | | |
| 79 | 149 | 80 | 77 | 117 | 119 | 107 | 78 | 100 | 40 | 30 | 25 | 25 | 25 | 20 | Captan | C9H8Cl3NO2S | M:299,301,303(2,2,1%) | | |
| 79 | <u>151</u> | 80 | 77 | 123 | 39 | 78 | 122 | 100 | 85 | 65 | 20 | 20 | 20 | 15 | Captafol/captan related | C8H9NO2 | M:151(85%) | | |
| 81 | 133 | 209 | 132 | 134 | 211 | 117 | <u>277</u> | 100 | 90 | 75 | 65 | 45 | 25 | 15 | 15 | Metazachlor | C14H16ClN3O | M:277,279(15,5%) | |
| 82 | 81 | 109 | 65 | 27 | 44 | 47 | 91 | 100 | 30 | 25 | 25 | 20 | 15 | 10 | 10 | *Ethephon | C2H6ClO3P | M:144,146(0,0%) | |
| 83 | 55 | 41 | 57 | 29 | 81 | 113 | 120 | 100 | 85 | 65 | 30 | 25 | 20 | 15 | 10 | Thiofanox sulphone oxime | C7H15NO3S | M:193(0%) | |
| 83 | 55 | 41 | 57 | 113 | 58 | 45 | 81 | 100 | 55 | 35 | 30 | 25 | 25 | 15 | | *Thiofanox sulphone | C9H18N2O4S | M:250(0%) | |
| 83 | 55 | 82 | 39 | - | - | - | - | 100 | 15 | 5 | 5 | - | - | - | - | Binapacryl | C15H18N2O6 | M:322(0%) | |
| 83 | 154 | 55 | 41 | 72 | <u>215</u> | 186 | 27 | 100 | 55 | 40 | 15 | 15 | 5 | 5 | 5 | Cycloate | C11H21NOS | M:215(5%) | |
| <u>84</u> | 28 | 57 | 43 | 42 | 85 | - | - | 100 | 45 | 40 | 20 | 15 | 3 | - | - | *Aminotriazole | C2H4N | M:84(100%) | |
| 84 | <u>162</u> | 133 | 161 | 85 | 42 | - | - | 100 | 20 | 15 | 10 | 5 | 5 | - | - | Nicotine | C10H14N2 | M:162(20%) | |
| 86 | 41 | 85 | 58 | 68 | 55 | 43 | 143 | 100 | 50 | 40 | 30 | 25 | 15 | 15 | 10 | *Aldoxycarb | C7H14N2O4S | M:222(0%) | |
| 86 | 41 | 85 | 144 | 58 | 87 | 76 | 100 | 100 | 70 | 55 | 50 | 45 | 40 | 30 | 30 | *Aldicarb | C7H14N2O2S | M:190(0%) | |
| 86 | 42 | 28 | 57 | 108 | 27 | 69 | 149 | 100 | 80 | 60 | 55 | 25 | 25 | 20 | 10 | Butoxycarboxim related | C5H11NO3S | M:165(0%) | |
| 86 | 99 | 87 | 109 | 71 | 42 | 58 | 141 | 100 | 50 | 20 | 15 | 15 | 10 | 10 | 10 | Amiton / VG nerve agent (CW) | C10H24NO3PS | M:269(0%) | |
| 87 | 41 | 74 | 55 | 44 | 144 | 42 | 75 | 100 | 75 | 60 | 60 | 55 | 55 | 55 | 50 | *Butocarboxim | C7H14N2O2S | M:190(0.5%) | |
| 87 | 57 | 42 | 41 | 55 | <u>133</u> | 71 | 75 | 100 | 75 | 55 | 40 | 35 | 30 | 25 | 25 | Butocarboxim related | C5H11NOS | M:133(30%) | |
| 87 | 93 | 125 | <u>229</u> | 143 | 47 | 79 | 104 | 100 | 35 | 30 | 5 | 5 | 5 | 5 | 5 | Dimethoate | C5H12NO3PS2 | M:229(5%) | |
| 87 | 145 | 146 | 142 | 109 | 88 | 58 | 60 | 100 | 45 | 20 | 15 | 15 | 15 | 10 | 10 | *Vamidothion | C8H18NO4PS2 | M:287(1%) | |
| 87 | 169 | 109 | 125 | 58 | 142 | 86 | 79 | 100 | 40 | 25 | 20 | 15 | 10 | 10 | 10 | *Vamidothion sulphone | C8H18NO6PS2 | M:319(1%) | |
| 88 | 43 | 240 | 44 | 120 | 42 | 73 | 121 | 100 | 40 | 35 | 35 | 30 | 30 | 20 | 20 | *Thiram | C6H12N2S4 | M:240(35%) | |
| 88 | 60 | 29 | 89 | 61 | 114 | 115 | 93 | 100 | 42 | 14 | 13 | 13 | 10 | 9 | 9 | Demeton-S | C8H19O3PS2 | M:258(0.8%) | |
| 88 | 60 | 142 | 109 | 89 | 61 | 79 | 112 | 100 | 54 | 12 | 12 | 10 | 9 | 8 | 8 | Demeton-S-methyl | C6H15O3PS2 | M:230(1%) | |
| 88 | 89 | 60 | 61 | 29 | 171 | 115 | 59 | 100 | 53 | 39 | 27 | 12 | 10 | 9 | 8 | Demeton-O | C8H19O3PS2 | M:258(0.3%) | |
| 88 | 89 | 60 | 61 | 153 | 186 | 142 | <u>274</u> | 100 | 35 | 20 | 15 | 10 | 10 | 10 | 10 | Disulfoton | C8H19O2PS3 | M:274(10%) | |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|---------------------------------|--|-------------------|------------------------------|
| 88 89 60 125 61 <u>246</u> 90 158 | 100 20 20 10 10 5 5 5 | Thiometon | C6H15O2PS3 | M:246(5%) |
| 91 57 190 106 92 134 142 <u>233</u> | 100 60 25 10 5 5 5 5 | Tebutam | C15H23NO | M:233(5%) |
| 91 204 41 123 122 107 246 45 | 100 35 25 15 15 10 10 10 | Iprobenfos | C13H21O3PS | M:288(5%) |
| 92 65 <u>200</u> 39 93 108 64 121 | 100 65 45 30 25 15 10 5 | Dichlofluanid related | C8H12N2O2S | M:200(45%) |
| 92 140 196 60 168 <u>255</u> 81 227 | 100 65 55 55 45 35 30 25 | Phosfolan | C7H14NO3PS2 | M:255(35%) |
| 93 43 119 <u>179</u> 137 120 91 65 | 100 85 55 50 40 35 25 20 | Propham | C10H13NO2 | M:179(50%) |
| 93 125 <u>282</u> 63 79 47 173 188 | 100 40 20 20 20 20 10 10 | Tetramethyl pyrophosphorotrithioate | C4H12O4P2S3 | M:282(20%) |
| 93 <u>230</u> 121 110 65 109 29 185 | 100 25 25 25 25 20 20 5 | Fonofos oxon | C10H15O2PS | M:230(25%) |
| 94 95 <u>141</u> 64 47 79 46 110 | 100 60 40 20 20 10 10 5 | *Methamidophos | C2H8NO2PS | M:141(40%) |
| <u>94</u> <u>96</u> 15 93 95 79 81 91 | 100 95 45 20 15 5 5 5 | Methyl bromide | CH3Br | M:94,96(100,95%) |
| 94 <u>246</u> 110 109 97 105 141 190 | 100 78 63 43 26 20 17 17 | O,O-Diethyl-O-phenyl phosphorothioate | C10H15O3PS | M:246(78%) |
| 95 242 152 <u>301</u> 180 146 39 132 | 100 30 10 10 10 10 10 10 | Furalaxyl | C17H19NO4 | M:301(10%) |
| 96 97 107 143 68 79 29 106 | 100 85 80 50 50 50 40 35 | *Thionazin | C8H13N2O3PS | M:248(20%) |
| 96 <u>283</u> 67 68 41 53 <u>285</u> 39 | 100 35 35 35 25 25 25 15 | Procymidone | C13H11Cl2NO2 | M:283,285(35,25%) |
| 97 55 125 181 208 83 209 141 | 100 55 45 40 30 30 20 20 | Fenpropathrin | C22H23NO3 | M:349(5%) |
| <i>97 57 99 43 83 123 69 137</i> | <i>100 60 20 20 15 15 15 10</i> | <i>unidentified GC vial septum contaminant</i> | <i>C?H?O?</i> | <i>M:292(5%)</i> |
| 97 121 65 93 125 29 <u>338</u> 153 | 100 90 80 65 50 50 45 35 | Tetraethyl pyrophosphorotrithioate | C8H20O4P2S3 | M:338(45%) |
| 97 121 154 65 29 93 <u>234</u> 47 | 100 90 50 50 50 35 30 25 | Chlormephos | C5H12ClO2PS2 | M:234,236(30,10%) |
| 97 125 153 199 29 65 171 75 | 100 85 80 75 20 15 15 10 | *Phorate sulphoxide | C7H17O3PS3 | M:276(0%) |
| 97 125 153 271 65 185 270 86 | 100 60 70 65 35 30 25 15 | Dioxathion | C12H26O6P2S4 | M:456(0%) |
| 97 153 199 125 109 171 65 45 | 100 80 70 70 30 20 20 20 | Carbophenothion sulphoxide | C11H16ClO3PS3 | M:358(0%) |
| 97 197 199 314 316 125 258 286 | 100 80 80 60 50 40 30 30 | Chlorpyrifos | C9H11Cl3NO3PS | M:349,351,353(2,2,1%) |
| 97 279 223 162 109 251 164 125 | 100 80 75 50 45 35 35 30 | Dichlofenthion | C10H13Cl2O3PS | M:314,316(0,0%) |
| 97 359 29 303 357 301 125 242 | 100 50 50 40 40 30 25 25 | Bromophos-ethyl | C10H12BrCl2O3PS | M:392(0%) |
| 97 341 125 285 343 109 153 313 | 100 85 56 53 36 33 32 32 | Chlorthiophos I sulphoxide | C11H15Cl2O4PS2 | M: 376,378,380(0.2,0.2,0.1%) |
| 97 341 269 325 271 343 285 297 | 100 86 80 58 40 37 36 34 | Chlorthiophos III sulphoxide | C11H15Cl2O4PS2 | M: 376,378,380(1.0,0.8,0.2%) |
| 97 357 301 125 109 329 359 240 | 100 81 60 49 46 39 35 32 | Chlorthiophos III sulphone | C11H15Cl2O5PS2 | M:392,394,396(4,3,1%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|----------------------------|--|-------------------|-----------------------------|
| 97 313 257 315 259 125 285 109 | 100 64 59 47 40 35 33 33 | O,O-Diethyl-O-(2,4,5-trichlorophenyl) phosphorothioate | C10H12Cl3O3PS | M:348(0%) |
| <u>98</u> 42 72 69 58 97 83 54 | 100 60 55 50 45 45 30 35 | Oxamyl metabolite, DMCF | C4H6N2O | M:98(100%) |
| 98 99 41 55 <u>273</u> 42 - - | 100 5 5 5 2 2 - - | Fenpropidin | C19H31N | M:273(2%) |
| 99 67 54 41 39 82 81 55 | 100 20 15 10 5 5 5 5 | Cyclosarin nerve agent (CW) | C7H14FO2P | M:180(0%) |
| 99 125 81 43 41 39 - - | 100 35 10 10 10 5 - - | Sarin / GB nerve agent (CW) | C4H10FO2P | M:140(0%) |
| 98 271 184 157 156 125 82 309 | 100 30 30 25 25 20 15 15 | *Hexythiazox | C17H21ClN2O2S | M:352,354(5,2%) |
| 99 <i>155 211 125 57 41 137 56</i> | <i>100 25 10 5 5 5 5 2</i> | <i>tri-n-butyl phosphate</i> | <i>C12H27O4P</i> | <i>M:266(0%)</i> |
| 100 59 43 60 42 44 118 142 | 15 100 50 45 20 20 10 10 | *Daminozide | C6H12N2O3 | M:160(5%) |
| 100 272 274 65 102 270 237 135 | 100 60 45 35 30 30 20 15 | Heptachlor | C10H5Cl7 | M:370,372,374,376(2,6,7,3%) |
| 101 30 127 44 <u>142</u> 99 70 56 | 80 100 80 50 45 45 40 30 | Iprodione related v) | C6H10N2O2 | M:142(45%) |
| <u>102</u> 30 73 45 42 72 <u>103</u> <u>104</u> | 100 30 15 10 10 10 5 5 | *Ethylene thiourea (ETU) | C3H6N2S | M:102(100%) |
| 103 109 135 76 77 81 <u>298</u> 50 | 100 50 40 30 30 30 10 10 | *Phoxim | C12H15N2O3PS | M:298(10%) |
| 103 <u>130</u> 129 76 51 104 77 27 | 100 45 30 25 25 20 15 15 | Phoxim related | C8H6N2 | M:130(45%) |
| 103 311 313 309 105 375 377 275 | 100 65 50 30 30 25 25 25 | Isobenzan | C9H4Cl8O | M:408,410,412,414(2,5,5,3%) |
| 104 42 <u>202</u> 77 30 174 63 89 | 100 65 60 40 40 35 25 90 | *Metamitron | C10H10N4O | M:202(60%) |
| 104 76 260 130 117 262 79 147 | 100 80 55 55 55 50 35 25 | Folpet | C9H4Cl3NO2S | M:295,297,299(10,10,3%) |
| 105 45 163 132 120 77 133 91 | 60 100 55 35 25 20 15 15 | Oxadixyl | C14H18N2O4 | M:278(10%) |
| 105 58 42 88 47 45 57 59 | 80 100 35 30 30 25 15 15 | *Methomyl | C5H10N2O2S | M:162(1%) |
| <u>105</u> 58 47 45 42 88 31 59 | 55 100 45 45 45 35 35 20 | *Methomyl oxime | C3H7NOS | M:105(55%) |
| 105 172 57 106 104 77 41 83 | 100 55 50 45 40 40 35 30 | Buprofezin | C16H23N3OS | M:305(20%) |
| 106 <u>214</u> 79 77 107 78 135 92 | 100 50 40 25 15 10 5 5 | Tolylfluanid related | C9H14N2O2S | M:214(50%) |
| 107 27 109 26 28 79 81 93 | 80 100 80 15 10 5 5 5 | 1,2-Dibromoethane | C2H4Br2 | M:186,188,190(1,2,1%) |
| 107 79 80 78 77 183 149 150 | 10 100 35 15 15 10 10 10 | Captafol | C10H9Cl4NO2S | M:347,349,351(2,3,1%) |
| 107 96 97 143 68 79 29 106 | 80 100 85 50 50 50 40 35 | *Thionazin | C8H13N2O3PS | M:248(20%) |
| 107 121 149 167 93 150 135 91 | 100 80 70 50 50 30 20 20 | Cinerin II | C21H28O5 | M:360(1%) |
| 107 168 78 57 77 106 108 62 | 100 30 20 20 15 10 10 10 | *Ethiofencarb | C11H15NO2S | M:225(2%) |
| 107 200 77 78 79 108 52 - | 100 10 10 5 5 5 5 - | *Ethiofencarb sulphone | C11H15NO4S | M:257(0%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

Appendix II - Page 7

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|--------------------------|--|-------------------|-----------------------------|
| 107 235 203 139 123 <u>314</u> 112 237 | 100 80 80 70 40 40 30 25 | Nuarimol | C17H12ClFN2O | M:314,316(40,10%) |
| 108 79 82 81 263 277 279 77 | 15 100 30 25 15 10 10 10 | Dieldrin | C12H8Cl6O | M:378,380,382,384(3,6,5,2%) |
| 108 80 69 41 65 149 86 134 | 100 70 60 60 35 25 25 20 | *Butoxycarboxim | C7H14N2O4S | M:222(0%) |
| 108 86 42 28 57 27 69 149 | 25 100 80 60 55 25 20 10 | Butoxycarboxim related | C5H11NO3S | M:165(0%) |
| 109 79 110 145 80 139 112 82 | 100 85 45 35 30 30 25 20 | *Trichlorfon | C4H8Cl3O4P | M:256(0%) |
| 109 79 185 47 145 <u>220</u> 187 <u>222</u> | 100 15 15 10 10 5 5 5 | Dichlorvos | C4H7Cl2O4P | M:220,222(5,3%) |
| 109 81 149 <u>275</u> 99 139 127 247 | 100 95 95 60 55 45 45 20 | Parathion oxon, "Paraoxon" | C10H14NO6P | M:275(60%) |
| 109 82 81 65 27 44 47 91 | 25 100 30 25 20 15 10 10 | *Ethephon | C2H6ClO3P | M:144,146(0,0%) |
| 109 86 99 87 71 42 58 141 | 15 100 50 20 15 10 10 10 | Amiton / VG nerve agent (CW) | C10H24NO3PS | M:269(0%) |
| 109 96 79 30 63 230 <u>247</u> 200 | 100 75 35 35 30 20 15 15 | Parathion-methyl oxon, "Paraoxon methyl" | C8H10NO6P | M:247(15%) |
| 109 111 63 <u>158</u> 27 47 65 <u>160</u> | 100 40 35 25 25 20 15 15 | Mustard Gas (CW) | C4H8Cl2S | M:158,160,162(25,15,5%) |
| 109 125 215 155 183 139 61 45 | 100 80 60 50 40 35 30 30 | *Azamethiphos | C9H10ClN2O5PS | M:324,326(15,5%) |
| 109 125 <u>243</u> 79 47 93 63 102 | 100 60 50 30 30 15 15 10 | Cyanophos | C9H10NO3PS | M:243(50%) |
| 109 125 <u>263</u> 79 93 47 63 200 | 100 80 65 30 20 20 10 5 | Parathion-methyl | C8H10NO5PS | M:263(65%) |
| 109 137 <u>246</u> 110 81 63 174 77 | 100 60 35 20 15 10 5 5 | Fonofos | C10H15OPS2 | M:246(35%) |
| 109 145 79 147 185 301 47 189 | 100 40 20 15 10 10 10 10 | Naled | C4H7Br2Cl2O4P | M:378,380,382(0%) |
| 109 181 183 219 111 217 221 185 | 100 90 85 85 70 65 40 25 | beta-HCH | C6H6Cl6 | M:288,290,292(1,2,1%) |
| 109 183 75 137 155 139 81 127 | 100 46 35 25 25 25 20 20 | *Phorate oxon sulphoxide | C7H17O4PS2 | M:260(0%) |
| 109 183 139 81 137 75 155 127 | 100 61 32 31 29 27 21 15 | Carbophenothion oxon sulphoxide | C11H16ClO4PS2 | M:342,344(0,0%) |
| 109 183 139 137 81 75 155 127 | 100 90 40 30 30 30 30 20 | Phorate oxon sulphone | C7H17O5PS2 | M:276(0%) |
| 109 197 141 29 81 61 169 45 | 100 95 73 40 32 28 28 27 | Demeton-S sulphone | C8H19O5PS2 | M:290(0%) |
| 109 197 141 29 81 137 45 61 | 100 89 77 28 27 26 24 23 | Demeton-S sulphoxide | C8H19O4PS2 | M:274(0%) |
| 109 244 79 127 63 <u>261</u> 90 77 | 100 55 20 15 15 15 15 15 | Fenitrothion oxon | C9H12NO6P | M:261(15%) |
| 109 297 269 93 299 271 81 137 | 100 40 30 25 20 20 20 15 | Trichloronat | C10H12Cl3O2PS | M:332,334(0,0%) |
| 109 329 331 333 79 240 204 93 | 100 65 65 20 15 10 10 5 | Tetrachlorvinphos | C10H9Cl4O4P | M:364,366,368(0,5,1,0,5%) |
| 110 57 41 39 52 56 152 80 | 100 50 35 25 20 20 15 10 | Propoxur | C11H15NO3 | M:209(1%) |
| 110 109 79 80 113 47 145 137 | 100 30 30 15 10 10 10 5 | Ethephon, dimethyl | C4H10ClO3P | M:172,174(0,0%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

Appendix II - Page 8

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|--------------------------|------------------------------------|-------------------|-------------------------|
| 111 44 30 29 70 167 128 183 | 30 100 90 40 30 20 15 10 | Cymoxanil | C7H10N4O3 | M:198(1%) |
| 111 75 128 <u>191</u> 113 175 50 92 | 100 75 55 55 30 25 25 20 | Chlorsulfuron related ii) | C6H6ClNO2S | M:191,193(55,15%) |
| 111 175 69 74 140 42 110 112 | 100 55 55 50 40 40 40 35 | *Chlorsulfuron | C12H12ClN5O4S | M:357(0%) |
| <u>112</u> 82 55 26 54 27 29 41 | 100 80 40 25 25 20 20 10 | *Maleic hydrazide | C4H4N2O2 | M:112(100%) |
| 112 168 128 70 57 43 130 169 | 100 90 35 35 30 15 10 10 | *Triadimenol | C14H18ClN3O2 | M:295(0%) |
| 113 43 267 162 309 155 164 41 | 85 100 65 65 55 55 45 40 | Prothiofos | C11H15Cl2O2PS2 | M:344,346(1,1%) |
| 113 83 55 41 57 29 81 120 | 15 100 85 65 30 25 20 10 | Thiofanox sulphone oxime | C7H15NO3S | M:193(0%) |
| 113 83 55 41 57 58 45 81 | 25 100 55 35 30 25 25 15 | *Thiofanox sulphone | C9H18N2O4S | M:250(0%) |
| 114 88 60 29 89 61 115 93 | 13 100 42 14 13 10 9 | Demeton-S | C8H19O3PS2 | M:258(0.8%) |
| 115 41 55 60 83 <u>161</u> 40 57 | 85 100 95 90 90 50 40 35 | Thiofanox oxime | C7H15NOS | M:161(50%) |
| 115 41 57 83 61 55 42 87 | 100 95 90 65 65 60 45 35 | *Thiofanox | C9H18N2O2S | M:218(0%) |
| <u>115</u> 68 41 100 41 47 69 73 | 70 100 80 70 70 20 10 10 | Aldicarb related | C5H9NS | M:115(70%) |
| 115 185 187 149 51 387 389 117 | 100 75 70 50 40 40 40 30 | Oxychlorane | C10H4Cl8O | M:420,422,424(2,4,5%) |
| 117 119 121 82 47 84 35 49 | 100 95 35 30 25 20 15 10 | Carbon tetrachloride | CCl4 | M:152,154,156(0,0,0%) |
| 116 131 59 132 145 222 186 206 | 100 60 45 30 25 20 20 20 | Trifloxystrobin | C20H19F3N2O4 | M:408(0,0%) |
| 116 131 206 59 132 89 117 77 | 100 55 50 20 20 15 15 15 | Kresoxim-methyl | C18H19NO4 | M:313(3%) |
| 118 54 43 39 53 27 76 59 | 25 100 70 50 35 35 20 15 | Dimethipin | C6H10O4S2 | M:210(5%) |
| 119 44 45 29 72 91 73 120 | 100 35 35 30 25 25 25 20 | Carbetamide | C12H16N2O3 | M:236(5%) |
| 119 93 43 <u>179</u> 137 120 91 65 | 55 100 85 50 40 35 25 20 | Propham | C10H13NO2 | M:179(50%) |
| 119 175 43 91 93 147 64 <u>267</u> | 100 90 60 20 20 20 15 20 | *Oxycarboxin | C12H13NO4S | M:267(20%) |
| 119 198 161 92 121 182 64 225 | 100 80 50 45 30 20 20 15 | Bentazone | C10H12N2O3S | M:240(15%) |
| 120 176 93 57 77 43 169 196 | 100 40 35 30 25 25 15 10 | Propachlor | C11H14ClNO | M:211,213(10,3%) |
| 121 75 97 93 47 <u>260</u> 65 29 | 25 100 10 10 10 10 10 5 | Phorate | C7H17O2PS3 | M:260(10%) |
| 121 97 45 153 191 125 65 199 | 100 80 75 65 50 50 45 40 | Phenkapton | C11H15Cl2O2PS3 | M:376,378,380(15,10,3%) |
| 121 97 65 93 125 29 <u>338</u> 153 | 90 100 80 65 50 50 45 35 | Tetraethyl pyrophosphorotrithioate | C8H20O4P2S3 | M:338(45%) |
| 121 162 132 147 <u>293</u> 120 106 161 | 100 85 65 50 45 30 25 20 | Amitraz | C19H23N3 | M:293(45%) |
| 121 197 54 65 29 93 <u>234</u> 47 | 90 100 50 50 50 35 30 25 | Chlormephos | C5H12ClO2PS2 | M:234,236(30,10%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|--------------------------|---|-------------------|------------------------|
| 121 200 57 137 185 91 56 77 | 100 80 75 45 40 30 25 20 | Methiocarb sulphone | C11H15NO4S | M:257(0%) |
| 121 <u>200</u> 185 137 91 77 39 65 | 100 90 60 55 35 25 10 10 | Methiocarb sulphone related | C9H12O3S | M:200(90%) |
| 122 107 121 77 79 57 91 123 | 100 45 15 15 10 5 5 5 | Xylylcarb | C10H13NO2 | M:179(2%) |
| 123 93 79 135 41 107 81 168 | 100 25 25 20 20 20 15 10 | Pyrethrin I | C21H28O3 | M:328(1%) |
| 123 97 57 99 43 83 69 137 | 15 100 60 20 20 15 15 10 | unidentified GC vial septum contaminant | C?H?O? | M:292(5%) |
| 123 150 121 93 81 43 107 168 | 100 30 30 25 25 20 20 10 | Cinerin I | C20H28O3 | M:316(1%) |
| 123 164 81 93 55 41 107 135 | 100 30 20 20 20 20 15 15 | Jasmolin I | C21H30O3 | M:330(1%) |
| 123 167 <u>224</u> <u>226</u> 92 124 77 108 | 100 50 40 30 20 15 15 10 | Dichlofluanid | C9H11Cl2FN2O2S2 | M:332,334(7,5%) |
| 123 171 143 128 91 81 43 172 | 100 50 35 35 30 30 30 15 | Resmethrin | C22H26O3 | M:338(5%) |
| 123 183 81 184 43 124 <u>350</u> 168 | 100 55 20 15 10 10 5 5 | Phenothrin | C23H26O3 | M:350(5%) |
| 123 209 181 77 43 80 198 141 | 100 50 30 30 25 25 20 20 | Cyphenothrin | C24H25NO3 | M:375(5%) |
| 124 89 126 127 215 <u>250</u> 109 <u>252</u> | 100 35 35 20 15 15 10 5 | Heptenophos | C9H21ClO4P | M:250,252(15,5%) |
| 124 <u>233</u> 108 109 93 79 63 31 | 100 95 85 75 60 55 35 35 | Parathion-methyl, Amino- | C8H12NO3PS | M:233(50%) |
| <u>125</u> 67 82 97 41 54 56 69 | 20 100 90 75 70 50 50 30 | Hexythiazox related i) | C7H11NO | M:125(20%) |
| 125 70 250 83 57 127 252 163 | 100 80 70 60 45 30 25 20 | Tebuconazole | C16H22ClN3O | M:307,309(5,2%) |
| 125 87 93 <u>229</u> 143 47 79 104 | 30 100 35 5 5 5 5 5 | Dimethoate | C5H12NO3PS2 | M:229(5%) |
| 125 88 89 60 61 <u>246</u> 90 158 | 10 100 20 20 10 5 5 5 | Thiometon | C6H15O2PS3 | M:246(5%) |
| 125 93 <u>282</u> 63 79 47 173 188 | 40 100 20 20 20 20 10 10 | Tetramethyl pyrophosphorotrithioate | C4H12O4P2S3 | M:282(20%) |
| 125 97 55 181 208 83 209 141 | 45 100 55 40 30 30 20 20 | Fenpropathrin | C22H23NO3 | M:349(5%) |
| 125 99 181 121 127 153 155 29 | 100 85 73 45 45 44 43 34 | Demeton-O oxon sulphone | C8H19O3PS | M:274(2%) |
| 125 109 108 29 97 80 65 <u>261</u> | 100 95 85 75 60 55 35 35 | Parathion, Amino- | C10H16NO3PS | M:261(35%) |
| 125 109 <u>277</u> 260 79 47 93 63 | 100 90 50 30 30 35 35 15 | Fenitrothion | C9H12NO5PS | M:277(50%) |
| 125 169 79 109 111 63 47 107 | 100 65 43 18 11 11 11 11 | Demephion-O sulphone | C5H13O5PS2 | M:248(1%) |
| 125 180 93 208 <u>240</u> 110 79 209 | 100 60 60 55 55 35 30 20 | Methacrifos | C7H13O5PS | M:240(55%) |
| 125 185 93 157 29 158 186 61 | 100 55 35 20 15 10 10 10 | Thiometon sulphone | C6H15O2PS3 | M:278(0.5%) |
| 125 185 157 93 59 159 187 88 | 100 85 80 15 15 10 10 5 | *Thiometon sulphoxide | C6H15O2PS3 | M:262(0%) |
| 125 197 53 199 29 65 171 75 | 85 100 80 75 20 15 15 10 | *Phorate sulphoxide | C7H17O3PS3 | M:276(0%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|---------------------------------|----------------------------------|-------------------|------------------------|
| 125 197 53 271 65 185 270 86 | 60 100 70 65 35 30 25 15 | Dioxathion | C12H26O6P2S4 | M:456(0%) |
| 125 213 153 97 185 61 157 29 | 100 85 80 80 60 40 35 25 | *Disulfoton sulphoxide | C8H19O3PS3 | M:290(0.5%) |
| 125 286 288 79 47 93 109 290 | 100 90 60 35 30 25 20 15 | Chlorpyrifos-methyl | C7H7Cl3NO3PS | M:321,323,325(5,5,2%) |
| 125 <u>310</u> 109 93 136 105 79 137 | 100 95 60 35 35 30 25 15 | Fenthion sulphone | C10H15O5PS2 | M:310(95%) |
| 125 434 109 93 233 435 <u>482</u> 466 | 100 65 25 23 15 15 15 10 | *Temephos sulphoxide | C16H20O7P2S3 | M:482(15%) |
| <i>126 59 72 55 41 67 83 98</i> | <i>10 100 45 35 25 15 15 10</i> | <i>oleamide</i> | <i>C18H35NO</i> | <i>M:281(5%)</i> |
| 126 93 125 87 170 115 <u>224</u> <u>257</u> | 100 70 50 50 35 20 15 15 | Formothion | C6H12NO4PS2 | M:257(15%) |
| 126 99 82 69 41 57 43 83 | 100 85 55 50 35 20 15 15 | Soman / GD nerve agent (CW) | C7H16FO2P | M:182(0%) |
| 126 151 <u>166</u> 39 51 52 108 123 | 100 90 60 25 20 15 15 10 | Bendiocarb related | C9H10O3 | M:166(60%) |
| 127 43 <u>213</u> 171 129 154 41 27 | 50 100 15 15 15 15 15 10 | Chlorpropham | C10H12ClNO2 | M:213,215(15,5%) |
| 127 57 43 41 29 128 88 371 | 100 90 30 15 10 10 5 5 | Ioxynil octanoate | C15H17I2NO2 | M:497(0.5%) |
| 127 67 97 192 109 58 193 <u>223</u> | 100 35 20 15 15 15 10 5 | Monocrotophos | C7H14NO5P | M:223(5%) |
| 127 72 264 138 109 67 193 158 | 100 60 25 25 20 15 10 10 | Phosphamidon | C10H19ClNO5P | M:299(0%) |
| 127 99 109 55 142 195 268 79 | 100 45 25 20 15 15 15 15 | Malaoxon | C10H19O7PS | M:314(1%) |
| 127 99 55 128 173 47 283 79 | 100 50 30 25 20 20 20 15 | Isomalathion, see malathion | C10H19O6PS2 | M:330(1%) |
| <u>127</u> <u>129</u> 65 92 - - - - | 100 35 25 15 - - - - | Diflubenzuron related i) | C6H6ClN | M:127,129(100,35%) |
| 127 145 109 72 <u>271</u> 43 147 110 | 100 30 25 15 15 15 10 10 | Phosphamidon, N-desethyl | C8H15ClNO5P | M:271,273(15,5%) |
| 127 192 109 67 164 193 141 79 | 100 30 20 15 10 5 5 5 | Mevinphos | C7H13O6P | M:224(2%) |
| 128 43 91 86 41 65 <u>251</u> 162 | 60 100 65 35 20 15 15 10 | *Prosulfocarb | C14H21NOS | M:251(15%) |
| 128 43 129 42 <u>303</u> - - - | 100 10 10 5 5 - - - | Fenpropimorph | C20H33NO | M:303(5%) |
| 128 129 43 55 115 70 84 <u>297</u> | 100 10 5 5 5 5 5 2 | Tridemorph | C19H39NO | M:297(2%) |
| 128 141 <u>268</u> 130 <u>270</u> 143 233 77 | 100 60 40 35 25 20 15 15 | *Dichlorophen | C13H10Cl2O2 | M:268,270(40,25%) |
| <i>129 57 70 71 112 147 113 55</i> | <i>100 40 35 30 25 15 15 15</i> | <i>bis(2-ethylhexyl) adipate</i> | <i>C22H42O4</i> | <i>M:370(1%)</i> |
| 129 58 31 42 59 <u>188</u> 72 84 | 5 100 20 10 10 5 5 5 | *Propamocarb | C9H20N2O2 | M:188(5%) |
| 130 214 43 172 131 75 41 <u>256</u> | 100 80 50 50 50 50 20 | Bensulide related | C9H21O2PS2 | M:256(20%) |
| 130 <u>299</u> 148 209 243 194 271 102 | 100 85 75 60 55 50 35 25 | Ditalimfos | C12H14NO4PS | M:299(85%) |
| 131 41 68 64 47 63 42 39 | 5 100 80 75 20 10 10 10 | *Aldicarb sulphoxide | C7H14N2O3S | M:206(0%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|---------------------------------|-----------------------------------|-------------------|--------------------------|
| <u>131</u> 41 68 64 47 63 42 39 | 5 100 80 75 20 10 10 10 | Aldicarb sulphoxide related | C5H9NOS | M:131(5%) |
| 131 159 97 160 125 <u>329</u> 116 121 | 100 70 60 50 45 35 35 35 | Mecarbam | C10H20NO5PS2 | M:329(35%) |
| 132 160 77 105 104 97 129 65 | 100 75 65 25 25 20 15 15 | Azinphos-ethyl | C12H16N3O3PS2 | M:345(0%) |
| 132 160 232 <u>281</u> 77 146 105 204 | 100 85 70 50 50 45 45 40 | Ofurace | C14H16ClNO3 | M:281,283(50,15%) |
| 132 164 111 77 133 104 75 325 | 100 25 11 9 9 6 5 4 | Pyraclostrobin | C19H18ClN3O4 | M:387,389(0,0%) |
| 133 81 209 132 134 211 117 <u>277</u> | 90 100 75 65 45 25 15 15 | Metazachlor | C14H16ClN3O | M:277,279(15,5%) |
| <u>133</u> 87 57 42 41 55 71 75 | 30 100 75 55 40 35 25 25 | Butocarboxim related | C5H11NOS | M:133(30%) |
| <u>133</u> <u>134</u> 105 106 79 132 78 90 | 100 20 20 15 10 5 5 5 | Carbendazim related | C7H7N3 | M:133(100%) |
| 133 135 167 104 132 78 52 122 | 100 65 50 40 30 20 15 10 | *Phenmedipham | C16H16N2O4 | M:300(0%) |
| 133 160 161 107 166 91 105 41 | 100 85 80 80 75 70 55 45 | Pyrethrin II | C22H28O5 | M:372(1%) |
| 135 44 153 92 199 243 <u>286</u> 200 | 65 100 45 45 40 20 20 20 | Schradan | C8H24N4O3P2 | M:286(20%) |
| 135 81 173 39 57 41 150 <u>350</u> | 100 50 50 50 50 45 20 15 | Propargite | C19H26O4S | M:350(15%) |
| <u>135</u> 108 69 82 63 91 45 54 | <i>100 40 25 15 10 10 10 10</i> | <i>benzothiazole</i> | <i>C7H5NS</i> | <i>M:135(100%)</i> |
| 135 150 57 91 136 107 117 151 | 100 65 15 15 10 10 10 10 | Promecarb | C12H17NO2 | M:207(1%) |
| 136 42 43 94 41 95 96 47 | 100 80 50 50 30 30 25 25 | *Acephate | C4H10NO3PS | M:183(5%) |
| 137 102 75 139 77 138 103 <u>302</u> | 100 50 30 30 15 10 5 5 | Clofentezine | C14H8Cl2N4 | M:302,304(5,3%) |
| 137 180 147 151 162 57 161 39 | 100 45 25 20 20 15 10 10 | *Carbofuran, 3-hydroxy | C12H15NO4 | M:237(2%) |
| 137 238 181 240 106 45 214 92 | 100 40 35 25 15 15 10 10 | Tolylfluanid | C10H13Cl2FN2O2S2 | M:346(5,3%) |
| 138 44 194 236 110 122 156 111 | 100 60 35 25 25 25 15 15 | Propetamphos | C10H20NO4PS | M:281(0%) |
| 138 111 <u>198</u> 170 109 82 93 142 | 100 80 60 55 50 35 35 30 | Triethyl-(O,O,S) phosphorothioate | C6H15O3PS | M:198(60%) |
| 139 43 97 208 339 337 206 125 | 100 90 85 70 55 55 45 45 | Profenofos | C11H15BrClO3PS | M:372,374,376(25,30,10%) |
| 139 107 219 251 <u>330</u> 141 253 111 | 100 80 65 50 30 30 30 25 | Fenarimol | C17H12Cl2N2O | M:330,332(30,20%) |
| 139 141 111 <u>250</u> <u>252</u> 75 113 215 | 100 35 30 30 20 15 10 10 | Dicofol related | C13H8Cl2O | M:250,252(30,20%) |
| 139 251 253 111 141 75 252 140 | 100 60 45 35 30 15 10 10 | *Dicofol | C14H9Cl5O | M:368(0%) |
| 139 251 43 253 111 141 75 <u>266</u> | 100 95 90 60 40 35 30 15 | Chlorfenethol | C14H12Cl2O | M:266,268(15,5%) |
| <u>140</u> 69 110 42 58 139 43 68 | 75 100 70 55 25 20 20 15 | Chlorsulfuron related i) | C5H8N4O | M:140(75%) |
| 140 92 196 60 168 <u>255</u> 81 227 | 65 100 55 55 45 35 30 25 | Phosfolan | C7H14NO3PS2 | M:255(35%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|--------------------------------|-----------------------------------|-------------------|--------------------------|
| 140 112 142 342 253 289 <u>342</u> <u>344</u> | 100 30 30 15 10 10 10 10 | Boscalid | C18H12Cl2N2O | M:342,344,346(15,10,5) |
| 140 196 81 46 109 168 45 29 | 100 85 55 50 50 45 45 35 | Fosthietan | C6H12NO3PS2 | M:241(0%) |
| 140 <u>306</u> 139 43 125 156 307 97 | 100 90 35 20 20 15 15 15 | Sulprofos oxon | C12H19O3PS2 | M:306(90%) |
| 141 43 71 143 41 140 142 <u>239</u> | 100 70 65 30 20 15 15 15 | Pentanochlor | C13H18ClNO | M:239,241(15,5%) |
| <i>141 77 170 30 158 171 78 <u>213</u></i> | <i>100 95 85 20 15 10 10 5</i> | <i>N-butylbenzenesulphonamide</i> | <i>C10H15NO2S</i> | <i>M:213(5%)</i> |
| <u>141</u> 94 95 64 47 79 46 110 | 40 100 60 20 20 10 10 5 | *Methamidophos | C2H8NO2PS | M:141(40%) |
| 141 <u>157</u> 113 63 - - - - | 100 50 35 20 - - - - | Diflubenzuron related iii) | C7H5F2NO | M:157(50%) |
| 142 127 <u>329</u> 43 99 <u>331</u> 187 56 | 100 85 60 40 40 35 30 30 | Iprodione related iii) | C13H13Cl2N3O3 | M:329,331(60,35%) |
| 142 169 <u>228</u> 107 144 171 <u>230</u> 141 | 100 95 90 45 35 30 30 25 | Mecoprop-methyl | C11H13ClO3 | M:228,230(90,30%) |
| 142 <u>214</u> 107 141 169 144 77 <u>216</u> | 100 65 50 35 35 35 25 20 | *Mecoprop acid | C10H11ClO3 | M:214,216(65,20%) |
| 142 74 112 75 109 41 76 79 | 15 100 13 12 10 9 8 7 | Demephion-S | C5H13O3PS2 | M:216(3%) |
| 142 88 60 109 89 61 79 112 | 12 100 54 12 10 9 8 | Demeton-S-methyl | C6H15O3PS2 | M:230(1%) |
| 143 43 87 <u>235</u> 77 115 91 132 | 100 55 50 40 10 10 10 5 | Carboxin | C12H13NO2S | M:235(40%) |
| 143 86 41 85 58 68 55 43 | 10 100 50 40 30 25 15 15 | *Aldoxycarb | C7H14N2O4S | M:222(0%) |
| 143 74 75 41 76 125 47 109 | 9 100 33 7 6 5 4 3 | Demephion-O | C5H13O3PS2 | M:216(0.5%) |
| <u>144</u> 115 116 89 72 <u>145</u> 63 58 | 100 65 40 10 10 10 10 10 | Carbaryl related, 1-naphthol | C10H8O | M:144(100%) |
| 144 115 116 145 <u>201</u> 89 127 63 | 100 40 25 10 5 5 5 5 | Carbaryl | C12H11NO2 | M:201(5%) |
| 144 86 41 85 58 87 76 100 | 50 100 70 55 45 40 30 30 | *Aldicarb | C7H14N2O2S | M:190(0%) |
| 144 87 41 74 55 44 42 75 | 55 100 75 60 60 55 55 50 | *Butocarboxim | C7H14N2O2S | M:190(0.5%) |
| 144 245 176 246 117 89 116 214 | 100 65 60 35 30 25 25 25 | Imazamethabenz-methyl | C16H20N2O3 | M:288(10%) |
| 145 85 125 93 58 47 63 <u>302</u> | 100 85 25 15 15 10 10 5 | Methidathion | C6H11N2O4PS3 | M:302(5%) |
| 145 87 146 142 109 88 58 60 | 45 100 20 15 15 15 10 10 | *Vamidothion | C8H18NO4PS2 | M:287(1%) |
| 145 110 <u>206</u> <u>208</u> 147 180 182 171 | 100 90 75 70 60 40 40 35 | Lewisite (CW) | C2H2AsCl3 | M:206,208,210(75,70,30%) |
| 146 72 <u>206</u> 191 161 128 91 57 | 50 100 30 20 15 15 10 10 | *Isoproturon | C12H18N2O | M:206(30%) |
| 146 157 156 118 97 129 <u>298</u> 158 | 100 65 50 40 30 25 25 25 | Quinalphos | C12H15N2O3PS | M:298(25%) |
| 146 <u>161</u> 128 91 77 103 147 118 | 100 35 30 15 10 10 10 10 | Isoproturon related | C10H11NO | M:161(35%) |
| <u>147</u> 76 104 50 103 - - - | 100 100 80 45 30 - - - | Folpet related, phthalimide | C8H5NO2 | M:147(100%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|---------------------------------|------------------------------------|-------------------|------------------------|
| 147 149 112 76 110 75 50 85 | 100 65 50 45 25 20 20 15 | *Clopyralid acid | C6H3Cl2NO2 | M:191,193,195(10,7,2%) |
| 148 91 204 206 <u>325</u> 234 266 176 | 100 35 30 25 15 15 15 10 | Benalaxyl | C20H23NO3 | M:325(15%) |
| <i>149 29 150 41 57 56 223 205</i> | <i>100 10 10 10 5 5 5 5</i> | <i>di-n-butyl phthalate</i> | <i>C16H22O4</i> | <i>M:278(1%)</i> |
| <i>149 69 151 41 55 70 121 123</i> | <i>85 100 85 40 15 10 5 5</i> | <i>dibromopentane</i> | <i>C5H10Br2</i> | <i>M:228(0%)</i> |
| 149 79 80 77 117 119 107 78 | 40 100 30 25 25 25 25 20 | Captan | C9H8Cl3NO2S | M:299,301,303(2,2,1%) |
| <i>149 167 57 71 43 70 279 113</i> | <i>100 45 35 25 25 20 20 15</i> | <i>bis(2-ethylhexyl) phthalate</i> | <i>C24H38O4</i> | <i>M:390(0%)</i> |
| <i>149 177 150 65 176 76 105 29</i> | <i>100 25 10 10 10 10 10 5</i> | <i>diethyl phthalate</i> | <i>C12H14O4</i> | <i>M:222(5%)</i> |
| 150 73 44 72 86 159 43 30 | 100 40 25 20 20 20 20 20 | *Thiophanate-methyl | C12H14N4O4S2 | M:342(0%) |
| 151 43 69 68 <u>166</u> 109 165 56 | 100 95 60 50 45 40 30 30 | Cyromazine | C6H10N6 | M:166(45%) |
| <u>151</u> 79 80 77 123 39 78 122 | 85 100 65 20 20 20 20 15 | Captafol/captan related | C8H9NO2 | M:151(85%) |
| 151 126 166 51 39 <u>223</u> 58 123 | 100 60 50 20 15 15 10 10 | Bendiocarb | C11H13NO4 | M:223(15%) |
| 153 51 222 87 69 41 127 104 | 100 85 65 65 50 40 35 35 | Barban | C11H9Cl2NO2 | M:257,259(10,7%) |
| 153 56 69 140 112 <u>168</u> 124 99 | 100 75 50 50 45 35 25 25 | Etrimfos related | C8H12N2O2 | M:168(35%) |
| 153 57 97 29 125 41 199 186 | 55 100 85 50 50 40 35 30 | *Terbufos sulphoxide | C9H21O3PS3 | M:304(0%) |
| 153 88 89 60 61 186 142 <u>274</u> | 10 100 35 20 15 10 10 10 | Disulfoton | C8H19O2PS3 | M:274(10%) |
| 153 97 199 125 159 65 171 45 | 100 80 70 70 25 25 15 15 | Carbophenothion sulphone | C11H16ClO4PS3 | M:374,376(3,1%) |
| 153 97 199 125 171 65 29 93 | 100 85 80 80 15 15 15 15 | Phorate sulphone | C7H17O4PS3 | M:292(5%) |
| 153 97 299 301 125 166 263 115 | 100 85 50 50 40 30 30 25 | Chlorethoxyfos | C6H11Cl4O3PS | M:334,336,338(5,8,3%) |
| 153 109 127 79 96 95 154 63 | 100 82 64 15 10 9 7 7 | Demephion-O oxon sulphone | C5H13O6PS | M:232(0%) |
| <u>153</u> 125 <u>155</u> 90 63 127 - - | 100 40 35 30 20 15 - - | Diflubenzuron related ii) | C7H4ClNO | M:153,155(100,35%) |
| 153 141 155 157 113 63 125 127 | 100 80 30 25 25 25 25 25 | *Diflubenzuron | C14H19ClF2N2O2 | M:310,312(10,3%) |
| 153 197 99 125 109 171 65 45 | 80 100 70 70 30 20 20 20 | Carbophenothion sulphoxide | C11H16ClO3PS3 | M:358(0%) |
| 153 199 57 125 97 264 200 172 | 100 60 55 55 35 35 25 25 | Terbufos sulphone | C9H21O4PS3 | M:320(5%) |
| 153 <u>305</u> 180 44 124 95 43 71 | 100 70 40 35 30 30 25 25 | Pyrimitate | C11H20N3O3PS | M:305(70%) |
| 154 83 55 41 72 <u>215</u> 186 27 | 55 100 40 15 15 5 5 5 | Cycloate | C11H21NOS | M:215(5%) |
| <u>154</u> 153 152 76 155 78 115 63 | 100 35 25 20 15 10 5 5 | Biphenyl | C12H10 | M:154(100%) |
| <i>155 99 211 125 57 41 137 56</i> | <i>25 100 10 5 5 5 5 2</i> | <i>tri-n-butyl phosphate</i> | <i>C12H27O4P</i> | <i>M:266(0%)</i> |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|---------------------------|----------------------------|-------------------|--------------------------|
| 156 63 69 42 140 65 110 92 | 85 100 90 85 65 50 50 50 | *Triasulfuron | C14H16ClN5O5S | M:401,403(0,0%) |
| 156 100 57 91 <u>279</u> 250 190 134 | 100 65 60 50 20 15 10 10 | *Tiocarbazil | C16H25NOS | M:279(20%) |
| 156 110 79 109 80 126 46 141 | 100 100 30 25 15 15 10 10 | *Omethoate | C5H12NO4PS | M:213(2%) |
| 156 183 184 109 140 57 75 155 | 100 85 85 85 85 80 45 35 | Terbufos oxon sulphone | C9H21O5PS2 | M:304(0%) |
| 156 <u>227</u> 184 157 155 44 158 117 | 100 70 65 60 60 40 40 35 | Hexythiazox related ii) | C10H10ClNOS | M:227,229(70,25%) |
| 157 121 153 <u>342</u> 159 199 125 97 | 100 50 45 45 40 40 40 40 | Carbophenothion | C11H16ClO2PS3 | M:342,344(45,15%) |
| 157 125 45 93 159 <u>314</u> 171 108 | 100 45 40 40 35 15 10 10 | Methyl-trithion | C9H12ClOPS3 | M:314,316(15,5%) |
| 157 169 141 185 77 63 47 <u>303</u> | 100 55 35 35 25 25 15 15 | Cyanofenphos | C15H14NO2PS | M:303(15%) |
| 157 169 185 141 63 77 110 <u>323</u> | 100 60 40 40 25 20 15 10 | EPN | C14H14NO4PS | M:323(10%) |
| 158 43 97 41 139 126 74 93 | 90 100 70 60 50 50 40 40 | Ethoprophos | C8H19O2PS2 | M:242(25%) |
| 159 43 41 56 27 30 98 191 | 35 100 85 45 40 30 20 15 | *Benomyl | C14H18N4O3 | M:290(0%) |
| 159 104 <u>191</u> 131 31 160 77 105 | 100 25 20 15 15 15 10 10 | *Carbendazim | C9H9N3O2 | M:191(20%) |
| 159 111 75 227 229 <u>356</u> 161 127 | 100 80 55 50 50 35 35 30 | Tetradifon | C12H6Cl4O2S | M:354,356,358(25,35,20%) |
| 159 125 93 113 158 127 99 143 | 100 90 80 55 55 35 20 20 | Malathion "mixed ester" I | C9H17O6PS2 | M:316(1%) |
| 159 125 93 113 158 127 99 143 | 100 90 80 55 55 35 20 20 | Malathion "mixed ester" II | C9H17O6PS2 | M:316(1%) |
| 159 158 97 88 57 127 125 213 | 100 80 50 40 40 35 30 20 | Cadusafos | C10H23O2PS2 | M:270(15%) |
| 159 248 161 250 249 83 213 163 | 100 85 65 25 10 10 10 10 | Penconazole | C13H15Cl2N3 | M:283,285(0%) |
| 160 44 135 <u>294</u> 92 161 104 251 | 100 40 40 20 15 15 10 5 | Triamiphos | C12H19N6OP | M:294(20%) |
| 160 45 188 237 224 146 202 132 | 45 100 40 15 15 10 10 10 | Alachlor | C14H20ClNO2 | M:269(5%) |
| 160 77 93 76 161 <u>317</u> 104 133 | 100 15 15 15 10 5 5 5 | Phosmet | C11H12NO4PS2 | M:317(5%) |
| 160 118 163 164 57 84 135 149 | 100 95 50 50 30 20 20 20 | Carbosulfan | C20H32N2O3S | M:380(1%) |
| 160 132 77 105 93 76 104 125 | 100 95 95 30 30 30 20 20 | Azinphos-methyl | C10H12N3O3PS2 | M:317(0%) |
| 161 119 162 97 257 163 172 285 | 100 75 60 50 35 30 30 30 | Isazofos | C9H17ClN3O3PS | M:313,315(15,5%) |
| 161 162 172 177 257 97 285 91 | 100 75 50 30 30 25 25 25 | Triazophos | C12H16N3O3PS | M:313(5%) |
| 161 163 57 29 <u>217</u> 165 <u>219</u> 126 | 100 60 45 40 20 10 10 10 | *Propanil | C9H9Cl2NO | M:217,219,221(20,10,3%) |
| <u>161</u> <u>163</u> 90 63 99 126 165 125 | 100 70 25 25 20 20 10 10 | Iprodione related ii) | C6H5Cl2N | M:161,163(100,50%) |
| <u>162</u> 72 44 47 98 48 115 145 | 20 100 80 50 50 35 20 20 | Oxamyl oxime | C5H10N2O2S | M:162(20%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|---------------------------------|-------------------------------------|--------------------|------------------------|
| 162 72 44 115 57 145 47 98 | 55 100 95 35 35 25 25 20 | *Oxamyl | C7H13N3O3S | M:219(0%) |
| <u>162</u> 84 133 161 85 42 - - | 20 100 15 10 5 5 - - | Nicotine | C10H14N2 | M:162(20%) |
| 162 164 <u>220</u> <u>222</u> 161 163 175 133 | 100 65 65 45 40 35 30 30 | *2,4-D acid | C8H6Cl2O3 | M:220,222(65,45%) |
| 162 238 146 77 73 211 240 117 | 100 55 20 15 15 15 15 10 | Metolachlor | C15H22ClNO2 | M:283,285(0,0%) |
| <i>163 77 76 135 92 50 164 194</i> | <i>100 25 15 10 10 10 10 10</i> | <i>dimethyl phthalate</i> | <i>C10H10O4</i> | <i>M:194(10%)</i> |
| 163 107 135 166 121 93 55 164 | 100 85 75 70 60 55 55 50 | JasmolinII | C22H30O5 | M:374(1%) |
| 163 135 164 194 41 107 325 57 | 100 30 25 20 20 15 15 15 | Furathiocarb | C18H26N2O5S | M:382(5%) |
| 163 165 181 77 91 208 209 127 | 100 60 50 30 30 25 20 20 | Cypermethrin | C22H19Cl2N03 | M:415,417(2,1%) |
| 163 165 226 206 77 199 91 127 | 100 65 55 45 35 30 30 25 | Cyfluthrin | C22H18Cl2FNO3 | M:433,435(2,1%) |
| <i>163 273 37 89 341 59 253 429</i> | <i>65 100 60 35 30 25 20 20</i> | <i>silicones, linear (e.g. Si6)</i> | <i>C14H42O7Si6</i> | <i>M:490(0%)</i> |
| 164 123 81 165 107 79 43 41 | 100 40 15 10 10 10 10 10 | Tetramethrin | C19H25NO4 | M:331(0.5%) |
| 164 149 122 123 <u>221</u> 165 131 91 | 100 45 10 10 10 10 10 5 | Carbofuran | C12H15NO3 | M:221(10%) |
| <u>164</u> 149 131 103 122 77 123 121 | 100 80 40 40 40 35 35 35 | Carbofuran related | C10H12O2 | M:164(100%) |
| 165 68 163 96 150 41 164 162 | 100 20 15 10 10 10 10 10 | Isoxaben | C18H24N2O4 | M:332(1%) |
| <i>165 180 137 166 91 124 181 77</i> | <i>100 50 50 10 10 5 5 5</i> | <i>"BHA"</i> | <i>C11H16O2</i> | <i>M:180(50%)</i> |
| 166 72 <u>238</u> 167 123 138 152 110 | 100 90 25 10 10 10 10 5 | Pirimicarb | C11H18N4O2 | M:238(25%) |
| 166 96 <u>209</u> 42 55 167 71 194 | 100 25 20 15 15 10 10 5 | *Ethirimol | C11H19N3O | M:209(20%) |
| 167 72 165 239 152 166 168 <u>240</u> | 60 100 25 20 20 15 5 5 | Diphenamid | C16H17NO | M:240(5%) |
| 167 125 169 225 152 181 <u>419</u> 127 | 100 90 45 40 35 30 25 25 | Fenvalerate | C25H22ClNO3 | M:419,421(25,10%) |
| 167 <u>444</u> 282 290 121 163 277 129 | 100 75 50 50 50 35 25 20 | *Difenacoum | C31H24O3 | M:444(75%) |
| 168 153 109 45 57 91 <u>225</u> 77 | 100 60 25 20 15 15 10 5 | Methiocarb | C11H15NO2S | M:225(10%) |
| 169 87 109 125 58 142 86 79 | 40 100 25 20 15 10 10 10 | *Vamidothion sulphone | C8H18NO6PS2 | M:319(1%) |
| 169 107 184 108 57 168 123 153 | 100 80 75 55 35 30 20 20 | Methiocarb sulphoxide | C11H15NO3S | M:241(10%) |
| 169 107 <u>184</u> 108 168 153 123 79 | 100 95 85 70 40 25 20 20 | Methiocarb sulphoxide related | C9H12O2S | M:184(85%) |
| 169 109 125 58 87 143 142 86 | 100 50 25 20 20 15 15 10 | *Vamidothion sulphoxide | C8H18NO5PS2 | M:303(0%) |
| 169 109 125 74 91 171 142 110 | 100 69 42 10 7 6 5 5 | Demephion-S sulphoxide | C5H13O4PS2 | M:232(0%) |
| 169 109 125 110 168 105 60 142 | 100 90 50 15 10 10 10 5 | *Demeton-S-methyl sulphoxide | C6H15O4PS2 | M:246(0%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|---------------------------------|--------------------------------------|-------------------|---------------------------|
| 169 109 125 110 168 142 29 170 | 100 51 33 15 15 9 8 7 | Demeton-S-methyl sulphone | C6H15O5PS2 | M:262(0%) |
| 169 109 125 168 110 142 170 127 | 100 52 48 32 21 20 10 8 | Demephion-S sulphone | C5H13O5PS2 | M:246(0.5%) |
| <u>169</u> 168 167 51 84.5 77 170 66 | 100 50 30 20 15 15 15 10 | Diphenylamine | C12H11N | M:169(100%) |
| 170 57 168 112 171 268 169 141 | 100 30 15 15 15 5 5 5 | Bitertanol | C20H23N3O2 | M:337(1%) |
| <u>170</u> 169 141 115 31 171 142 139 | 100 60 35 25 20 15 10 10 | 2-Phenylphenol | C12H10O | M:170(100%) |
| 170 232 109 183 57 139 41 137 | 100 45 35 25 20 15 15 15 | *Terbufos oxon sulphoxide | C9H21O4PS2 | M:288(0%) |
| 171 44 83 71 128 98 <u>252</u> 127 | 100 65 55 45 45 25 20 20 | Hexazinone | C12H20N4O2 | M:252(20%) |
| 171 57 215 170 <u>272</u> 143 115 126 | 100 65 60 55 30 30 20 15 | Terbufos oxon | C9H21O3PS2 | M:272(30%) |
| 171 74 75 111 138 109 47 <u>244</u> | 45 100 70 30 15 15 15 15 | Phorate oxon | C7H17O3PS2 | M:244(15%) |
| 171 88 89 60 61 29 115 59 | 12 100 53 39 27 10 9 8 | Demeton-O | C8H19O3PS2 | M:258(0.3%) |
| 171 156 98 57 41 74 88 172 | 100 65 65 55 20 10 10 10 | *Tebuthiuron | C9H16N4OS | M:228(2%) |
| 171 377 375 77 155 109 63 124 | 100 50 40 35 25 20 20 15 | Leptophos | C13H10BrCl2O2PS | M:410,412,414(0,0,0%) |
| <u>172</u> 93 125 47 63 79 109 174 | 100 95 70 30 20 20 20 10 | Trimethyl-(O,O,S) phosphorodithioate | C3H9O2PS2 | M:172(100%) |
| 172 196 43 139 296 188 97 157 | 100 60 55 50 35 35 35 30 | Sulprofos oxon sulphone | C12H19O5PS2 | M:338(15%) |
| 173 69 259 41 175 261 191 128 | 50 100 40 40 30 25 20 15 | Propiconazole | C15H17Cl2N3O2 | M:341(0%) |
| 173 127 125 93 158 99 143 79 | 100 90 85 85 45 35 20 15 | Malathion | C10H19O6PS2 | M:330(1%) |
| 173 175 145 <u>255</u> 41 147 84 254 | 100 65 35 25 25 20 15 15 | Propyzamide | C12H11Cl2NO | M:255,257,259(25,15,3%) |
| 173 <u>220</u> 175 <u>222</u> 203 174 191 97 | 100 100 85 65 50 50 45 40 | *Dicamba acid | C8H6Cl2O3 | M:220,222,224(100,65,10%) |
| 173 <u>374</u> 165 174 89 166 201 105 | 100 15 15 10 10 10 10 5 | *Chlorophacinone | C23H15ClO3 | M:374,376(15,5%) |
| 174 176 147 146 56 41 148 192 | 100 65 55 50 50 50 30 30 | Clopyralid, n-butyl | C10H11Cl2NO2 | M:247,249(2,1%) |
| 175 41 177 57 43 258 260 302 | 100 85 65 65 55 50 30 30 | Oxadiazon | C15H18Cl2N2O3 | M:344,346(20,15%) |
| 175 111 177 113 <u>302</u> 75 <u>304</u> 127 | 100 95 40 30 25 25 15 20 | Chlorfenson | C12H8Cl2O3S | M:302,304(25,15%) |
| 176 177 149 45 57 193 <u>338</u> 119 | 100 25 10 10 10 5 5 5 | Piperonyl butoxide | C19H30O5 | M:338(5%) |
| <i>177 161 164 149 <u>340</u> 41 57 284</i> | <i>100 75 50 40 40 25 25 20</i> | <i>"Antioxidant 2246"</i> | <i>C23H32O2</i> | <i>M:340(40%)</i> |
| 177 197 141 127 178 199 91 225 | 100 80 60 55 55 55 45 30 | Tefluthrin | C17H14ClF7O2 | M:418,420(0,0%) |
| 178 <u>248</u> <u>250</u> 213 88 177 176 106 | 100 80 60 40 30 20 20 20 | DDNU | C14H10Cl2 | M:248,250(80,50%) |
| 178 280 41 101 136 150 179 67 | 100 45 35 30 20 20 15 15 | *Cycloxydim | C17H27NO3S | M:325(1%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|---------------------------------|-----------------------------------|-------------------|---------------------------|
| 179 82 150 181 55 206 <u>288</u> 152 | 100 55 45 35 35 30 25 25 | Myclobutanil | C15H17Cl4N | M:288,290(25,10%) |
| 179 137 152 <u>304</u> 199 93 153 97 | 100 95 85 65 50 45 40 35 | Diazinon | C12H21N2O3PS | M:304(65%) |
| 180 43 70 308 310 266 268 312 | 55 100 80 20 20 15 15 10 | *Prochloraz | C15H16Cl3N3O2 | M:375(0%) |
| <u>180</u> <u>182</u> 74 145 109 <u>184</u> 147 75 | 100 95 45 40 35 30 25 25 | HCH related, trichlorobenzene | C6H3Cl3 | M:180,182,184(100,95,30%) |
| 181 57 71 43 209 210 211 254 | 25 100 85 65 25 20 20 15 | Fluroxypyr-meptyl | C15H21Cl2FN2O3 | M:366,368,370(10,7,2%) |
| 181 166 182 165 180 167 141 179 | 100 25 20 15 10 5 5 5 | Bifenthrin | C23H22ClF3O2 | M:422,424(1,0,5%) |
| 181 183 185 111 146 147 145 219 | 100 90 30 25 25 25 25 20 | HCH related, gamma-PCCH | C6H5Cl5 | M:252,254,256(2,3,2%) |
| 181 183 219 109 217 111 221 185 | 100 90 90 75 65 60 40 30 | gamma-HCH | C6H6Cl6 | M:288,290,292(1,2,1%) |
| 181 183 219 217 109 111 221 185 | 100 90 85 65 55 45 40 30 | alpha-HCH | C6H6Cl6 | M:288,290,292(0,0,0%) |
| 181 197 208 209 199 77 141 180 | 100 85 85 45 25 25 25 20 | Cyhalothrin | C23H19ClF3NO3 | M:449,451(8,3%) |
| 182 121 97 200 154 111 65 <u>367</u> | 100 50 40 30 25 25 25 20 | Phosalone | C12H15ClNO4PS2 | M:367,369(20,8%) |
| 182 127 99 119 109 <u>308</u> 201 280 | 100 85 75 65 65 60 55 50 | Fensulfothion oxon sulphone | C11H17O6PS | M:308(60%) |
| 183 41 125 109 102 143 79 29 | 100 40 35 25 20 10 10 5 | *Oxydeprofos | C7H17O4PS2 | M:260(0%) |
| 183 109 139 137 75 155 127 184 | 100 45 30 23 19 18 9 7 | Carbophenothion oxon sulphone | C11H16ClO5PS2 | M:358,356(0,0%) |
| 183 109 <u>326</u> 139 157 111 155 75 | 100 95 55 53 44 44 42 40 | Carbophenothion oxon | C11H16ClO3PS2 | M:326,328(55,23%) |
| 183 163 165 184 77 91 127 51 | 100 30 20 15 15 15 10 10 | Permethrin | C21H20Cl2O3 | M:390,392(2,1%) |
| 183 185 76 <u>340</u> 155 157 75 <u>338</u> | 100 100 40 40 30 30 20 20 | Bromopropylate related | C13H8Br2O | M:338,340,342(20,40,20%) |
| <u>184</u> 156 155 183 <u>185</u> 92 129 64 | 100 30 30 25 25 15 15 10 | Fuberidazole | C11H8N2O | M:184(100%) |
| <u>184</u> <u>186</u> 101 93 64 143 129 156 | 100 35 30 30 25 20 15 10 | Azamethiphos related | C7H5ClN2O2 | M:184,186(100,35%) |
| 185 57 41 29 <u>276</u> 175 162 <u>278</u> | 50 100 45 40 30 25 25 20 | 2,4-D n-butyl | C12H14Cl2O3 | M:276,278(30,20%) |
| <i>185 129 57 259 29 111 147 56</i> | <i>100 80 45 35 25 15 15 10</i> | <i>tri-n-butyl citrate</i> | <i>C18H32O7</i> | <i>M:360(0%)</i> |
| <i>185 129 259 43 57 41 157 139</i> | <i>100 60 50 40 30 25 20 10</i> | <i>acetyl tri-n-butyl citrate</i> | <i>C20H35O8</i> | <i>M:402(0%)</i> |
| 187 39 54 213 <u>285</u> 212 53 198 | 85 100 90 80 80 80 73 65 | Vinclozolin | C12H9Cl2NO3 | M:285,287(80,50%) |
| 187 189 124 159 126 161 191 88 | 100 65 50 20 15 15 15 10 | Iprodione related iv) | C7H3Cl2NO | M:187,189(100,65%) |
| 187 <u>244</u> 189 <u>246</u> 188 124 56 190 | 100 65 60 45 35 30 20 20 | Iprodione related i) | C9H6Cl2N2O2 | M:244,246(65,45%) |
| 187 <u>256</u> 144 117 89 116 214 41 | 100 85 80 55 50 40 35 30 | Imazamethabenz-methyl related | C15H16N2O2 | M:256(85%) |
| 188 312 43 113 172 141 125 155 | 100 70 40 30 30 20 15 15 | Sulprofos sulphone | C12H19O4PS3 | M:354(15%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|---------------------------------|-----------------------------------|-------------------|-------------------------------|
| 190 91 57 106 92 134 142 <u>233</u> | 25 100 60 10 5 5 5 5 | Tebutam | C15H23NO | M:233(5%) |
| <i>191 175 178 <u>368</u> 163 57 135 169</i> | <i>100 70 60 45 40 35 25 20</i> | <i>"Antioxidant 425"</i> | <i>C25H36O2</i> | <i>M:368(45%)</i> |
| 193 195 66 263 147 197 261 265 | 100 95 80 40 35 35 25 25 | Isodrin | C12H8Cl6 | M:362,364,366,368(5,10,10,3%) |
| 195 197 159 160 241 237 207 89 | 100 75 70 65 60 60 60 50 | beta-Endosulfan | C9H6Cl6SO3 | M:404,406,408(1,1,1%) |
| 195 197 241 239 207 237 160 69 | 100 75 75 65 65 60 60 60 | alpha-Endosulfan | C9H6Cl6SO3 | M:404,406,408(1,1,1%) |
| <u>196</u> 44 181 117 152 42 154 <u>198</u> | 85 100 50 50 40 30 30 25 | Chlordimeform | C10H13ClN2 | M:196,198(85,25%) |
| 196 140 106 74 41 168 227 81 | 100 95 90 90 70 60 45 35 | Mephosfolan | C8H16NO3PS2 | M:269(10%) |
| 196 198 <u>254</u> <u>256</u> 200 209 211 167 | 100 95 55 55 30 20 20 20 | *2,4,5-T acid | C8H5Cl3O3 | M:254,256,258(55,55,20%) |
| 197 153 29 45 141 125 97 121 | 100 89 84 77 71 51 44 42 | Demeton-O sulphone | C8H19O5PS2 | M:290(1%) |
| 197 197 99 314 316 125 258 286 | 80 100 80 60 50 40 30 30 | Chlorpyrifos | C9H11Cl3NO3PS | M:349,351,353(2,2,1%) |
| <u>198</u> 51 77 169 197 141 181 115 | 100 45 40 40 40 35 20 15 | Cypermethrin (etc) related | C13H10O2 | M:198(100%) |
| <u>198</u> 72 153 45 <u>200</u> 44 125 155 | 50 100 20 15 15 10 5 5 | *Monuron | C9H11ClN2O | M:198,200(50,15%) |
| <u>198</u> 105 121 51 53 168 106 30 | 100 35 30 20 20 20 15 15 | *DNOC | C7H6N2O5 | M:198(100%) |
| <u>198</u> 121 93 109 115 114 126 65 | 100 95 75 40 40 40 40 35 | Triethyl-(O,O,O) phosphorothioate | C6H15O3PS | M:198(100%) |
| 198 199 57 41 103 144 <u>214</u> 182 | 100 20 20 20 20 15 10 10 | *Metribuzin | C8H14N4OS | M:214(10%) |
| 199 157 184 181 <u>451</u> 225 55 107 | 100 60 30 25 20 20 20 15 | Flucythrinate | C26H23F2NO4 | M:451(20%) |
| 199 175 <u>234</u> 45 177 <u>236</u> 161 201 | 100 65 65 45 40 35 30 30 | 2,4-D methyl | C9H8Cl2O3 | M:234,236(65,40%) |
| 200 58 <u>215</u> 173 43 202 92 68 | 100 70 70 35 30 30 25 25 | Atrazine | C8H14ClN5 | M:215,217(70,20%) |
| <u>200</u> 92 65 39 93 108 64 121 | 45 100 65 30 25 15 10 5 | Dichlofluanid related | C8H12N2O2S | M:200(45%) |
| 200 <u>229</u> 214 186 202 68 72 <u>231</u> | 100 65 60 55 35 25 25 20 | Trietazine | C9H16ClN5 | M:229,231(65,20%) |
| <u>201</u> 44 186 173 43 68 <u>203</u> 158 | 90 100 55 45 35 30 30 25 | Simazine | C7H12ClN5 | M:201,203(90,30%) |
| 202 174 173 203 <u>217</u> 145 144 188 | 100 50 20 20 20 15 10 5 | Ethoxyquin | C14H19NO | M:217(20%) |
| <u>201</u> 174 202 63 90 129 175 100 | 100 75 15 15 10 10 10 10 | Thiabendazole | C10H7N3S | M:201(100%) |
| 202 201 44 265 109 186 93 <u>309</u> | 100 69 39 21 18 18 12 9 | Famphur oxon | C10H16NO6PS | M:309(9%) |
| 203 125 <u>498</u> 109 93 388 265 <u>499</u> | 100 65 50 50 40 15 15 10 | *Temephos sulphone | C16H20O8P2S3 | M:498(50%) |
| 203 201 205 96 61 <u>238</u> <u>240</u> <u>236</u> | 100 75 50 30 25 25 15 15 | Dienochlor related | C5HCl5 | M:236,238,240(15,25,15%) |
| 203 205 <u>234</u> 188 <u>236</u> 201 190 175 | 100 65 25 20 15 15 10 10 | Dicamba, methyl ester | C9H8Cl2O3 | M:234,236(25,15%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|--------------------------------|------------------------|-------------------|---------------------------|
| 203 215 <u>261</u> 201 30 <u>259</u> 213 205 | 100 85 80 70 70 60 55 45 | Tecnazene | C6HCl4NO2 | M:259,261,263(60,80,35%) |
| 204 91 41 123 122 107 246 45 | 35 100 25 15 15 10 10 10 | Iprobenfos | C13H21O3PS | M:288(5%) |
| 205 207 42 70 162 164 231 233 | 100 95 35 20 15 15 15 15 | *Bromacil | C9H13BrN2O2 | M:260,262(5,5%) |
| 205 <u>220</u> 57 206 145 105 177 55 | <i>100 25 25 15 15 10 10 5</i> | "BHT" | <i>C15H24O</i> | <i>M:220(25%)</i> |
| 206 45 192 220 249 234 146 160 | 35 100 25 20 20 15 15 15 | Metalaxyl | C15H21NO4 | M:279(10%) |
| <u>206</u> 124 176 <u>208</u> 160 178 126 133 | 100 95 70 65 55 45 30 25 | Dicloran | C6H4Cl2N2O2 | M:206,208,210(100,65,10%) |
| 206 <u>234</u> 116 174 173 148 89 103 | 100 95 60 45 30 30 20 10 | Quinomethionate | C10H6N2OS2 | M:234(95%) |
| 208 57 41 85 29 128 110 181 | 50 100 40 35 30 20 20 20 | Triadimefon | C14H16ClN3O2 | M:293,295(2,1%) |
| 208 210 76 97 357 65 129 130 | 100 35 10 10 10 10 10 10 | Dialifos | C14H17ClNO4PS2 | M:393(1%) |
| 210 69 140 42 110 90 77 199 | 100 65 50 40 40 35 30 30 | *Metsulfuron-methyl | C14H15N5O6S | M:381(0%) |
| 210 154 42 56 124 90 69 77 | 100 75 30 30 30 25 20 20 | *Tribenuron-methyl | C15H17N5O6S | M:395(0%) |
| 210 212 182 146 45 <u>269</u> <u>271</u> 59 | 100 90 40 40 40 30 30 25 | Triclopyr-methyl | C8H6Cl3NO3 | M:269,271,273(30,30,5%) |
| 211 43 41 163 240 205 147 212 | 45 100 15 10 10 10 10 5 | Dinobuton | C14H18N2O7 | M:326(0%) |
| 211 43 240 44 163 147 117 205 | 10 100 10 10 5 5 5 5 | Dinoseb acetate | C12H14N2O6 | M:282(1%) |
| 211 163 147 117 <u>240</u> 29 41 57 | 100 45 25 20 15 15 15 15 | *Dinoseb | C10H12N2O5 | M:240(15%) |
| 212 44 225 68 173 198 <u>240</u> 172 | 100 100 90 85 75 65 65 65 | Cyanazine | C9H13ClN6 | M:240,242(65,20%) |
| <u>212</u> 72 44 45 77 132 167 104 | 10 100 20 10 10 5 5 5 | *Chlorotoluron | C10H13ClN2O | M:212,214(10,3%) |
| 212 <u>282</u> <u>284</u> 176 214 247 <u>286</u> 88 | 100 80 80 45 45 30 30 25 | DDMU ("TDE-olefin") | C14H9Cl3 | M:282,284,286(80,80,30%) |
| 213 58 121 185 255 96 43 138 | 60 100 55 40 40 40 30 20 | Isofenphos | C15H24NO4PS | M:345(5%) |
| 213 153 61 125 97 157 185 186 | 100 75 40 30 30 20 15 10 | Disulfoton sulphone | C8H19O4PS3 | M:306(1%) |
| <u>213</u> 198 171 57 82 124 99 156 | 100 65 35 35 25 20 15 15 | Desmetryn | C8H15N5S | M:213(100%) |
| <u>214</u> 61 46 153 127 126 99 90 | 15 100 15 15 15 15 10 5 | *Monolinuron | C9H11ClN2O2 | M:214,216(15,5%) |
| 214 173 216 <u>229</u> 68 43 175 132 | 100 40 35 30 15 15 15 15 | Terbuthylazine | C9H16ClN5 | M:229,231(30,10%) |
| 215 41 173 217 175 81 159 54 | 25 100 15 15 10 10 5 5 | Imazalil | C14H14Cl2N2O | M:296,298(2,1%) |
| 215 172 131 77 214 173 141 130 | 100 75 75 70 70 55 50 50 | *Bensulide | C14H24NO4PS3 | M:397(0%) |
| 216 69 140 110 42 247 205 126 | 100 90 80 65 55 45 45 40 | *Thifensulfuron-methyl | C12H13N5O6S2 | M:387(0%) |
| <u>216</u> 183 78 153 201 138 137 121 | 100 55 45 30 25 20 20 15 | Dioxabenzofos | C8H9O3PS | M:216(100%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|--------------------------|----------------------|-------------------|---------------------------|
| 218 93 125 217 44 109 219 79 | 100 30 25 25 15 15 10 5 | Famphur | C10H16NO5PS2 | M:325(1%) |
| <u>218</u> 119 144 185 77 183 219 <u>220</u> | 100 20 15 10 10 5 5 5 | Cymiazole | C12H14N2S | M:218(100%) |
| 220 57 56 41 29 85 175 222 | 20 100 40 25 20 15 15 15 | 2,4-D butoxyethyl | C14H18Cl2O4 | M:320,322(8,5%) |
| 220 57 71 43 70 41 <u>222</u> <u>332</u> | 50 100 65 65 40 35 25 20 | 2,4-D i-octyl | C16H22Cl2O3 | M:332,334(20,15%) |
| 221 232 <u>373</u> 237 222 265 193 97 | 100 40 30 20 15 15 10 10 | Pyrazophos | C14H20N3O5PS | M:373(30%) |
| 222 97 224 257 45 <u>360</u> 289 259 | 100 97 77 61 45 43 41 40 | Chlorthiophos II | C11H15Cl2O3PS2 | M:360,362,364(43,32,7%) |
| 223 224 165 179 193 104 115 178 | 100 20 5 5 5 5 5 5 | Perthane | C18H20Cl2 | M:306,308(2,1%) |
| <u>225</u> 43 139 68 182 58 210 47 | 80 100 75 65 55 45 40 40 | *Aziprotryne | C7H11N7S | M:225(80%) |
| 225 177 131 <u>240</u> 161 41 103 226 | 100 45 25 15 15 10 10 10 | *Dinoterb | C10H12N2O5 | M:240(15%) |
| 226 125 43 184 228 93 154 171 | 100 75 65 55 35 35 30 30 | Anilofos | C13H19ClNO3PS2 | M:367,369(1,0.5%) |
| 226 185 <u>241</u> 170 106 157 71 43 | 100 90 80 50 25 20 15 15 | Terbutryn | C10H18N5S | M:241(80%) |
| <u>227</u> 58 212 68 99 170 69 185 | 100 75 70 50 40 35 30 25 | Ametryn | C9H17N5S | M:227(100%) |
| 227 228 114 212 152 141 <u>344</u> <u>346</u> | 100 20 10 5 5 5 5 5 | Methoxychlor | C16H15Cl3O2 | M:344,346,348(5,5,2%) |
| <u>230</u> 93 121 110 65 109 29 185 | 25 100 25 25 25 20 20 5 | Fonofos oxon | C10H15O2PS | M:230(25%) |
| 231 57 29 103 153 41 65 186 | 40 100 25 20 15 15 15 10 | Terbufos | C9H21O2PS3 | M:288(5%) |
| 231 153 97 121 125 93 65 <u>384</u> | 100 65 50 45 45 25 20 20 | Ethion | C9H22O4P2S4 | M:384(20%) |
| <u>231</u> <u>229</u> <u>233</u> 158 160 235 169 196 | 100 80 45 20 15 10 10 10 | Tecnazene related i) | C6H3Cl4N | M:229,231,233(80,100,45%) |
| 231 <u>323</u> 76 203 77 105 196 50 | 100 35 35 25 20 15 15 15 | Benodanil | C13H10INO | M:323(35%) |
| <u>232</u> 72 <u>234</u> 44 73 187 189 45 | 15 100 10 5 5 5 5 5 | *Diuron | C9H10Cl2N2O | M:232,234(15,10%) |
| 233 73 45 235 <u>268</u> <u>270</u> 209 211 | 100 85 80 70 65 65 60 50 | 2,4,5-T methyl | C9H7Cl3O3 | M:268,270,272(65,65,20%) |
| 233 206 47 234 <u>315</u> 123 220 300 | 100 35 25 25 10 10 10 5 | Flusilazole | C16H15F2N3Si | M:315(10%) |
| 235 237 165 200 199 236 <u>266</u> 239 | 100 65 30 15 10 10 5 5 | *DDOH | C14H12Cl2O | M:266,268(5,2%) |
| 235 237 165 236 199 239 200 212 | 100 65 35 15 15 10 10 10 | TDE (DDD) | C14H10Cl4 | M:318,320,333(1,2,1%) |
| 235 237 165 236 199 239 200 246 | 100 65 40 15 15 10 10 10 | DDT | C14H9Cl5 | M:352,354,356(1,2,1%) |
| 235 237 165 236 <u>280</u> 201 199 <u>282</u> | 100 65 30 10 10 10 10 5 | *DDA | C15H12Cl2O2 | M:280,282(10,7%) |
| 235 237 165 236 <u>284</u> <u>286</u> 199 200 | 100 65 30 15 5 5 5 5 | DDMS | C14H11Cl3 | M:284,286,288(5,5,2%) |
| 235 237 165 <u>294</u> 199 200 <u>296</u> 72 | 100 65 30 15 10 10 10 5 | DDA, methyl ester | C15H12Cl2O2 | M:294,296(15,10%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|--|---------------------------------|---------------------------------------|-------------------|------------------------------------|
| 236 125 82 238 167 57 70 127 | 100 60 35 30 30 25 20 20 | Paclobutrazol | C15H20ClN3O | M:293(0%) |
| 236 212 194 43 254 59 237 42 | 100 65 60 55 55 35 30 30 | Nitrothal-isopropyl | C14H17NO6 | M:295(5%) |
| 237 157 145 141 172 252 156 236 | 100 80 70 60 60 60 40 30 | Quintiofos | C17H16NO2PS | M:329(20%) |
| 237 239 235 404 402 406 332 334 | 100 65 65 50 45 30 30 25 | Dienochlor | C10Cl10 | M:470,472,474,476,478(2,5,10,7,3%) |
| 237 <u>295</u> 30 214 249 212 235 251 | 100 90 90 85 80 60 55 50 | Quintozene | C6Cl5NO2 | M:293,295,297,299(50,90,45,15%) |
| 239 241 143 178 90 62 111 240 | 100 60 40 35 15 10 10 10 | Anilazine | C9H5Cl3N4 | M:274,276,278(10,10,3%) |
| <u>240</u> 88 43 44 120 42 73 121 | 35 100 40 35 30 30 20 20 | *Thiram | C6H12N2S4 | M:240(35%) |
| <u>241</u> 58 184 226 43 106 68 69 | 90 100 65 60 55 45 40 35 | Prometryn | C10H19N5S | M:241(90%) |
| <i>241 185 56 57 98 41 123 125</i> | <i>100 75 65 55 40 40 35 35</i> | <i>dibutyl sebacate/decanedioate</i> | <i>C18H34O4</i> | <i>M:314(0.1%)</i> |
| 242 95 152 <u>301</u> 180 146 39 132 | 30 100 10 10 10 10 10 10 | Furalaxyl | C17H19NO4 | M:301(10%) |
| <u>246</u> 94 110 109 97 105 141 190 | 78 100 63 43 26 20 17 17 | O,O-Diethyl-O-phenyl phosphorothioate | C10H15O3PS | M:246(78%) |
| 246 248 <u>318</u> <u>316</u> <u>320</u> 176 281 283 | 100 65 55 40 25 25 15 15 | DDT, Aspergillus niger metabolite | C14H8Cl4 | M:316,318,320(40,55,25%) |
| 246 <u>318</u> 248 <u>316</u> 176 <u>320</u> 210 247 | 100 80 65 60 45 40 20 15 | DDE | C14H8Cl4 | M:316,318,320(60,80,40%) |
| <u>248</u> 61 46 <u>250</u> 187 200 189 202 | 10 100 10 5 5 5 2 2 | Linuron | C9H10Cl2N2O2 | M:248,250(10,6%) |
| 249 63 251 27 143 205 65 223 | 85 100 45 45 40 40 35 25 | tris-(2-chloroethyl) phosphate | C6H12Cl3O4P | M:284,286(0,0%) |
| 251 139 253 111 141 235 165 255 | 100 85 60 30 25 25 10 10 | Chlorobenzilate | C16H14Cl2O3 | M:324,326(1,0.5%) |
| 252 162 29 57 253 43 192 119 | 100 15 15 15 15 15 10 10 | Pendimethalin | C13H9N3O4 | M:281(10%) |
| 253 181 251 255 208 93 77 172 | 100 85 50 50 45 40 30 30 | Deltamethrin | C22H19Br2NO3 | M:503,505,507(1,2,1%) |
| 254 <u>327</u> 146 255 227 282 226 328 | 100 85 60 50 35 25 25 15 | *Fluazifop acid | C15H12F3NO4 | M:327(85%) |
| 256 57 43 71 41 70 254 55 | 25 100 70 50 40 40 25 25 | 2,4,5-T i-octyl | C16H21Cl3O3 | M:366,368,370(12,12,4%) |
| <u>256</u> 64 160 128 192 <u>258</u> 96 162 | 95 100 75 70 40 35 25 20 | Sulphur | S8 | M:256,258(95,35%) |
| 256 108 276 169 182 278 41 171 | 100 95 80 65 60 25 25 25 | Crufomate | C12H19ClNO3P | M:291,293(20,7%) |
| 257 259 97 313 222 45 224 315 | 100 66 64 42 35 33 29 27 | Chlorthiophos II sulphoxide | C11H15Cl2O4PS2 | M: 376,378,380(0,0,0%) |
| 257 259 97 313 315 285 287 179 | 100 64 49 43 35 25 22 22 | Chlorthiophos II sulphone | C11H15Cl2O5PS2 | M:392,394,396(0,0,0%) |
| 258 260 249 178 250 120 92 348 | 100 95 85 55 50 35 35 25 | *Bromadiolone | C30H23BrO4 | M:526,528(0,0%) |
| 259 43 29 188 <u>331</u> 187 261 186 | 30 100 70 30 25 25 20 20 | Chlozolate | C13H11Cl2NO5 | M:331,333,335(25,15,5%) |
| 261 66 91 263 265 79 101 293 | 30 100 40 40 30 30 25 20 | Aldrin | C12H8Cl6 | M:362,364,366(1,2,1%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

Appendix II - Page 22

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|---------------------------|-----------------------------|-------------------|----------------------------------|
| 262 125 79 47 63 109 93 216 | 100 65 25 20 20 20 15 15 | Dicaphon | C8H9ClNO5PS | M:297,299(0,0%) |
| <u>262</u> 247 <u>263</u> <u>264</u> 135 217 109 215 | 100 30 20 10 10 10 10 5 | Fenthion oxon | C10H15O4PS | M:262(100%) |
| <u>262</u> <u>260</u> <u>264</u> 227 229 45 210 212 | 100 75 50 40 40 40 35 35 | Tecnazene related ii) | C7H4Cl4S | M:260,262,264(75,100,50%) |
| 263 109 <u>278</u> 262 127 79 45 77 | 100 70 25 25 20 15 109 10 | Fenthion oxon sulphoxide | C10H15O5PS | M:278(25%) |
| 263 161 235 179 207 162 99 81 | 100 85 80 75 65 55 40 40 | TEPP | C8H20O7P2 | M:290(10%) |
| 265 43 121 45 <u>308</u> 266 187 213 | 100 65 60 55 45 35 30 25 | *Warfarin | C19H16O4 | M:308(45%) |
| <u>265</u> <u>263</u> <u>267</u> <u>269</u> 194 192 133 96 | 100 65 65 20 15 15 15 10 | Quintozene related i) | C6H2Cl5N | M:263,265,267,269(65,100,65,20%) |
| 265 267 125 79 93 250 47 63 | 100 35 30 20 15 15 10 10 | Tolclofos-methyl | C9H11Cl2O3PS | M:300(0%) |
| <u>266</u> <u>264</u> <u>268</u> 109 124 229 270 194 | 100 80 50 20 15 10 10 10 | Chlorothalonil | C8Cl4N2 | M:264,266,268(80,100,50%) |
| 266 <u>394</u> 101 267 169 145 218 246 | 100 25 25 20 15 15 15 15 | Diflufenican | C19H11F5N2O2 | M:394(25%) |
| 267 323 269 81 325 109 29 295 | 100 70 65 60 45 45 45 25 | Chlorfenvinphos | C12H14Cl3O4P | M:358,360(1,1%) |
| 268 43 86 128 270 143 145 84 | 20 100 85 20 15 10 10 5 | Tri-allate | C10H16Cl3NOS | M:303,305,307(0,0,0%) |
| <u>268</u> 57 152 170 153 184 76 269 | 35 100 15 15 15 10 5 5 | Bitertanol related | C18H20O2 | M:268(35%) |
| 268 70 57 270 41 29 165 269 | 100 80 70 65 35 25 20 20 | Diniconazole | C15H17Cl2N3O | M:325(0%) |
| 269 271 246 248 273 318 176 316 | 100 95 65 45 40 35 35 30 | Tetrachloro-DDT | C14H8Cl6 | M:386,388,390(0,0,0%) |
| 269 97 325 297 <u>360</u> 271 109 125 | 100 99 79 51 44 43 42 35 | Chlorthiophos I | C11H15Cl2O3PS2 | M:360,362,364(44,33,8%) |
| 269 325 97 271 297 327 65 299 | 100 81 55 42 37 34 18 15 | Chlorthiophos III | C11H15Cl2O3PS2 | M:360,362,364(13,10,2%) |
| 271 98 184 157 156 125 82 309 | 30 100 30 25 25 20 15 15 | *Hexythiazox | C17H21ClN2O2S | M:352,354(5,2%) |
| 272 274 229 387 227 270 239 237 | 100 80 75 60 55 50 45 45 | Endosulfan sulphate | C9H6Cl6SO4 | M:420,422,424,426(8,17,15,5%) |
| 272 274 270 237 276 239 235 332 | 100 80 50 50 35 30 30 10 | Mirex | C10Cl12 | M:540,542,544,546(1,2,2,1%) |
| 273 98 99 41 55 42 - - | 2 100 5 5 5 2 - - | Fenpropridin | C19H31N | M:273(2%) |
| 273 208 166 <u>316</u> 108 96 44 150 | 100 65 35 35 30 25 20 20 | Bupirimate | C13H24N4O3S | M:316(35%) |
| 274 93 125 121 107 92 79 246 | 100 95 90 70 55 55 55 30 | Phenthoate | C12H17O4PS2 | M:320(5%) |
| <u>275</u> <u>273</u> <u>277</u> 133 240 <u>279</u> 238 203 | 100 65 65 25 20 20 15 15 | Chlorothalonil related | C7Cl5N | M:273,275,277,279(65,100,65,20%) |
| <u>276</u> 140 220 248 125 202 139 109 | 100 75 60 40 25 20 15 15 | Fensulfothion oxon sulphide | C11H17O4PS | M:276(100%) |
| <u>277</u> 88 <u>275</u> <u>279</u> 62 168 170 117 | 100 60 50 50 20 20 20 15 | *Bromoxynil | C7H3Br2NO | M:275,277,279(50,100,50%) |
| 277 141 249 109 221 <u>292</u> 278 81 | 100 40 25 25 20 20 15 15 | Fensulfothion oxon | C11H17O5PS | M:292(20%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|--------------------------|--------------------------|-------------------|----------------------------------|
| 277 184 88 279 275 63 53 91 | 100 75 70 55 50 45 40 35 | *Bromofenoxim | C13H7Br2N3O6 | M:459,461,463(1,2,1%) |
| <u>278</u> 109 <u>279</u> 169 <u>280</u> 125 245 137 | 100 20 15 15 10 10 10 10 | Fenthion | C10H15O3PS2 | M:278(100%) |
| 279 77 51 50 277 78 - - | 5 100 35 15 5 5 - - | *Phenylmercury acetate | C8H8HgO2 | M:338(0%) |
| 279 125 <u>294</u> 109 169 138 153 93 | 100 65 60 40 25 25 20 15 | Fenthion sulphoxide | C10H15O4PS2 | M:294(60%) |
| 279 297 23 162 109 251 164 125 | 80 100 75 50 45 35 35 30 | Dichlofenthion | C10H13Cl2O3PS | M:314,316(0,0%) |
| 282 <u>383</u> 254 255 146 238 227 91 | 100 50 45 30 20 20 20 15 | Fluazifop n-butyl | C19H20F3NO4 | M:383(50%) |
| <u>283</u> 96 67 68 41 53 <u>285</u> 39 | 35 100 35 35 25 25 25 15 | Procymidone | C13H11Cl2NO2 | M:283,285(35,25%) |
| 284 29 138 126 146 285 43 91 | 100 80 55 25 25 20 20 20 | *Tralkoxydim | C20H27NO3 | M:329(1%) |
| <u>284</u> <u>286</u> <u>282</u> <u>288</u> 142 249 106 144 | 100 80 55 35 30 25 20 15 | Hexachlorobenzene | C6Cl6 | M:282,284,286,288(55,100,80,40%) |
| 285 287 125 79 109 93 47 289 | 100 80 60 25 25 25 20 15 | Fenchlorphos | C8H8Cl3O3PS | M:320,322,324(2,2,1%) |
| 286 96 200 72 152 232 202 29 | 100 95 90 60 50 50 50 50 | Butamifos | C13H21N2O4PS | M:332(0%) |
| 288 57 204 41 29 184 232 290 | 50 100 30 30 25 20 15 15 | Diniconazole ketone | C15H15Cl2N3O | M:323(0%) |
| 288 <u>361</u> 289 290 180 316 <u>363</u> 63 | 100 70 60 40 35 30 25 20 | *Haloxypop acid | C15H11ClF3NO4 | M:361,363(70,25%) |
| 288 <u>361</u> 290 261 119 <u>363</u> 289 182 | 100 70 35 30 25 25 20 15 | Fenoxaprop-ethyl | C18H16ClNO5 | M:361,363(70,25%) |
| 290 276 <u>305</u> 125 233 180 262 93 | 100 90 85 50 40 30 30 30 | Pirimiphos-methyl | C11H20N3O3PS | M:305(85%) |
| <u>291</u> 109 97 137 139 125 155 123 | 100 95 95 60 55 45 45 20 | Parathion | C10H14NO5PS | M:291(100%) |
| <u>292</u> 156 140 97 264 125 109 236 | 100 60 45 35 25 20 20 20 | Fensulfothion sulphide | C11H17O3PS2 | M:292(100%) |
| <u>292</u> 181 56 125 153 168 79 277 | 100 75 65 55 50 45 35 30 | Etrimfos | C10H17N2O4PS | M:292(100%) |
| <u>292</u> 188 130 121 129 115 91 175 | 100 70 55 55 25 25 15 15 | *Coumatetralyl | C19H16O3 | M:292(100%) |
| 293 97 125 141 <u>308</u> 109 153 265 | 100 95 85 85 50 50 50 25 | Fensulfothion | C11H17O4PS2 | M:308(50%) |
| <u>294</u> 215 104 109 231 230 295 279 | 100 60 30 25 20 20 20 15 | Fenthion oxon sulphone | C10H15O6PS | M:294(100%) |
| <u>296</u> 76 240 104 50 295 268 297 | 100 90 50 50 40 30 30 20 | *Dithianon | C14H4N2O2S2 | M:296(100%) |
| 296 141 43 281 139 156 113 140 | 100 95 85 80 75 75 70 65 | Sulprofos sulphoxide | C12H19O3PS3 | M:338(40%) |
| <u>296</u> <u>298</u> <u>294</u> 246 244 263 45 248 | 100 65 60 55 40 40 35 30 | Quintozene related ii) | C7H3Cl5S | M:294,296,298,300(60,100,65,20%) |
| 301 299 303 <u>332</u> <u>330</u> <u>334</u> 221 223 | 100 80 45 30 20 15 15 10 | Chlorthal-dimethyl | C10H6Cl4O4 | M:330,332,334(20,30,15%) |
| 301 97 357 303 329 359 125 65 | 100 85 79 44 41 35 31 18 | Chlorthiophos I sulphone | C11H15Cl2O5PS2 | M:392,394,396(0,0,0%) |
| <u>303</u> 288 260 154 195 44 217 <u>304</u> | 100 40 30 30 25 20 15 15 | Fenamiphos | C13H22NO3PS | M:303(100%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|--------------------------|--|-------------------|------------------------------|
| 304 122 303 <u>319</u> 154 196 80 44 | 100 85 35 30 30 25 25 20 | Fenamiphos sulphoxide | C13H22NO4PS | M:319(30%) |
| 306 264 43 41 290 <u>335</u> 307 248 | 100 80 65 35 15 15 15 15 | Trifluralin | C13H16F3N3O4 | M:335(15%) |
| 306 326 264 63 43 328 310 248 | 100 75 55 50 45 20 15 15 | Fluchloralin | C12H13ClN3O3F3 | M:355,357(5,2%) |
| 307 139 167 43 97 141 125 140 | 100 75 50 40 35 30 30 20 | Sulprofos oxon sulphoxide | C12H19O4PS2 | M:322(20%) |
| <u>310</u> 57 29 41 <u>312</u> 219 196 211 | 15 100 40 40 15 15 10 10 | 2,4,5-T n-butyl | C12H13Cl3O3 | M:310,312,314(15,15,5%) |
| <u>310</u> 57 41 29 <u>312</u> 196 198 211 | 10 100 35 30 10 10 10 10 | 2,4,5-T i-butyl | C12H13Cl3O3 | M:310,312,314(10,10,3%) |
| <u>311</u> 187 174 <u>313</u> 103 145 75 172 | 100 95 70 70 55 50 45 35 | Flurochloridone | C12H10Cl2F3NO | M:311,313(100,70%) |
| 313 97 257 315 259 125 285 109 | 64 100 59 47 40 35 33 33 | O,O-Diethyl-O-(2,4,5-trichlorophenyl) phosphorothioate | C10H12Cl3O3PS | M:348(0%) |
| 314 43 56 58 316 187 70 189 | 100 90 70 65 65 45 35 25 | Iprodione | C13H13Cl2N3O3 | M:329,331(4,3%) |
| 316 45 302 288 <u>433</u> 289 91 318 | 100 85 75 75 60 50 45 35 | Haloxypop 2-ethoxyethyl | C19H19ClF3NO5 | M:433,435(60,20%) |
| 316 <u>375</u> 288 289 91 290 180 318 | 100 90 85 45 40 35 35 35 | Haloxypop methyl | C16H13ClF3NO4 | M:375,377(90,30%) |
| 316 <u>417</u> 288 289 318 91 290 272 | 100 55 45 40 35 30 20 20 | Haloxypop n-butyl | C19H19ClF3NO4 | M:417,419(55,20%) |
| 317 43 275 41 301 318 258 259 | 100 85 55 25 15 15 10 10 | *Oryzalin | C12H18N4O6S | M:346(5%) |
| 317 67 315 319 345 281 79 147 | 55 100 35 35 30 30 25 25 | Endrin | C12H8Cl6O | M378,380,382(1,2,1%) |
| <u>318</u> 261 234 276 152 137 303 110 | 100 60 55 40 35 20 20 15 | Tebupirimphos / Phostebupirim | C13H23N2O3PS | M:318(100%) |
| 320 292 58 44 321 122 293 <u>335</u> | 100 65 20 15 15 10 10 10 | Fenamiphos sulphone | C13H22NO5PS | M:335(10%) |
| <u>322</u> 156 140 139 113 43 125 280 | 100 80 60 55 30 25 20 15 | Sulprofos | C12H19O2PS3 | M:322(100%) |
| <u>322</u> 202 121 93 65 174 97 238 | 100 55 55 50 45 40 40 35 | Sulfotep | C8H20O5P2S3 | M:322(100%) |
| <u>324</u> 188 109 97 125 172 157 219 | 100 60 60 60 50 35 30 30 | Fensulfothion sulphone | C11H17O5PS2 | M:324(100%) |
| <u>324</u> <u>326</u> 309 311 289 325 215 291 | 100 70 55 35 35 25 20 15 | Dichlorophen related | C15H14Cl2O2Si | M:324,326,328(100,70,15%) |
| <u>326</u> 325 77 170 94 233 215 65 | 100 65 45 35 30 25 20 20 | <i>triphenyl phosphate</i> | <i>C18H15O4P</i> | <i>M:326(100%)</i> |
| 331 329 125 79 93 109 333 47 | 100 75 75 35 35 30 30 30 | Bromophos | C8H8BrCl2O3PS | M:364(0%) |
| <u>333</u> 318 304 168 180 152 166 109 | 100 95 80 45 40 40 35 25 | Pirimiphos-ethyl | C13H24N3O3PS | M:333(100%) |
| <u>334</u> 120 162 107 55 124 335 143 | 100 20 20 20 20 20 20 20 | *Strychnine | C21H22N2O2 | M:334(100%) |
| <u>340</u> 97 199 188 77 125 204 109 | 100 85 80 70 60 50 45 25 | Pyridaphenthion | C14H17N2O4PS | M:340(100%) |
| <u>340</u> 253 <u>342</u> 255 254 256 281 283 | 100 90 65 65 50 30 30 25 | Diclofop-methyl | C16H14Cl2O4 | M:340,342,344(100,65,10%) |
| 341 97 125 285 343 109 153 313 | 85 100 56 53 36 33 32 32 | Chlorthiophos I sulphoxide | C11H15Cl2O4PS2 | M: 376,378,380(0.2,0.2,0.1%) |

Molecular ion m/z underlined

Contaminants in italics

* denotes poor/negligible GC transmission

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| Eight most abundant ions (m/z) | Relative abundances (%) | Name | Empirical Formula | Molecular ion, m/z (%) |
|---|---------------------------|------------------------------|-------------------|-----------------------------------|
| 341 97 269 325 271 343 285 297 | 86 100 80 58 40 37 36 34 | Chlorthiophos III sulphoxide | C11H15Cl2O4PS2 | M: 376,378,380(1.0,0.8,0.2%) |
| 341 183 185 339 343 155 157 76 | 100 50 50 50 50 15 15 15 | Bromopropylate | C17H16Br2O3 | M:426,428,430(0.5,1,0.5%) |
| <u>341</u> 282 254 146 255 227 342 238 | 100 90 75 35 30 25 20 15 | Fluazifop methyl | C16H14F3NO4 | M:341(100%) |
| 344 388 345 75 372 329 172 <u>403</u> | 100 30 30 15 15 10 10 10 | Azoxystrobin | C22H17N3O5 | M:403(10%) |
| 349 297 <u>494</u> 30 350 296 55 475 | 100 60 40 25 25 15 15 5 | Hydramethylnon | C25H24F6N4 | M:494(40%) |
| 353 81 355 351 357 263 237 151 | 100 90 80 50 35 25 25 20 | Heptachlor epoxide | C10H5Cl7O | M:386,388,390,392(3,6,8,4%) |
| 357 97 301 125 109 329 359 240 | 81 100 60 49 46 39 35 32 | Chlorthiophos III sulphone | C11H15Cl2O5PS2 | M:392,394,396(4,3,1%) |
| 359 97 29 303 357 301 125 242 | 50 100 50 40 40 30 25 25 | Bromophos-ethyl | C10H12BrCl2O3PS | M:392(0%) |
| 361 109 363 <u>396</u> <u>398</u> 79 97 93 | 100 55 35 25 15 15 10 5 | Iodofenphos oxon | C8H8Cl2IO4P | M:396,398(25,15%) |
| <u>362</u> 109 97 226 210 29 125 <u>364</u> | 100 95 90 70 50 50 35 35 | Coumaphos | C14H16ClO5PS | M:362,364(100,35%) |
| 367 369 213 351 255 215 353 85 | 100 70 40 35 25 25 20 20 | Fipronil | C12H4Cl2F6N4OS | M:436,438(0,0%) |
| <u>371</u> 117 88 62 89 61 <u>372</u> 216 | 100 50 15 15 10 10 5 5 | *Ioxynil | C7H3I2NO | M:371(100%) |
| 373 375 377 371 237 272 100 379 | 100 95 50 45 25 20 20 20 | Chlordane | C10H6Cl8 | M:406,408,410,412(2,4,5,2%) |
| 377 379 125 93 79 109 47 250 | 100 40 35 20 20 20 15 10 | Iodofenphos | C8H8Cl2IO3PS | M:412,414(2,1%) |
| 409 407 411 405 413 237 272 109 | 100 90 65 35 25 20 20 20 | Nonachlor | C10H5Cl9 | M:440,442,444,446,448(2,5,5,3,2%) |
| 429 173 47 221 355 281 430 431 | 45 100 35 25 25 15 15 15 | silicones, cyclic (e.g. Si9) | C18H54O9Si9 | M:666(0%) |
| <u>466</u> 93 203 125 <u>467</u> <u>468</u> 357 155 | 100 20 20 20 20 20 5 5 | *Temephos | C16H20O6P2S3 | M:466(100%) |
| <u>522</u> <u>524</u> 290 163 277 360 362 157 | 100 100 70 45 35 35 35 25 | *Brodifacoum | C31H23BrO3 | M:522,524(100,100%) |