APPENDICES

The analysis of pesticides & related compounds using Mass Spectrometry

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Introduction to the Appendices

The purpose of these data compilations is to provide a convenient source of data for analysts involved in the identification of pesticides using mass spectrometry. Data for related compounds, such as metabolites and degradation products produced during analysis, have been included when relevant. Where direct GC-MS techniques are unlikely to be of use, alternative analytical strategies are sometimes suggested.

The MS data in Appendices I and II are presented in two ways: alphabetically by compound name in Appendix I (with data for commonly encountered GC contaminants at the end); and by most intense ion, in a style similar to that of *The Eight Peak Index of Mass Spectra* (MSDC, 1983), in Appendix II, in order to facilitate the identification of unknowns, without recourse to dedicated MS search software.

Where possible, mass spectra were obtained following GC separation. When this was not possible, direct insertion (DI) introduction into the mass spectrometer was used. Most of the data are the averaged results of several acquisitions, generated at different times and (in many cases) on different mass spectrometers. Two magnetic sector instruments were used by the author to generate the data; a VG7070 (for packed column GC introduction) and a JEOL DX300 (for capillary GC introduction). An ion source temperature of 200°C and electron ionisation energy of 70eV was used throughout. Spectra were recorded from m/z 20 to beyond the expected molecular ion region.

Although the mass spectra obtained for most compounds on different instruments are fairly consistent, some variation in the data, even when obtained under apparently similar conditions, is unavoidable. This fact must be borne in mind when using the data in this compilation. Many spectra reported elsewhere, especially those obtained using quadrupole instruments of early design, exhibit exaggerated intensities for low mass ions, at the expense of the more characteristic and diagnostically useful high mass ions. Comparison of the data obtained for many pesticides in this collection with those obtained using bench-top GC-MS instruments (a Finnigan-MAT ITD800 [ion-trap] and a Hewlett-Packard 5971A Mass Selective Detector quadrupole) demonstrated good overall agreement.

Compounds prone to degradation reactions, such as dehydration or reduction, tend to be most susceptible to mass spectral irreproducibility. For these compounds, *e.g.* alcohols, epoxides, sulphoxides and nitro-compounds, the design, temperature and state of cleanliness of the ion source are critical factors in determining the appearance of their mass spectra. An interesting example is the behaviour of methiocarb sulphoxide. Data obtained on the two different GC-MS systems used are included in order to illustrate this effect. Poor reproducibility of mass spectra may also be observed

with compounds that undergo many energetically similar MS fragmentations, e.g. endrin. These compounds produce many ionic species, none of which is particularly abundant, so the overall appearance of the mass spectrum can be particularly sensitive to factors which affect the fragmentation pathways.

Appendix I has a supplement which contains accurate mass MS data for 25 pesticides, generated at Cardiff using GCT MS. These mass spectra had proved difficult to interpret.

Appendix III contains mass-ordered, accurate mass, molecular weight information for nearly 2,000 pesticides, for use in the identification of unknown compounds.

How to use the Appendices

Data are presented in three sections:

Appendix I Pesticides and chemical warfare agents are listed in alphabetical order of their common name, with related metabolites and significant degradation products. The name of the compound is followed by the empirical formula and the nominal molecular ion mass or masses (*not* the average molecular weight) and the observed EI+ MS relative intensity/intensities in brackets.
On the next line are the theoretical molecular ion accurate masses and their relative abundances.

The **molecular structure** is given. This is followed by **pesticide chemical class** (organophosphorus, carbamate, organochlorine etc.) and **pesticide type** (insecticide, acaricide, fungicide, herbicide etc.), plus typical **applications** (veterinary, public health, food production etc.). The online *Compendium of Pesticide Common Names* (Wood 2015) is a convenient source of information.

The **regulatory approval status** is given, plus the **acute oral LD50** (median lethal dose) for the rat, as an indication of acute mammalian toxicity. These data derive mainly from the online *Pesticide Properties DataBase* (PPDB 2015).

Supplementary analytical information, concerning amenability to GC, isomerism or susceptibility to degradation etc., is included when relevant. Relative retention times on packed and/or capillary column GC are expressed, where determined, as *n*-alkane equivalent retention time:

KI(SE-30/OV-17/OV-210) = n for packed column GC data
and
KI(CPSil5/19) = n for capillary GC data.

The eight most intense ions in the electron impact mass spectrum are given (with the molecular ion(s), if present, underlined) and their relative intensities presented beneath (generally rounded to the nearest 5%, if >5%).

Additional data for diagnostic or significant high mass ions are given, plus tentative empirical formula assignments and accurate mass data, in decreasing mass order.

N.B. The empirical formula assignments are generally based on rational interpretation of the nominal mass data and isotope fingerprints. The ion formulae and accurate mass assignments are predictions,

not experimental data (apart from the 25 pesticides described in the supplementary section, whose spectra were obtained using OA TOF MS at Cardiff School of Chemistry).

Result of comparison with reported data, e.g. with the NIST WebBook (NIST 2015), is included when possible. Links to specific mass spectra, and critical appraisals, are provided.

A collection of data for frequently encountered GC contaminants is included at the end of Part I, and these data are also included in Appendix II (in which contaminant names appear in *italics* to distinguish them from pesticides and related compounds).

Supplementary accurate mass MS data for 25 selected pesticides are also included. These data were collected in order to investigate and confirm the empirical formula assignments.

Appendix II - where the mass spectral data are sorted by most abundant ion, compiled in "Eight Peak Index" format, to facilitate the identification of unidentified spectra without resort to computerised systems. As such spectra will generally have been obtained following gas chromatographic separation, those compounds that are not readily amenable to GC are distinguished (by an asterisk). For spectra in which the base peak is at low mass, and which therefore may be difficult to observe (either because it is outside the acquired 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 (>m/z 100). 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. Some spectra exhibit no ions of any significant intensity of m/z greater than 100 (particularly those whose molecular weight is less than 100), but the only pesticides in this category in this collection were 2-aminobutane, aminotriazole, binapacryl, dinocap, metaldehyde, methyl bromide, methyl isothiocyanate and thiodicarb.

Appendix III - is intended to facilitate the identification of pesticides by their molecular weights. It contains mass-ordered, accurate mass, molecular weight information for pesticides described in the ***Pesticide Manual*** (Worthing 1990).

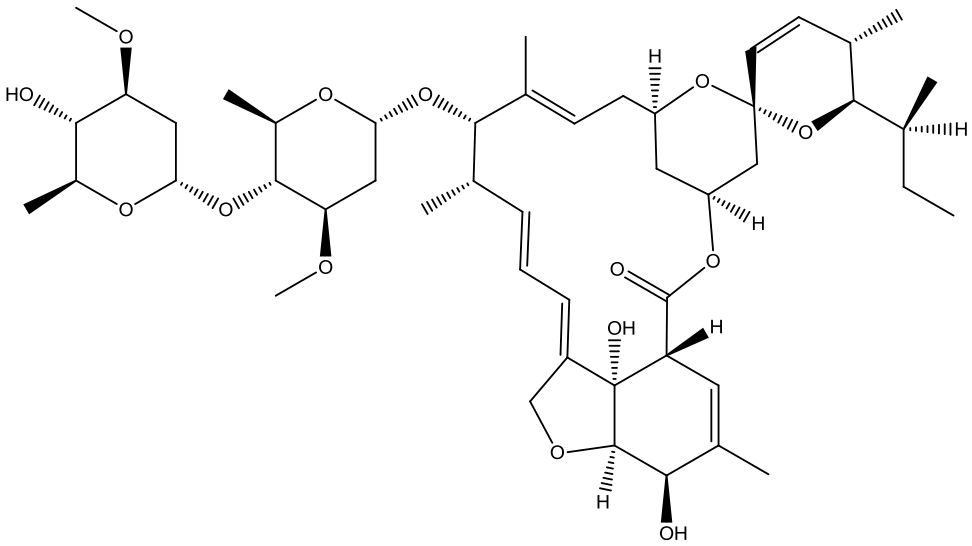
Happy Hunting!

John Wilkins

Appendix I. The compilation of EI+ MS data

Abamectin / Avermectin **$C_{48}H_{72}O_{14}$** **M:872(0%)**

Theoretical molecular ion: m/z 872.4922 (100%), m/z 873.49556 (51.9%), m/z 874.49892 (13.2%), m/z 874.49645 (2.9%), m/z 875.50227 (2.2%), m/z 875.49981 (1.5%).
Average MW: 873.077



Macrocyclic lactone disaccharide insecticide, acaricide and nematicide.
Originally isolated from the Japanese soil bacterium *Streptomyces avermitilis*.
Abamectin is a 4:1 mixture of avermectin B_{1a} ($C_{48}H_{72}O_{14}$, mw 872) and B_{1b} ($C_{47}H_{70}O_{14}$, mw 858). It is not amenable to GC analysis.
Residues may be determined by HPLC/ESP+ MS/MS.
See e.g. European Community Reference Laboratory method:
http://www.crl-pesticides.eu/library/docs/srm/meth_Abamectin_CrlSrm.PDF
Electrospray+ MS/MS ions:
Avermectin B1a: m/z 890.5 → 567.4, m/z 890.5 → 305.1, m/z 891.5 → 568.1
Avermectin B1b: m/z876.6 → 553.3, m/z 876.6 → 291.2

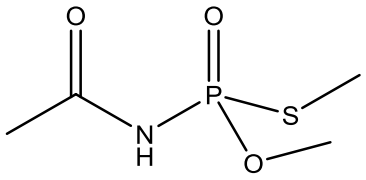
For plant commodities, the total residue is defined as the sum of avermectin B1a + avermectin B1b, plus the photo-isomers 8,9-Z-avermectin B1a + 8,9-Z-avermectin B1b.

Typical values of Maximum Residue Level, MRL, (ex Codex Alimentarius): 0.005 mg/kg in milk to 0.05 mg/kg in lettuce.

No NIST mass spectrum available.

Acephate **$C_4H_{10}NO_3PS$** **M:183(5%)**

Theoretical molecular ion: m/z 183.0119 (100%), 184.0153 (4.3%), 185.0077 (4.5%)
Average MW: 183.17



Organophosphorus insecticide, with systemic action in plants.

Acute oral LD50 for rat approx. 1000 mg/kg (moderate toxicity).

N.B. Acephate can be hydrolysed to **methamidophos**.

Chiral molecule. Acephate sometimes exhibits poor GC peak shape/transmission.

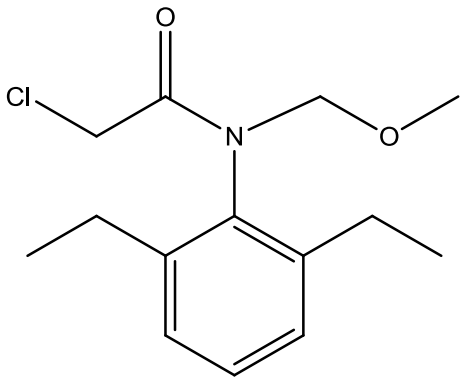
m/z	136	42	43	94	41	95	96	47
%	100	80	50	50	30	30	25	25

183 (5) – M^+
142 (10) – $[M-41]^+$ due to loss of ketene C_2H_2O to $[H_2N.P{=}OH(SCH_3)(OCH_3)]^+$ $C_2H_9NO_2PS^+$ m/z 142.0092
equivalent to $M+H^+$ of methamidophos (MW 141).
136 (100) – $[M-47]^+$ loss of (CH_3S) to $C_3H_7NO_3P^+$ m/z136.0164
125 (15) – [M58] loss of CH_3CONH to $(CH_3O)(CH_3S)P{=}O^+$ m/z 124.9826
94 (50) – [M-89] loss of CH_3CO +CH_2S to give $H2N.P{=}O.(OCH_3)^+$ $CH_5NO_2P^+$ m/z 94.0058
42 (80) – [M-141] $CH_2{=}C{=}O^+$ $C_2H_2O^+$ m/z 42.0106

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C30560191&Mask=200#Mass-Spec

Alachlor / Lasso **$C_{14}H_{20}ClNO_2$** **M:269,271(5,1.5%)**

Theoretical molecular ion: m/z: 269.11826 (100.0%), 271.11531 (32.0%)
Average MW: 269.767



Chloroacetanilide pre-emergence herbicide used for control of grassy and broadleaved weeds in maize, soybeans and peanuts. No longer approved for use in EU because of chronic toxicity concerns.

Acute oral LD50 for rat approx. 1000 mg/kg.

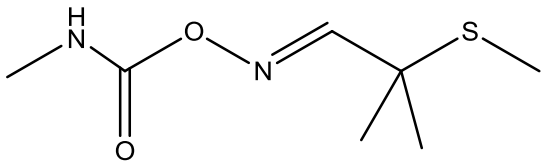
m/z	45	160	188	237	224	146	202	132
%	100	45	40	15	15	10	10	10

269,271 (5,1.5) – M^+
237,239 (15,10) – [M-32] due to loss of CH_3OH to $C_{13}H_{16}ClNO^+$ m/z 237.0920 etc.
224,226 (15,10) – [M-45] due to loss of CH_3OCH_2 to $C_{12}H_{15}ClNO^+$ m/z 224.0842 etc.
202 (10) – [M-67] due to loss of CH_3OH+Cl to $C_{13}H_{16}NO^+$ m/z 202.1232 etc.
188 (40) – [M-81] loss of CH_3O+CH_2Cl to $(C_2H_5)_2C_6H_3$-$NCO(CH)^+$ $C_{12}H_{16}N^+$ m/z 188.1075
160 (45) – [M-109] loss of $ClCH_2CO$+CH_3OH to $(C_2H_5)_2C_6H_3$-NCH^+ $C_{11}H_{14}N^+$ m/z 160.1126
45 (100) – [M-224] $(CH_2OCH_3)^+$ m/z 45.0340

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C15972608&Mask=200

Aldicarb / Temik **$C_7H_{14}N_2O_2S$** **M:190(0%)**

Theoretical molecular ion: m/z: 190.0776 (100%), 191.0810 (8%), 192.0734 (5%)
Average MW: 190.26



Carbamate insecticide with high acute human/mammalian toxicity (WHO Class 1a "extremely hazardous", with rat LD_{50} of 0.93 mg/kg).
Very susceptible to GC degradation to nitrile (described below).
May be oxidised to aldicarb sulphoxide and aldicarb sulphone (see Aldoxycarb).
The MRL for aldicarb includes the sulphoxide and sulphone.

m/z	86	41	85	144	58	87	76	100
%	100	70	55	50	45	40	30	30

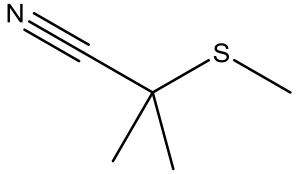
190 (0) – M^+ absent
144 (50) – [M-46] due to loss of CH_2S, $C_6H_{12}N_2O_2^+$ m/z 144.0899
100 (30) – [M-90] due to $C_4H_6NS^+$ m/z 100.0221 (see nitrile spectrum below)
86 (100) - [M-104] due to loss of CH_3NHCO & CH_2S to $HON{=}CHC(CH_3)_2^+$, $C_4H_8NO^+$ m/z 86.0606
58 (45) – [M-132] CH_3NHCO^+ $C_2H_4NO^+$ m/z 58.0293
41 (70) – [M-149] $C_3H_5^+$ m/z 41.0391

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C116063&Mask=200

Aldicarb related **C_5H_9NS** **M:115(70%)**

2-methyl-2-(methylthio)propanenitrile

Theoretical molecular ion: m/z 115.04557 (100.0%), 116.04892 (5.4%), 117.04137 (4.5%)
Average MW: 115.19666



Aldicarb degradation product.
Determination of the nitrile pyrolysis product (which may be produced on GC) may be more convenient than determination of the parent compound (high injection temperature, say 300C, and injection liner filled with glass wool encourages conversion): KI(OV-17) = 10.7

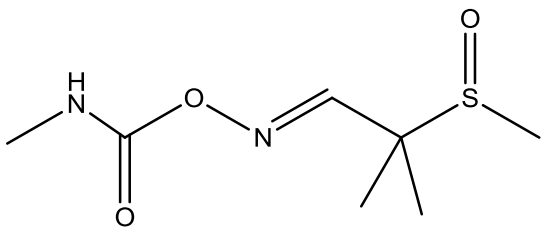
m/z	68	41	115	100	41	47	69	73
%	100	80	70	70	70	20	10	10

115 (70) – M^+
100 (70) – [M-15] loss of CH_3 to $C_4H_6NS^+$ m/z 100.0221
68 (100) – [M-47] NC-$C(CH_3)_2^+$, $C_4H_6N^+$ m/z 69.0500
47 (20) – [M-68] CH_3S^+ m/z 46.9956

No NIST spectrum available for comparison.

Aldicarb sulphone, see Aldoxycarb - Pesticide and oxidation product of Aldicarb

Aldicarb sulphoxide **$C_7H_{14}N_2O_3S$** **M:206(0%)**
Theroetical molecular ion: m/z: 206.0725 (100%), 207.0759 (7.6%), 208.0683 (4.5%)
Average MW: 206.26



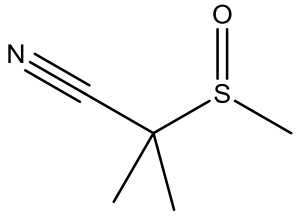
An oxidative metabolite of aldicarb.
Very susceptible to GC degradation. May be determined by HPLC/MS

m/z	41	68	64	47	63	42	39	131
%	100	80	75	20	10	10	10	5

206 (0) – M^+ absent
131 (5) – [M-75] due to loss of methylcarbamic acid ($CH_3NHCOOH$) to $C_5H_9NOS^+$, m/z 131.0405
68 (80) – [M-138] NC-$C(CH_3)_2^+$ $C_4H_6N^+$ m/z 68.0500
63 (10) – [M-143] CH_3SO^+ m/z 62.9905
41 (100) – [M-165] $C_3H_5^+$ m/z 41.0391

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1646873&Mask=200), which appears to be due to **aldicarb sulphone / aldoxycarb**. It exhibits m/z 86 (100%), 41 (70%) and high mass ion at m/z 143 (15%).

Aldicarb sulphoxide related **C5H9NOS** **M:131(5%)**
2-methyl-2-(methylsulfinyl)propanenitrile
Theoretical molecular ion: m/z: 131.04048 (100.0%), 132.04384 (5.4%), 133.03628 (4.5%)
Average MW: 131.19606



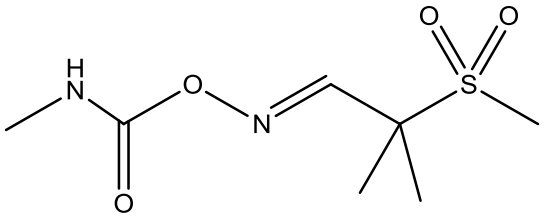
Aldicarb sulphoxide may produce several degradation products on GC.
This, the major one, has an EI mass spectrum very similar to that of aldicarb sulphoxide.

m/z	41	68	64	47	63	42	39	131
%	100	80	75	20	10	10	10	5

131 (5) – M^+
68 (80) – [M-63] loss of CH_3SO to $NC\text{-}C(CH_3)_2^+$ $C_4H_6N^+$ m/z 68.0500
63 (10) – [M-68] CH_3SO^+ m/z 62.9905
41 (100) – [M-90] loss of CH_3SO+HCN to $C_3H_5^+$ m/z 41.0391

No NIST spectrum available for comparison.

Aldoxycarb / aldicarb sulphone **$C_7H_{14}N_2O_4S$** **M:222(0%)**
Theoretical molecular ion: m/z: 222.0674 (100%), 223.0708 (7.6%), 224.0632 (4.5%)
Average MW: 222.26



Carbamate insecticide and nematicide currently used outside the EU to control honey locust gall midge. Chemically identical to aldicarb sulphone, an oxidative metabolite of aldicarb.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

Very susceptible to GC degradation. May be determined as the GC degradation product (nitrile) described below, or directly by LC-MS (e.g. Wang 2006).

m/z	86	41	85	58	68	55	43	143
%	100	50	40	30	25	15	15	10

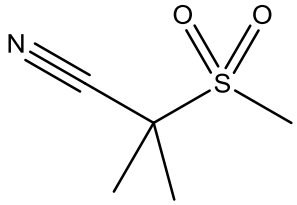
222 (0) – M^+ absent
143 (10) – [M-79] loss of CH_3SO_2 to $C_6H_{11}N_2O_2^+$ m/z143.0821
86 (100) – [M-136] loss CH_3NCO+CH_3SO_2 to $HON{=}CHC(CH_3)_2^+$ $C_4H_8NO^+$ m/z 86.0606
68 (80) – [M-154] $NC\text{-}C(CH_3)_2^+$ $C_4H_6N^+$ m/z 68.0500

Cf. similar spectrum in NIST database http://webbook.nist.gov/cgi/cbook.cgi?ID=C1646884&Mask=200

Aldoxycarb related **$C_5H_9NO_2S$** **M:147(0%)**

2-methyl-2-(methylsulfonyl)propanenitrile

Theoretical molecular ion: m/z: 147.0354 (100%), 148.0388 (5.4%), 149.0312 (4.5%)
Average MW: 147.20



Aldoxycarb may exhibit several degradation products on GC, the major one being the nitrile. The degradation is encouraged by elevated injector temperatures, e.g. 300°C):
KI(OV-17) = 14.3

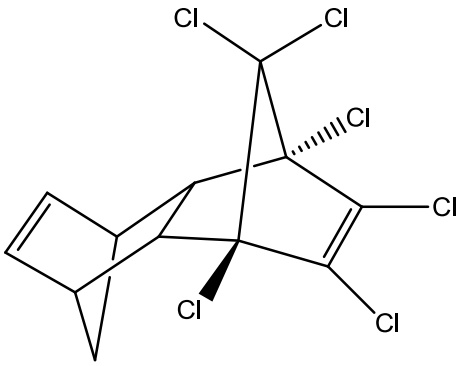
m/z	68	41	80	69	65	39	79	52
%	100	85	20	10	10	5	5	5

147 (0) – M^+ absent
80 (20) – [M-67] loss of $(CH_3)(CH_2)CN$ to $CH_3SO_2H^+$ at m/z 79.9932
79 (5) – [M-68] loss of $(CH_3)_2CN$ to $CH_3SO_2^+$ at m/z 78.9854
68 (100) – [M-79] loss of CH_3SO_2 to $NC\text{-}C(CH_3)_2^+$, $C_4H_6N^+$ m/z 68.0500
41 (85) – [M-106] $C_3H_5^+$ m/z 41.0391

No NIST MS spectrum available.

Aldrin **$C_{12}H_8Cl_6$** **M:362,364,366(1,2,1%)**

Theoretical molecular ion: m/z 361.87572 (52.1%), 363.87277 (100.0%), 365.86982 (79.9%), 367.86687 (34.1%), 369.86392 (8.2%)
Average MW: 364.90992



Cyclodiene organochlorine insecticide, named after Chemistry Nobel Prize winner Kurt Alder (of Diels-Alder fame). Over 270,000 tonnes were produced, 1946-1976. Persistent, bioaccumulative and toxic. It was banned in the US in 1990 and the EU in 1984.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

Aldrin is one of the “dirty dozen” organochlorine compounds/classes outlawed or restricted under the UN Stockholm Convention on Persistent Organic Pollutants, 2001. The others were dieldrin, endrin, heptachlor, hexachlorobenzene, mirex, toxaphene (camphechlor), polychlorinated biphenyls (PCBs), DDT, polychlorinated dibenzo-p-dioxins ("dioxins") and

polychlorinated dibenzofurans. Several other organohalogen compounds have since been added (e.g. isomers of HCH, chlordecone, endosulfan etc.).

Aldrin is rapidly metabolised to **dieldrin**.

m/z	66	91	263	261	265	79	101	293
%	100	40	40	30	30	30	25	20

362, 364, 366 (1, 2, 1) – M^+
327, 329, 331 (3, 5, 3) – $[M-Cl]^+$
296, 298, 300 (5, 10, 8) – $[M-C_5H_6]^+$
291, 293, 295 (12, 15, 7) – $[M-HCl_2]^+$
261, 263, 265 (30, 40, 30) – $[M-C_5H_6-Cl]^+$
91 (40) – $[C_7H_7]^+$ (tropylium ion)
66 (100) – $[C_5H_6]^+$ - accurate mass m/z 66.046950

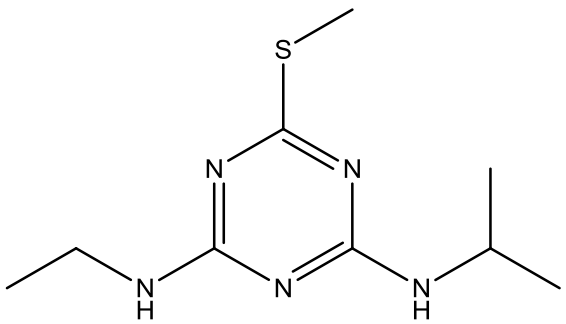
Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C309002&Units=SI&Mask=200#Mass-Spec

Optimal detection sensitivity is obtained using GC-NCI-MS, which may be several orders of magnitude more sensitive than GC-EI-MS under similar chromatographic conditions (Nakamura 2001).

For a comparison of detection limits for pesticides using GC-EI SIM MS and GC-MS/MS and GC-NCI MS, see Raina (2008).

Ametryn **$C_9H_{17}N_5S$** **M:227(100%)**

Theoretical molecular ion: m/z: 227.1205 (100%), 228.1238 (10%), 229.1163 (4.5%)
Average MW: 227.33



Methylthiotriazine herbicide used to control broadleaf weeds and grasses and as a desiccant in maize, sugar cane and pineapple cultivation. Banned in EU in 2006.

Acute oral LD50 for rat is approx. 1000 mg/kg (moderate toxicity)

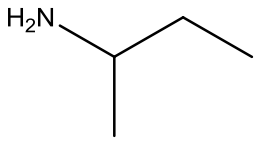
m/z	227	58	212	68	99	170	69	185
%	100	75	70	50	40	35	30	25

227 (100) – M^+
212 (70) - [M-15] loss of CH_3 to $C_8H_{14}N_3S^+$ m/z 212.0970
58 (75) - [M-169] $NHCH(CH_3)_2^+$, $C_3H_8N^+$ m/z 58.065674

Cf. similar but noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C834128&Mask=200#Mass-Spec

2-Aminobutane/ *sec*-Butylamine **$C_4H_{11}N$** **M:73(1%)**

Theoretical molecular ion: m/z: 73.08915 (100.0%), 74.09250 (4.3%)
Average MW: 73.14



Fumigant fungicide. Not approved for use in EU.

Acute oral LD50 for rat is approx. 350 mg/kg (moderate toxicity)

Very volatile. Poor GC transmission at low levels because of its polarity.

m/z	44	58	41	30	42	43	29	27
%	100	10	10	5	5	5	5	5

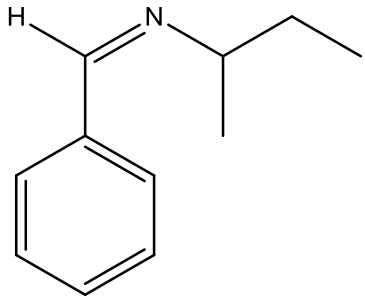
73 (1) – M^+
58 (10) – [M-15] due to loss of CH_3 to $C_3H_8N^+$ m/z 58.0657
44 (100) – [M-29] due to loss of CH_2CH_3 to $C_2H_6N^+$ m/z 44.0500

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C13952846&Units=SI&Mask=200#Mass-Spec

2-Aminobutane related **$C_{11}H_{15}N$** **M:161 (5%)**

N-*sec*-butyl-1-phenylmethanimine

Theoretical molecular ion: m/z 161.12045 (100.0%), 162.12380 (11.9%)
Average MW: 161.24



2-aminobutane benzaldehyde imine derivative

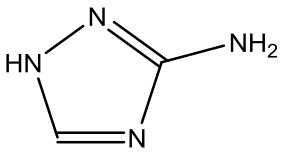
For analytical convenience 2-aminobutane may be determined by GC as its benzaldehyde imine.

m/z	132	146	133	104	91	160	89	161
%	100	30	15	15	15	5	5	5

161 (5) – M^+
146 (30) – [M-15] loss of CH_3 to $C_{10}H_{12}N^+$ m/z 146.0970
132 (100) – [M-29] loss of C_2H_5 to $C_9H_{10}N^+$ m/z 132.0813
104 (15) – [M-57] loss of C_4H_9 to $C_7H_6N^+$ m/z 104.0500

No NIST spectrum available

Aminotriazole /Amitrole **$C_2H_4N_4$** **M:84(100%)**
Theoretical molecular ion: m/z: 84.0436 (100%), 85.0470 (2%)
Average MW: 84.08



Triazole herbicide. Used to control a wide range of perennial grasses and broad-leaved weeds. Approved for use in EU.

Acute oral rat LD50 >5,000 mg/kg (low toxicity).

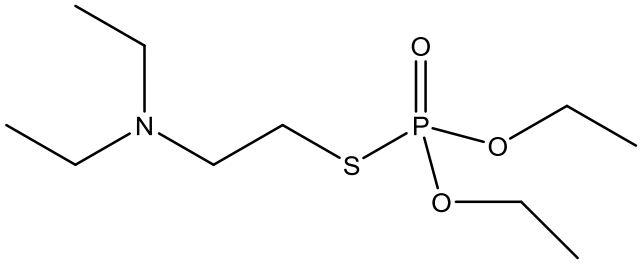
Aminotriazole is not directly amenable to GC analysis, but may be determined by LC-ESP+ MS/MS, monitoring transitions from $(M+H)^+$ m/z 85 → m/z 43 and 57 (EURL 2015).

m/z	84	28	57	43	42	85	-	-
%	100	45	40	20	15	3	-	-

84 (100) – M^+
57 (40) – [M-27] due to loss of HCN to $CH_3N_3^+$ m/z 57.0327
28 (45) – [M-56] H_2CN^+ m/z 28.0187

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C61825&Mask=200#Mass-Spec

Amiton / "VG" (nerve agent) **$C_{10}H_{24}NO_3PS$** **M:269(0%)**
Theoretical molecular ion: m/z 269.1215 (100%), 270.1248 11%), 271.1173 (4.5%)
Average MW: 269.34



Organophosphorus insecticide. Developed in the 1950s and found to be very effective against mites, but no longer in use, as too toxic.

Acute oral LD50 for rat approx. 3 mg/kg (high toxicity)

Latterly, a V series chemical warfare "nerve agent", VG.

m/z	86	99	87	109	71	42	58	141
%	100	50	20	15	15	10	10	10

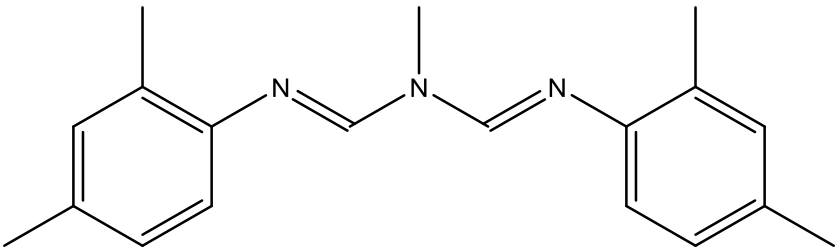
269 (0) – M^+
197 (5) – [M-72] $(CH_3CH_2O)_2P{=}O.SCH_2CH_2^+$ $C_6H_{14}O_3PS^+$ m/z 197.0401

169 (5) – [M-100] $(CH_3CH_2O)_2P{=}O.S^+$ $C_4H_{10}O_3PS^+$ m/z 169.0088
141 (10) – [M-128] $(CH_3CH_2O)(HO)P{=}O.S^+$ $C_2H_6O_3PS^+$ m/z 140.9775
109 (15) – [M-160] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0054
99 (50) – [M-160] $(C_2H_5)_2NCHCH_2^+$ $C_6H_{13}N^+$ m/z 99.1048
86 (100) – [M-183] $(C_2H_5)_2NCH_2^+$ $C_5H_{12}N^+$ m/z 86.0970
71 (15) – [M-198] $C_4H_9N^+$ m/z 71.0735

N.B. Mass spectral data from Borrett (2003). No NIST spectrum available.

Amitraz **$C_{19}H_{23}N_3$** **M:293(45%)**

Theoretical molecular ion: m/z: 293.1892 (100%), 294.1926 (21%), 295.1959 (2%),
Average MW: 293.41



Non-systemic formamide acaricide and insecticide. It is used as a pesticide mainly on top fruit, cotton and hops. In veterinary medicine it is applied topically as a spray, dip, or pour-on to pigs, cattle and sheep for the control of ectoparasites. In apiculture, amitraz is used as a sustained-release strip containing 500 mg amitraz which is suspended in the hive for the treatment of *Varroa* mite infestation.

Acute oral LD50 for rat is 800 mg/kg (moderate toxicity).

Sometimes poor GC transmission.

MRLs may include 2,4-dimethylaniline and/or formamidine $(CH_3)_2C_6H_3$-N=CH-NH-CH_3 metabolites (the latter is not directly amenable to GC but may be determined by HPLC).

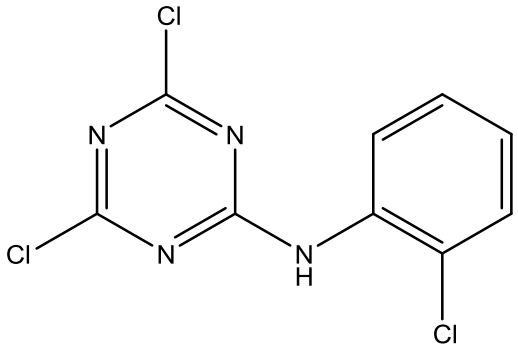
m/z	121	162	132	147	293	120	106	161
%	100	85	65	50	45	30	25	20

293 (75) – M^+
162 (85) – [M-131] $(CH_3)_2C_6H_4$-N=$CHNHCH_3^+$, $C_{10}H_{14}N_2^+$, m/z 162.1157
132 (65) – [M-161] $(CH_3)_2C_6H_4$-N=CH^+, $C_9H_{10}N^+$, m/z 132.0813
121 (100) – [M-172] $(CH_3)_2C_6H_4NH_2^+$, $C_8H_{11}N^+$, m/z 121.0892 (M^+ of 2,4-dimethylaniline)

Cf. similar though weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C33089611&Mask=200#Mass-Spec

Anilazine **$C_9H_5Cl_3N_4$** **M:274,276,278(10,10,3%)**

Theoretical molecular ion: m/z 273.9580 (100%), 275.9550 (95.9%), 277.9521 (30.6%)
Average MW: 275.52



Triazine non-systemic foliar fungicide, introduced in 1995. Banned in the EU in 2005.

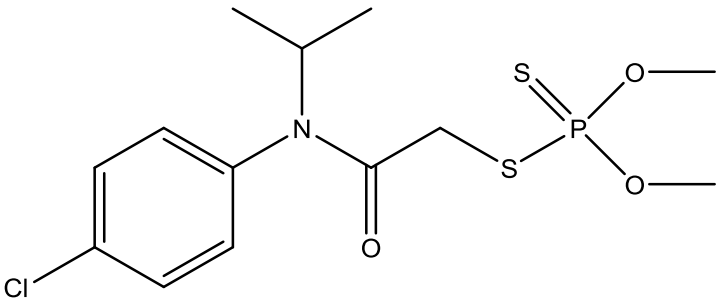
Acute oral LD_{50} for rat >4,000 mg/kg.

m/z	239	241	143	178	90	62	111	240
%	100	60	40	35	15	10	10	10

274,276,278 (10,10,3) – M^+
239,241,243 (100,60,10) – [M-35] loss of Cl to $C_9H_5Cl_2N_4^+$ m/z 238.9891 etc.
178,180 (35,10) – [M-101] loss of 2Cl+CN to $C_8H_5ClN_3^+$ m/z 178.0172 etc.
143 (40) – [M-136] loss of 3Cl+CN, to $C_8H_5N_3^+$ m/z 143.0484

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C101053&Mask=200#Mass-Spec

Anilofos **$C_{13}H_{19}ClNO_3PS_2$** **M:367,369(1,0.5%)**
Theoretical molecular ion: m/z: 367.0233 (100%), 369.0200 (32.0%)
Average MW: 367.84



Organophosphorus herbicide used as for pre-emergence and early post-emergence selective control of annual grasses, sedges and some broad-leaved weeds in transplanted and direct seeded rice.

Acute oral LD50 for rat approx. 1,700 mg/kg.

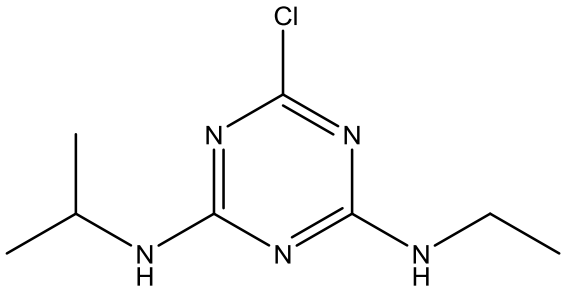
m/z	226	125	43	184	228	93	154	171
%	100	75	65	55	35	35	30	30

367,369 (1,0.5) – M^+
334,336 (10,3) – [M-33] due to rearrangement and loss of SH to $C_{13}H_{18}ClNO_3PS^+$ at m/z 334.0434 etc.
226,228 (100,35) – [M-141] loss of C_2H_6OPS to $ClC_6H_4N(iPr)COCH_2O^+$ $C_{11}H_{13}ClNO_2$ m/z 226.0635 etc.
184 (55) – [M-183] loss of C_2H_6OPS & C_3H_6 to $ClC_6H_4NHCOCH_2O^+$ $C_8H_7ClNO_2^+$ m/z 184.0165 etc.

125 (75) – [M-242] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ at m/z 124.9826
93 (35) – [M-274] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ at m/z 93.0105
43 (65) – [M-324] $C_3H_7^+$ at m/z 43.0548

No NIST spectrum available for comparison.

Atrazine **$C_8H_{14}ClN_5$** **M:215,217(70,20%)**
Theoretical molecular ion: m/z 215.0938 (100%), 217.0908 (32%)
Average MW: 215.69



Triazine herbicide, heavily used in US (40,000 tonnes p.a.), mainly for maize production. Banned in EU because of toxicity concerns, effects on aquatic organisms (especially frogs), residues in ground and drinking water, and the development of resistance.

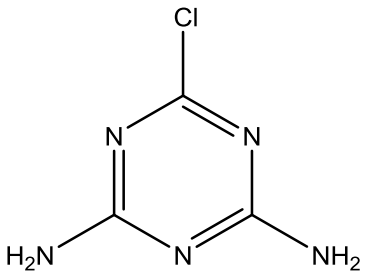
Acute oral LD50 for rat approx. 1,800 mg/kg (moderate toxicity).

m/z	200	58	215	173	43	202	92	68
%	100	70	70	35	30	30	25	25

215,217 (70,20) – M^+
200,202 (100,30) – [M-15] due to loss of CH_3 to $C_7H_{11}ClN_5^+$ m/z 200.0703
173,175 (35,10) – [M-42] loss of C_3H_6 to $C_5H_8ClN_5^+$ m/z 173.0468
58 (70) – [M-157] $(CH_3)_2CHNH^+$ $C_3H_7N^+$ m/z 57.0578

Cf. similar though weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912249&Mask=200#Mass-Spec

Atrazine metabolite **$C_3H_4ClN_5$** **M:145,147(100,30%)**
2-chloro-4,6-diamino-1,3,5-triazine
Theoretical molecular ion: m/z 145.0155 (100%), 147.0126 (32%)
Average MW: 145.55



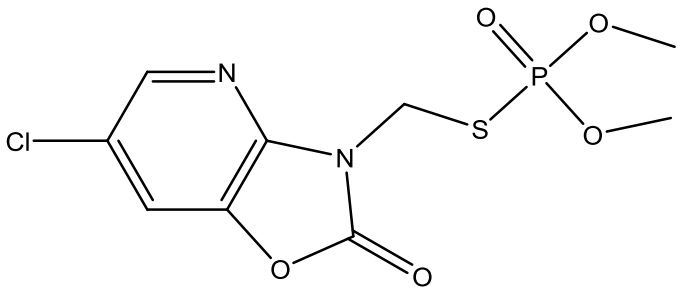
Atrazine metabolite, 2-chloro-4,6-diamino-1,3,5-triazine

m/z	145	147	110	68	43	42	62	146
%	100	30	30	30	25	20	10	5

145,147 (100,30) – M+
110 (30) – [M-35] loss of Cl to $C_3H_4N_5^+$ m/z 110.0467
68 (30) – [M-77] loss of Cl & CH_2N_2 to $C_2H_2N_3^+$ m/z 68.0249

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3397624&Units=SI&Mask=200#Mass-Spec
listed under "1,3,5-Triazine-2,4-diamine, 6-chloro-"

Azamethiphos **$C_9H_{10}ClN_2O_5PS$** **M:324,326(15,5%)**
Theoretical molecular ion: m/z: 323.9737 (100%), 325.9707 (32%)
Average MW: 324.67



(N.B. Structure incorrect in Wikipedia, Nov 2014)

Organophosphorus insecticide, used in fish farming to control external parasites of the Atlantic Salmon, and in pest/hygiene control in warehouses for flies and cockroaches.

Acute oral LD5 for rat approx. 1,000 mg/kg (moderate toxicity).

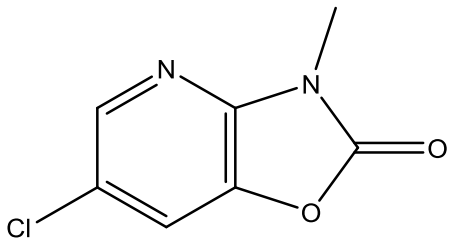
Poor GC transmission. Susceptible to GC degradation.

m/z	109	125	215	155	183	139	61	45
%	100	80	60	50	40	35	30	30

324,326 (15,5) – M^+
215,217 (60,20) – [M-109] loss of $(CH_3O)_2P{=}O$ to $C_7H_4ClN_2O_2S^+$ m/z 214.9682 etc.
183 (40) – [M-141] loss of $(CH_3O)_2P{=}O.S$ to $C_7H_4ClN_2O_2^+$ m/z 182.9961
155 (50) – [M-169] loss of $(CH_3O)_2P{=}O.S$ & CO to $C_6H_4ClN_2O^+$ m/z 155.0012
139 (35) – [M-185] loss of $(CH_3O)_2P{=}O.S$ & CO_2 to $C_6H_4ClN_2^+$ m/z 139.0063
125 (80) – [M-199] $(CH_3O)_2P{=}O.S^+$ $C_2H_6O_3PS^+$ m/z 124.9826
109 (100) – [M-183] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (20) – [M-213] $(CH_3O)(HO)P{=}O^+$ $CH_4O_2P^+$ m/z 78.9949

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C35575963&Units=SI&Mask=200#Mass-Spec

Azamethiphos contaminant **$C_7H_5ClN_2O_2$** **M:184,186(100,35%)**
6-chloro-3-methyloxazolo[4,5-b]pyridin-2(3H)-one
Theoretical molecular ion: m/z 184.0040 (100%), 186.0010 (32%)
Average MW: 184.58



Azamethiphos formulation contaminant
6-chloro-3-methyloxazolo[4,5-b]pyridin-2(3H)-one

Shorter RT compound observed on GC.

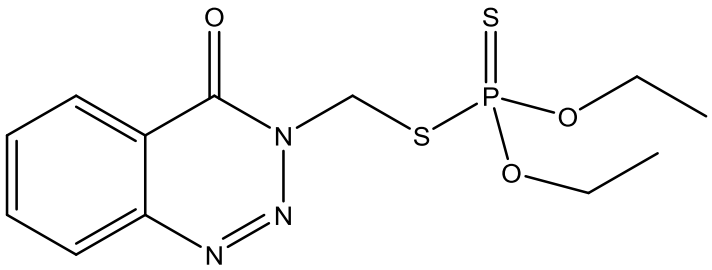
m/z	184	186	101	93	64	143	129	156
%	100	35	30	30	25	20	15	10

184,186 (100,35) – M^+
156 (10) – [M-28] loss of CO to $C_6H_5ClN_2O^+$ m/z 156.0090

No NIST spectrum available for comparison.

Azinphos-ethyl **$C_{12}H_{16}N_3O_3PS_2$** **M:345(0%)**

Theoretical molecular ion: m/z 345.0371 (100%), 346.0404 (13%), 347.0329 (9.0%)
Average MW: 345.37



Organophosphorus insecticide. Broad spectrum, non-cumulative and non-systemic insecticide/acaricide with good ovicidal properties. Not approved for use in EU.

Acute oral LD_{50} for rat approx.12 mg/mg (high toxicity).

Azinphos-ethyl and azinphos-methyl have superficially similar mass spectra, with dominant ions at m/z 77, 132 and 160. They can be distinguished by the presence of m/z 129 $(HO_2)PS_2^+$ and m/z 97 $(HO_2)PS^+$ in the azinphos-ethyl spectrum, and more abundant m/z 125 $(CH_3O)_2PS^+$ and m/z 93 $(CH_3O)_2P^+$ in the azinphos-methyl spectrum (as well as by GC retention time).

KI (SE-30) = 25.5

m/z	132	160	77	105	104	97	129	65
%	100	75	65	25	25	20	15	15

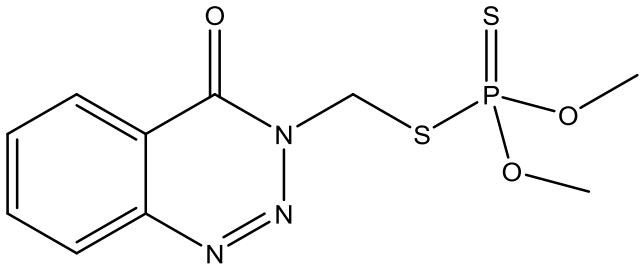
Main assignments confirmed by accurate mass (Cardiff GCT) of azinphos-methyl homologue (below).
345 (0) – M^+ absent
160 (75) – [M-185] loss of $SP{=}S.(OCH_2CH_3)_2$ to $C_8H_6N_3O^+$, m/z160.0511

132 (100) – [M-213] loss of SP=S.$(OCH_2CH_3)_2$ & N_2 to $C_8H_6NO^+$ m/z132.0449
129 (15) – [M-216] (HO) $_2PS_2^+$ $H_2O_2PS_2^+$ m/z 128.9234
105 (25) – [M-240] loss of SP=S.$(OCH_2CH_3)_2$ & N_2 & HCN to $C_6H_5CO^+$ m/z 105.0340
104 (25) – [M-241] loss of SP=S.$(OCH_2CH_3)_2$ & N_2 & NCH_2 to $C_6H_4CO^+$ m/z 104.0262
97 (20) – [M-248] $(HO_2)PS^+$ $H_2O_2PS^+$ m/z 96.9513
77 (65) – [M-268] $C_6H_5^+$ m/z 77.03913
65 (15) – [M-280] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2642719&Mask=200#Mass-Spec

Azinphos-methyl **$C_{10}H_{14}N_3O_3PS_2$** **M:317(0%)**

Theoretical molecular ion: 317.0058 (100%), 318.0091 (11%), 319.0016 (9%)
Average MW: 317.32



Organophosphorus insecticide. Highly persistent, broad spectrum. Not approved for use in EU.

Acute oral LD_{50} for rat approx. 10 mg/mg (high toxicity).

Azinphos-ethyl and azinphos-methyl have superficially similar mass spectra, with dominant ions at m/z 77, 132 and 160. They can be distinguished by the presence of m/z 97 [$(HO_2)PS^+$] in the azinphos-ethyl spectrum, and more abundant m/z 93 [$(CH_3O)_2P^+$] and 125 [$(CH_3O)_2PS^+$] in the azinphos-methyl spectrum (as well as by GC retention time).

KI (SE-30) = 24.5

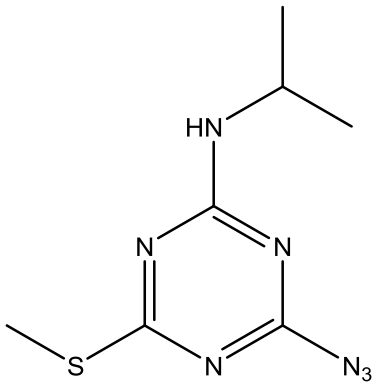
m/z	160	132	77	105	93	76	104	125
%	100	95	95	30	30	30	20	20

Assignments confirmed by accurate mass (Cardiff GCT).
317 (0) – M^+ absent
160 (100) – [M-157] loss of SP=S.$(OCH_3)_2$ to $C_8H_6N_3O^+$, m/z160.0511
132 (100) – [M-185] loss of SP=S.$(OCH_3)_2$ & N_2 to $C_8H_6N^+$ m/z132.0449
Not $C_7H_6N_3^+$ m/z132.0562 or $C_7H_4N_2O^+$ m/z132.0324 due to loss of CO or C_2H_4
125 (20) – [M-192] S=P$(OCH_3)_2^+$ $C_2H_6O_2PS^+$ m/z 124.9826 – (characteristic organophosphorus ion)
105 (25) – [M-212] loss of SP=S.$(OCH_3)_2$ & N_2 & HCN to $C_6H_5CO^+$ m/z 105.0340
104 (20) – [M-213] $C_6H_4N_2^+$ m/z 104.0352
(Not $C_6H_4CO^+$ m/z 104.0262 as predicted)
93 (30) – [M-224] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
77 (65) – [M-268] $C_6H_5^+$ m/z 77.03913
65 (15) – [M-280] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C86500&Mask=200#Mass-Spec

Aziprotryne **$C_7H_{11}N_7S$** **M:225(80%)**

Theoretical molecular ion: m/z 225.0797 (100%), 226.0830 (7.6%), 227.0755 (4.5%)
Average MW: 225.27



Methylthiotriazine herbicide once used as a post-emergence treatment for the control of broad-leaved weeds. Not approved for use in EU.

Acute oral LD50 for rat approx. >3,000 mg/kg (low toxicity)

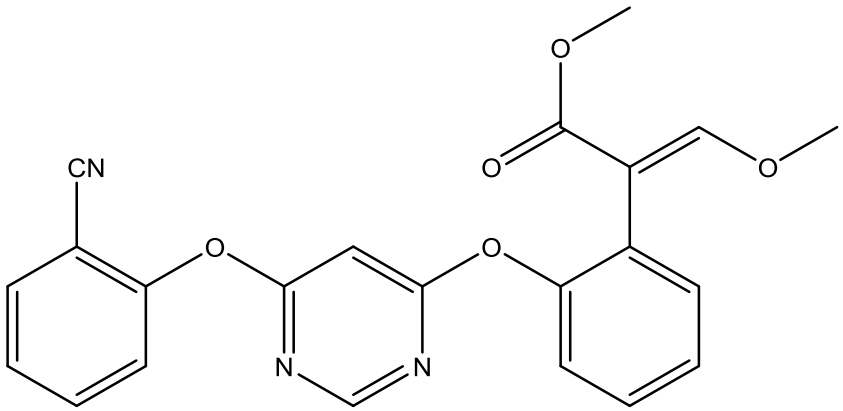
Susceptible to GC degradation (reduction of $-N_3$ moiety to $-NH_2$ either on GC or in mass spectrometer ion source, results in observation of M^+ at m/z 199).
For a comparison of GCMS performance using EI, methane CI and ammonia CI see H-J Stan (1991).

m/z	43	225	139	68	182	58	210	47
%	100	80	75	65	55	45	40	40

225 (80) – M^+
182 (55) – [M-43] loss of C_3H_7 to $C_4H_7N_7S^+$ m/z 182.0249
And/or due to loss of HN_3 to $C_7H_{10}N_4S^+$ m/z 182.0626
139 (75) – [M-86] loss of C_3H_7 & HN_3 to $C_4H_3N_4S^+$ m/z 139.0078
68 (65) – [M-157] $N{=}C{-}N_3^+$ CN_4^+ (!) m/z 68.0123 – unexpected ion
58 (45) – [M-167] $(CH_3)_2CHNH^+$ $C_3H_8N^+$ m/z 58.0657
47 (40) – [M-178] CH_3S^+ m/z 46.9955
43 (100) – [M-182] $C_3H_7^+$ m/z 43.0548
And/or hydrazoic acid, HN_3^+ m/z 43.0171

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C4658280&Units=SI&Mask=200#Mass-Spec
though with less abundant high mass ions.

Azoxystrobin **$C_{22}H_{17}N_3O_5$** **M:403(####7%)**
Theoretical molecular ion: m/z 403.1168 (100%), 404.1208 (24%)
Average MW: 403.39



Strobilurin fungicide. Broad spectrum QoI (*Quinone outside Inhibitor*) fungicide with protectant, curative, eradicant and systemic properties. Strobilurins were derived from a naturally occurring compound found in wood-rotting fungi (Anke 1977). They act by inhibiting fungal mitochondrial respiration. Azoxystrobin was introduced in 1992. Approved for use in EU.

See other strobilurins: kresoxim-methyl, pyracolostrobin & trifloxystrobin.

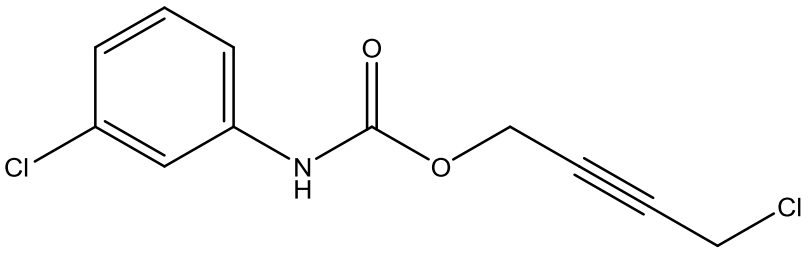
Acute oral LD50 for rat approx. >5,000 mg/kg (low toxicity).

m/z	344	388	345	75	372	329	172	403
%	100	30	30	15	15	10	10	10

403 (10) – M^+ $C_{22}H_{17}N_3O_5^+$
388 (30) – [M-15] loss of CH_3 to $C_{21}H_{14}N_3O_5^+$ m/z 388.0934
372 (15) – [M-31] loss of CH_3O to $C_{21}H_{14}N_3O_4^+$ m/z 372.0984
344 (100) – [M-59] loss of $COOCH_3$ to $C_{20}H_{14}N_3O_3^+$ m/z 344.1035
172 (15) – [M-328] $C_{11}H_8O_2^+$ m/z 172.0524 (but many options so confirm with acc mass)
102 (10) – [M-301] $NC.C_6H_4^+$ $C_7H_4N^+$ m/z 102.0344
75 (15) – [M-328] $C_6H_3^+$ m/z 75.0235

Data taken from NIST spectrum, http://webbook.nist.gov/cgi/cbook.cgi?ID=C131860338&Mask=200#Mass-Spec

Barban **$C_{11}H_9Cl_2NO_2$** **M:257,259(10,7%)**
Theoretical molecular ion: m/z 257.0010 (100%), 258.0044 (12%), 258.9981 (64%), 260.9951 (10%)
Average MW: 258.10



Carbanilate herbicide, used as post-emergence herbicide for general weed control, including wild oats in cereals, particular barley, and sugar beet. No longer approved for use in EU.

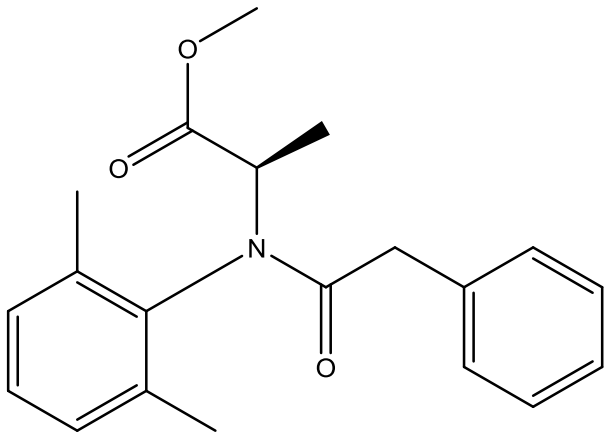
Acute oral LD50 for rat approx. >500 mg/kg (moderate toxicity).

m/z	153	51	222	87	69	41	127	104
%	100	85	65	65	50	40	35	35

257,259 (10,7) – M^+
222,224 (65,20) – [M-35] loss of Cl to $C_{11}H_9Cl_2NO_2^+$ m/z 222.0322 etc.
153,155 (100,30) – [M-104] $C_7H_5ClNO^+$ m/z 152.9981 (3-chlorophenyl isocyanate M^+)
104 (35,10) – [M-153] complementary ion to m/z153: $HOCH_2$-C≡C-CH_2Cl m/z 104.0029
87,89 (65,20) – [M-170] $^+CH_2$-C≡C-CH_2Cl, $C_4H_4Cl^+$ m/z 87.0002 etc.
51 (85) – [M-206] CH_2-C≡C-CH^+ $C_4H_3^+$ m/z 51.0235

Cf. similar spectrum, though with less abundant high mass ions, at
http://webbook.nist.gov/cgi/cbook.cgi?ID=C101279&Mask=200#Mass-Spec

Benalaxyl **$C_{20}H_{23}NO_3$** **M:325(15%)**
Theoretical molecular ion: m/z 325.1678 (100%), 326.17115 (22%)
Average MW: 325.41



Broad spectrum phenylamide/acylaniline fungicide, used to control blight on potatoes and mildew on grapes. The more active (R)-isomer of this compound (depicted) is sold as Benalaxyl-M (*Kiralaxyl*). Approved for use in EU.

Acute oral LD_{50} for rat approx. 500 mg/kg (moderate toxicity).

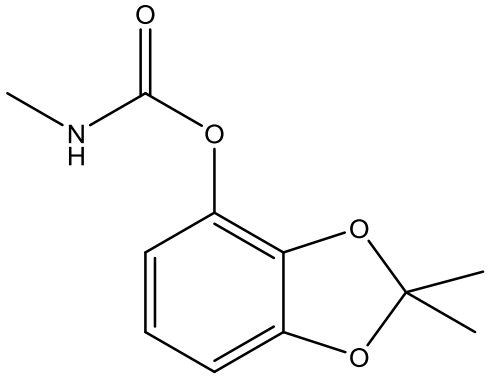
m/z	148	91	204	206	325	234	266	176
%	100	35	30	25	15	15	15	10

325 (15) – M^+
294 (5) – [M-31] loss of CH_3O to $C_{19}H_{20}NO_2^+$ m/z 294.1494
266 (15) – [M-59] loss of CH_3OCO to $C_{18}H_{20}NO^+$ m/z 266.1545
234 (15) – [M-91] loss of $C_6H_5CH_2$ to $C_{13}H_{16}NO_3^+$ m/z 234.1130
148 (100) – [M-177] $(CH_3)_2C_6H_3$-$NCOH^+$, $C_9H_{10}NO^+$ m/z 148.0762
91 (35) – [M-234] $C_7H_7^+$ tropylium ion, m/z 91.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C71626114&Mask=200#Mass-Spec

Bendiocarb **$C_{11}H_{13}NO_4$** **M:223(15%)**

Theoretical molecular ion: m/z223.08446 (100.0%), 224.08781 (11.9%)
Average MW: 223.23



Carbamate insecticide. Used in agriculture and public health applications, to control beetles, mosquitoes, cockroach, ants, wasps etc., and snails and slugs. No longer approved for use in EU or US.

Acute oral LD_{50} for rat approx. 30 mg/kg (high toxicity).

m/z	151	126	166	51	39	223	58	123
%	100	60	50	20	15	15	10	10

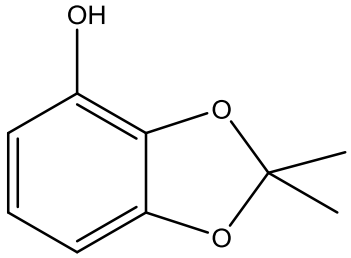
223 (15) – M^+
166 (50) – [M-57] due to loss of CH_3NCO (methyl isocyanate) to $HOC_6H_3.O_2C(CH_3)_2$ (2,2-dimethyl-1,3-benzodioxol-4-ol), i.e. reverse of synthesis. $C_9H_{10}O_3^+$ m/z 166.0630
151 (100) – [M-72] loss of CH_3NCO & CH_3 to $HO\text{-}C_6H_4.O_2CCH_3^+$, $C_8H_7O_2^+$ m/z151.0395
126 (60) – [M-97] loss of CH_3NCO & C_3H_4 to 1,2,3-trihydroxybenzene (pyrogallol), $C_6H_6O_3^+$ m/z 126.01234

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C22781233&Mask=200#Mass-Spec

Bendiocarb related **$C_9H_{10}O_3$** **M:166(60%)**

2,2-dimethyl-1,3-benzodioxol-4-ol

Theoretical molecular ion: m/z166.06299 (100.0%), 167.06635 (9.7%)
Average MW: 166.07



2,2-dimethyl-1,3-benzodioxol-4-ol

GC degradation product (due to loss of methyl isocyanate). Cf. carbofuran.

m/z	126	151	166	39	51	52	108	123
%	100	90	60	25	20	15	15	10

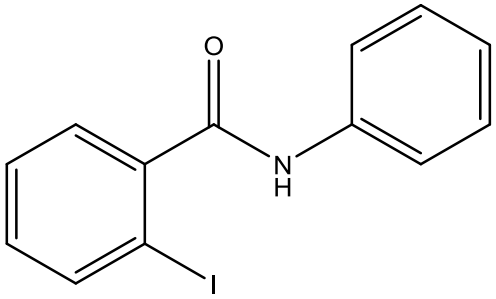
166 (60) – M^+
151 (100) – [M-15] loss of CH_3 to $C_8H_7O_2^+$ m/z 151.0395

126 (60) – [M-40] loss of C_3H_4 to 1,2,3-trihydroxybenzene (pyrogallol), $C_6H_6O_3^+$ m/z 126.0317
108 (15) – [M-58] loss of acetone $(CH_3)_2CO$ to $C_6H_4O_2^+$ m/z 108.0211

No NIST spectrum available.

Benodanil **$C_{13}H_{10}INO$** **M:323(35%)**

Theoretical molecular ion: m/z322.9807 (100%), 323.9841 (14%)
Average MW: 323.31



Benzanilide fungicide previously used to control rust diseases. No longer approved for use in EU.

Acute oral LD50 for rat approx. >6,400 mg/kg (low toxicity).

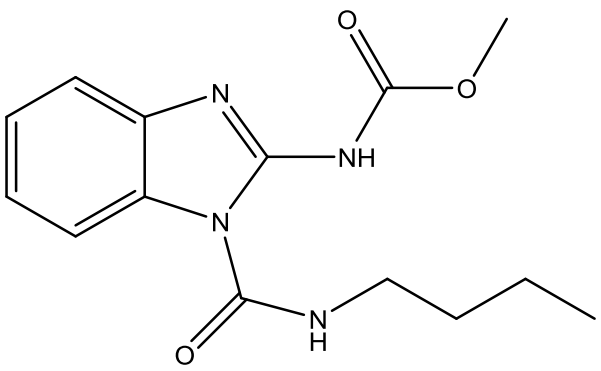
m/z	231	323	76	203	77	105	196	50
%	100	35	35	25	20	15	15	15

323 (35) – M^+
231 (100) – [M-92] loss of C_6H_5NH to $C_7H_4IO^+$ m/z 230.9307
203 (25) – [M-120] $C_6H_4I^+$ m/z 202.9358
196 (15) – [M-127] loss of iodine to $C_{13}H_{10}NO+$ m/z 196.0762
76 (35) – [M-247] $C_6H_4^+$ (benzyne) m/z 76.0313

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C15310017&Mask=200#Mass-Spec

Benomyl **$C_{14}H_{18}N_4O_3$** **M:290(0%)**

Theoretical molecular ion: m/z 290.1379 (100%), 291.1413 (15%)
Average MW: 290.32



Benzimidazole fungicide. Effective as a pre-harvest systemic fungicide, and as a post-harvest dip or dust treatment for the protection of fruits, seeds and vegetables in storage. It controls a wide range of fungal diseases of fruits, nuts, vegetables, field crops, turf and ornamentals, e.g. powdery mildew, apple scab and grey mould fungus. It is also effective against mites. No longer approved for use in EU.

Acute oral LD_{50} for rat is>10,000 mg/kg (low toxicity).

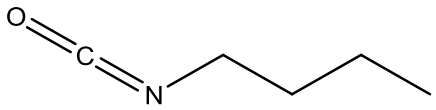
Benomyl is not directly amenable to GC analysis, but may be determined by HPLC. Benomyl decomposes to n-butyl isocyanate and 2-aminobenzimidazole on GC (see carbendazim for details of latter compound). For efficient conversion, the injector must be hot (300°C) and contain a dense plug of glass wool (to increase analyte residence time).

m/z	43	41	56	27	159	30	98	191
%	100	85	45	40	35	30	20	15

290 (0) – M^+
191 (15) – [M-99] loss of C_4H_9NCO (n-butyl isocyanate) to $C_9H_9N_3O_2^+$ m/z 191.0695
159 (35) – [M-131] loss of C_4H_9NCO & CH_3OH to $C_6H_4N_2CHNCO^+$ $C_8H_5N_3O^+$ m/z 159.0433
(benzimidazole isocyanate M^+)
56 (45) – [M-234] $C_4H_8^+$ butene m/z 56.0626
43 (100) – [M-247] $C_3H_7^+$ m/z 43.0548

Cf. noisy (over enhanced) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C17804352&Mask=200#Mass-Spec with elevated high mass ion intensities (m/z 159 and 191), and some different ions e.g. m/z 105, 42 and 40 at low mass.

Benomyl related **C_5H_9NO** **M:99(3%)**
n-butyl isocyanate
Theoretical molecular ion: m/z 99.0684 (100%), 100.0718 (5%)
Average MW: 99.33



n-butyl isocyanate

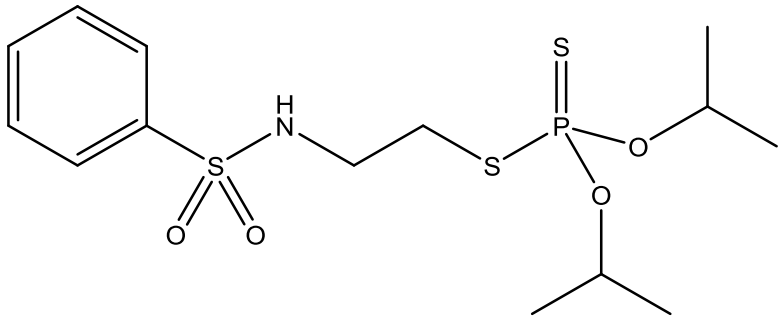
Very volatile. Short GC RT.

m/z	43	41	27	56	28	30	39	98
%	100	90	75	50	40	30	20	20

99 (3) – M^+
98 (20) – [M-1] $C_5H_8NO^+$ m/z 98.0606
56 (50) – [M-43] $C_4H_8^+$ m/z 56.0626 (and/or CH_2NCO^+ m/z 56.0136)
43 (100) – [M-56] $C_3H_7^+$ m/z 43.0548
41 (90) – [M-58] $C_3H_5^+$ m/z 41.0391

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C111364&Mask=200#Mass-Spec

Bensulide **$C_{14}H_{24}NO_4PS_3$** **M:397(0%)**
Theoretical molecular ion: m/z 397.06051 (100.0%), 398.06386 (15.1%), 399.05630 (13.6%)
Average MW: 397.50



Bensulide (N.B. Wikipedia structure is incorrect)

Organophosphorus herbicide (not insecticide), applied pre-emergence to control grasses and weeds in food crops (carrots, cucumbers, cabbages), and on lawns and golf courses.

Acute oral LD50 in rat approx. 500 mg/kg. Highly toxic to bees and fish.
Not amenable to GC.

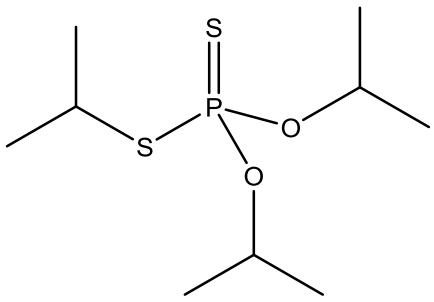
m/z	215	172	131	77	214	173	141	130
%	100	75	75	70	70	55	50	50

397 (0) – M^+ absent
256 (10) – [M-141] loss of $C_6H_5SO_2$ to $NHCH_2CH_2S.P{=}S(OC_3H_7)_2^+$ $C_8H_{19}NO_2PS_2^+$ m/z 256.0595
215 (100) – [M-182] loss of $C_6H_5SO_2NC_2H_3$ to $(C_3H_7O)_2(HS)_2P^+$ $C_6H_{16}O_2PS_2^+$ m/z 215.0329
214 (70) – [M-183] loss of $C_6H_5SO_2NC_2H_4$ to $(C_3H_7O)_2PS(SH)^+$ $C_6H_{15}O_2PS_2^+$ m/z 214.0251
184 (30) – [M-213] $C_6H_5SO_2NHCH_2CH_2^+$ $C_8H_{10}NO_2S^+$ m/z 184.0432
172 (75) – [M-225] $(C_3H_7O)(HO)P{=}S.SH^+$ $C_3H_9O_2PS_2^+$ m/z 171.9782
156 (10) – [M-241] $C_6H_5SO_2NH^+$ $C_6H_6NO_2S^+$ m/z 156.0229
141 (50) – [M-256] $C_6H_5SO_2^+$ m/z 141.0010
131 (75) – [M-266] $(HO)_2(HS)_2P^+$ $H_4O_2PS_2^+$ m/z 130.9390
77 (70) – [M-320] $C_6H_5^+$ m/z 77.0391

Cf. quite different (weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C741582&Mask=200#Mass-Spec which exhibits abundant ions at m/z 77, 170 and 141. Probably due to **N-butyl benzene sulphonamide**:

See GC artefact compound & http://webbook.nist.gov/cgi/cbook.cgi?ID=C3622842&Mask=200#Mass-Spec

Bensulide related **$C_9H_{21}O_2PS_2$** **M:256(20%)**
O,O,S-tri-*iso*-propyl phosphorodithioate
Theoretical molecular ion: 256.07206 (100%), 257.07541 (10%), 258.06785 (9%)
Average MW: 256.36



O,O,S-tri-*iso*-propyl phosphorodithioate

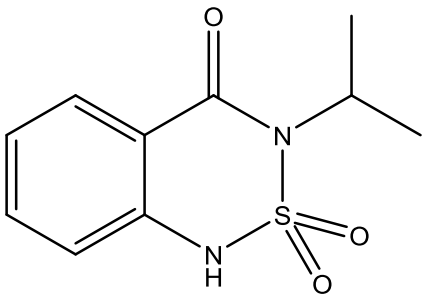
Technical contaminant or GC degradation product.

m/z	130	214	43	172	131	75	41	256
%	100	80	50	50	50	50	50	20

256 (20) – M^+
214 (80) – [M-42] $(C_3H_7O)_2(HS)P{=}S^+$ $C_6H_{15}O_2PS_2^+$ m/z 214.0251
172 (50) – [M-84] $(C_3H_7O)(HO)(HS)P{=}S^+$ $C_3H_9O_2PS_2^+$ m/z 171.9782
131 (50) – [M-125] $(HO)_2(HS)_2P^+$ $H_4O_2PS_2^+$ m/z 130.9390
130 (100) – [M-126] loss of $3C_3H_6$ to $(HO)_2(HS)P{=}S^+$ $H_3O_2PS_2^+$ m/z 129.9312
75 (50) – [M-181] $C_3H_7S^+$ m/z 75.0268
43 (100) – [213] $C_3H_7^+$ m/z 43.0548

No NIST spectrum available.

Bentazone **$C_{10}H_{12}N_2O_3S$** **M:240(15%)**
Theoretical molecular ion: 240.05686 (100.0%), 241.06022 (10.8%), 242.05266 (4.5%)
Average MW: 240.28



Herbicide with selective, contact, post emergence applications for use against broadleaved weeds and sedges in legume, potato etc. cultivation.

Acute oral LD_{50} for rat is approx. 1500 mg/kg.

m/z	119	198	161	92	121	182	64	225
%	100	80	50	45	30	20	20	15

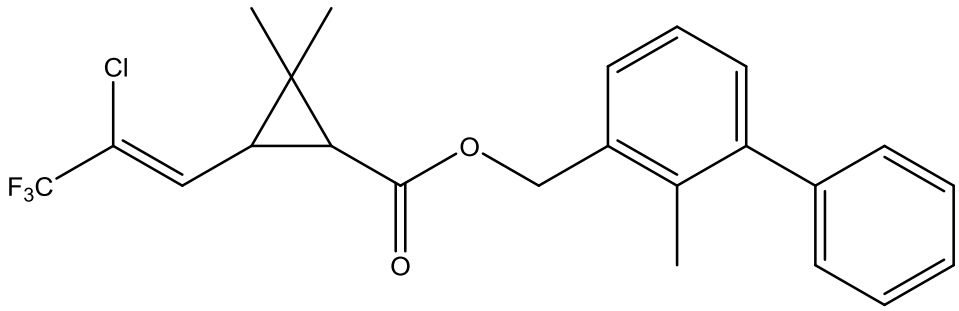
240 (15) – M^+
225 (15) – [M-15] loss of CH_3 to $C_9H_9N_2O_3S^+$ m/z 225.0334
198 (80) – [M-42] loss of C_3H_6 to $C_7H_6N_2O_3S^+$ m/z 198.0099
161 (50) – [M-79] loss of SO_2N to $C_{10}H_{11}NO^+$ m/z 161.0841
119 (100) – [M-121] $C_7H_5NO^+$ m/z 119.0371 (≡ phenyl isocyanate)

Cf. similar but noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C25057890&Mask=200#Mass-Spec

BHC, see HCH

Bifenthrin **$C_{23}H_{22}ClF_3O_2$** **M:422,424(1,0.5%)**

Theoretical molecular ion: m/z 422.12604 (100.0%), 424.12309 (32.0%)
Average MW: 422.87



Synthetic pyrethroid insecticide. Stereoisomer enriched to improve activity. Broad spectrum contact and ingestion activity, used on cereals, cotton, maize, grass, vegetables and some fruits. Approved for use in EU.

Acute oral LD_{50} for rat is approx. 50 mg/kg (high toxicity). Also highly toxic to fish and bees.

Generally one peak on capillary GC (unlike many other pyrethroids).

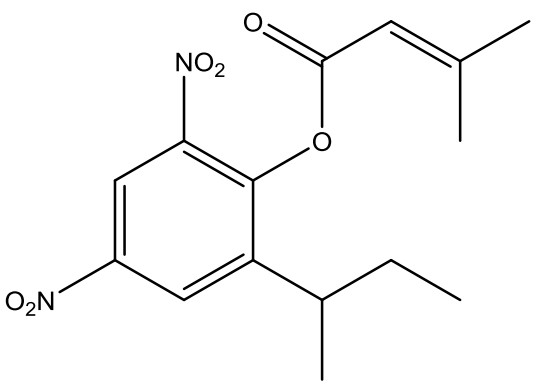
m/z	181	166	182	165	180	167	141	179
%	100	25	20	15	10	5	5	5

422,424 (1,0.5) – M^+
181 (100) – [M-241] C_6H_5-$C_6H_4(CH_3)CH_2^+$, $C_{14}H_{13}^+$ m/z 181.1017
166 (25) – [M-256] $C_{13}H_{10}^+$ m/z 166.0783
165 (15) – [M-256] $C_{13}H_9^+$ m/z 165.0704
141 (5) – [M-281] $C_{11}H_9^+$ m/z 114.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C82657043&Mask=200#Mass-Spec

Binapacryl **$C_{15}H_{18}N_2O_6$** **M:322(0%)**

Theoretical molecular ion: m/z 322.1165 (100%), 323.1198 (16%)
Average MW: 332.12



Dinitrophenol acaricide and fungicide. No longer approved for use in EU.
Binapacryl is the 3-methylbutenoate (3,3-dimethylacrylate) ester of **dinoseb**.
It is metabolized to dinoseb which is more toxic (suspect carcinogen).

Acute oral LD50 for rats approx. 200 mg/kg (moderate toxicity).

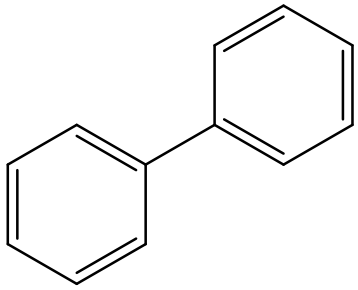
m/z	83	55	82	39	-	-	-	-
%	100	15	5	5	-	-	-	-

Remarkably uninformative EI mass spectrum. Only two significant ions, and both associated with the dimethylacrylic acid moiety

322 (0) – M^+ absent
83 (100) – [M-239] $OC\text{-}CH{=}C(CH_3)_2^+$ $C_5H_7O^+$ m/z 83.1100
55 (15) – [M-267] $HC{=}C(CH_3)_2^+$ $C_4H_7^+$ m/z 55.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C485314&Mask=200#Mass-Spec

Biphenyl **$C_{12}H_{10}$** **M:154(100%)**
Theoretical molecular ion: m/z 154.07825 (100.0%), 155.08161 (13.0%)
Average MW: 154.21



Aromatic fungicide used mainly on citrus fruits.

Acute oral LD50 for rats approx. 2,000 mg/kg (low toxicity).

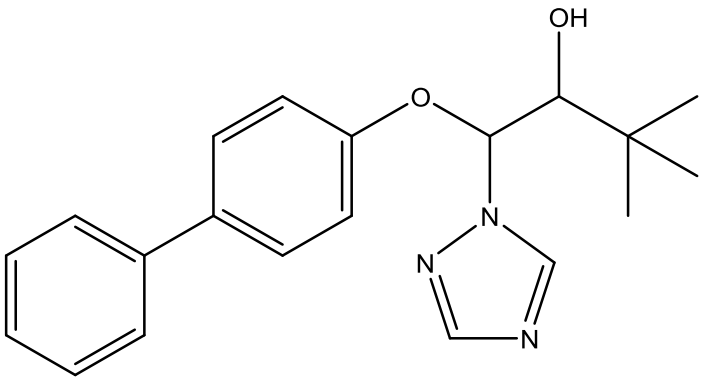
m/z	154	153	152	76	155	78	115	63
%	100	35	25	20	15	10	5	5

154 (100) – M^+
115 (15) – [M-39] $C_9H_7^+$ m/z 115.0548
76 (20) – [M-78] $C_6H_4^+$ m/z 76.0313

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C92524&Mask=200#Mass-Spec

Bitertanol **$C_{20}H_{23}N_3O_2$** **M:337(1%)**

Theoretical molecular ion: m/z 337.17903 (100%), 338.18238 (22%), 339.18574 (2%)
Average MW: 337.42



Triazole "conazole" fungicide, used to control a range of diseases including scab, powdery mildew, rusts and blackspot. Not approved for use in EU.

Acute oral LD50 for rats >5,000 mg/kg (low toxicity).

Technical bitertanol contains a pair of diastereoisomers (80:20), which may be resolved by capillary GC (e.g. using 25m CPSil19CB). KI (SE-30) = 26.3

m/z	170	57	168	112	171	268	169	141
%	100	30	15	15	15	5	5	5

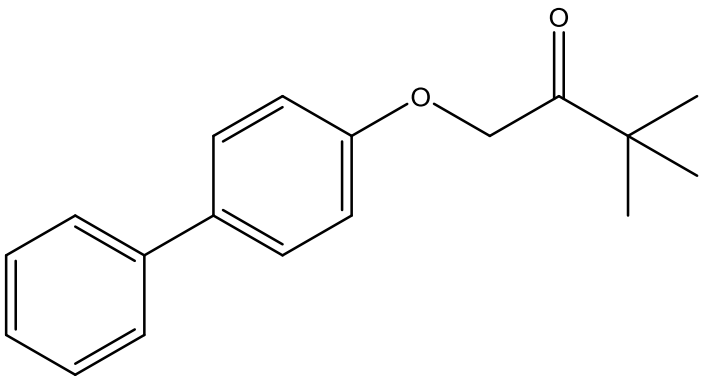
337 (1) – M^+
268 (5) – [M-69] loss of triazole $C_2N_3H_2$+H to $C_{18}H_{20}O_2^+$ m/z 268.1463
170 (100) – [M-167] C_6H_5-C_6H_4-OH^+ $C_{12}H_{10}O^+$ m/z 170.2110
57 (30) – [M-280] $(CH_3)_3C^+$ $C_4H_9^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C55179312&Mask=200#Mass-Spec

Bitertanol related **$C_{18}H_{20}O_2$** **M:268(35%)**

1-([1,1'-biphenyl]-4-yloxy)-3,3-dimethylbutan-2-one

Theoretical molecular ion: m/z 268.14633 (100.0%), 269.14968 (19.5%)
Average MW: 268.36



1-([1,1'-biphenyl]-4-yloxy)-3,3-dimethylbutan-2-one

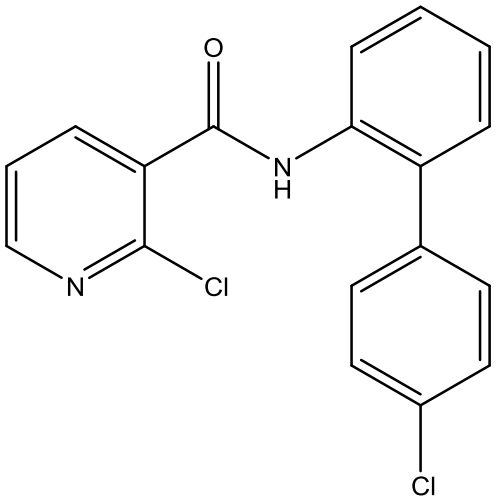
Bitertanol may undergo GC degradation : KI (SE-30) = 22.2

m/z	57	268	152	170	153	184	76	269
%	100	35	15	15	15	10	5	5

268 (35) – M^+
170 (15) – [M-98] C_6H_5-C_6H_4-OH^+ $C_{12}H_{10}O^+$ m/z 170. 2110
152 (15) – [M116] $C_{12}H_8^+$ m/z 152.0626

No NIST spectrum available.

Boscalid **$C_{18}H_{12}Cl_2N_2O$** **M:342,344,346(15,10,5)**
Theoretical molecular ion: 342.0327 (100%), 344.0297 (65%), 346.0268 (11%)
Average MW: 343.21



Anilide/pyridine carboxamide fungicide. Used to protect crops from grey mould, powdery mildew etc.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

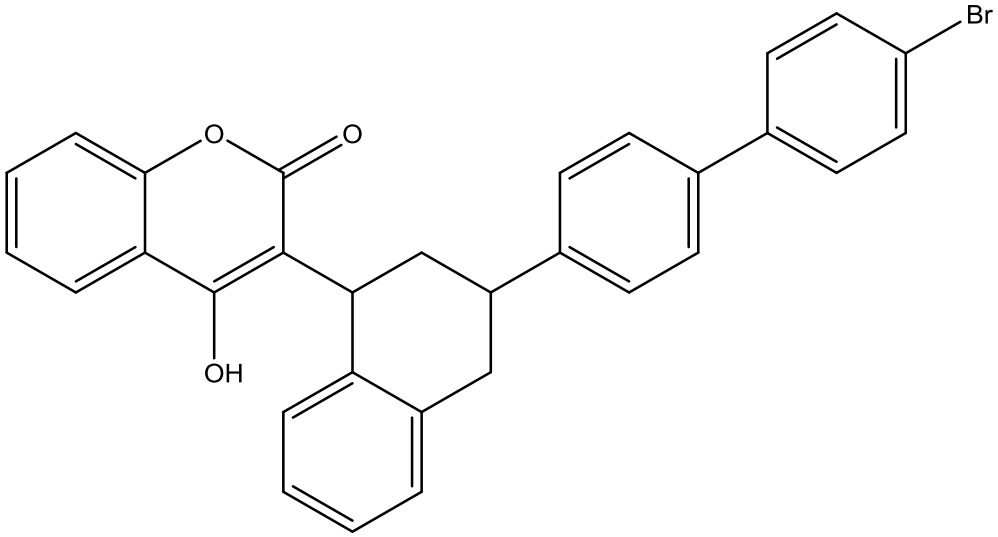
m/z	140	112	142	342	253	289	342	344
%	100	30	30	15	10	10	10	10

342,344,346 (15,10,5) – M^+
140,142 (100,30) – [M-202] $Cl.C_5H_3N.CO^+$ $C_6H_3ClNO^+$ m/z 139.9903 etc.
112 (30) – [M-230] $C_5H_3ClN^+$ m/z 111.9954 etc.

No NIST spectrum available. Data from Portoles (2011).

Brodifacoum **$C_{31}H_{23}BrO_3$** **M:522,524(100,100%)**

Theoretical molecular ion: 522.08306 (100%), 524.08101 (97%)
Average MW: 523.43



Anticoagulant rodenticide.

Acute oral LD50 for rat approx. 0.3 mg/kg.

Not amenable to GC.

May be determined by HPLC ESP- MS/MS, e.g. Fourel (2010).

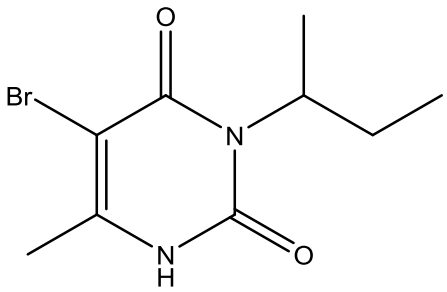
m/z	522	524	290	163	277	360	362	157
%	100	100	70	45	35	35	35	25

522,524 (100,100) – M^+
360,362 (35,35) – [M-162] $C_{22}H_{17}Br^+$ m/z 360.05136 (100.0%), 362.04932 (97.3%)
290 (70) – [M-232] loss of bromobiphenyl to $C_{19}H_{14}O_3^+$ m/z 290.0943
163 (45) – [M-359] 4-hydroxycoumarin moiety, $C_9H_7O_3^+$ m/z 163.0395

No NIST spectrum available.

Bromacil **$C_9H_{13}BrN_2O_2$** **M:260,262(5,5%)**

Theoretical molecular ion: m/z 260.01604 (100%), 262.01399 (97%)
Average MW: 261.12



Uracil herbicide. The technical material is a racemic mixture. Bromacil is used for brush control on non-cropland areas. It is especially useful against perennial grasses. It is used for

selective weed control in pineapple and citrus crops. It is sprayed or spread dry on the soil surface just before, or during, a period of active weed growth. Approved for use in EU.

Acute oral LD50 in rat approx. 5,200 mg/kg.

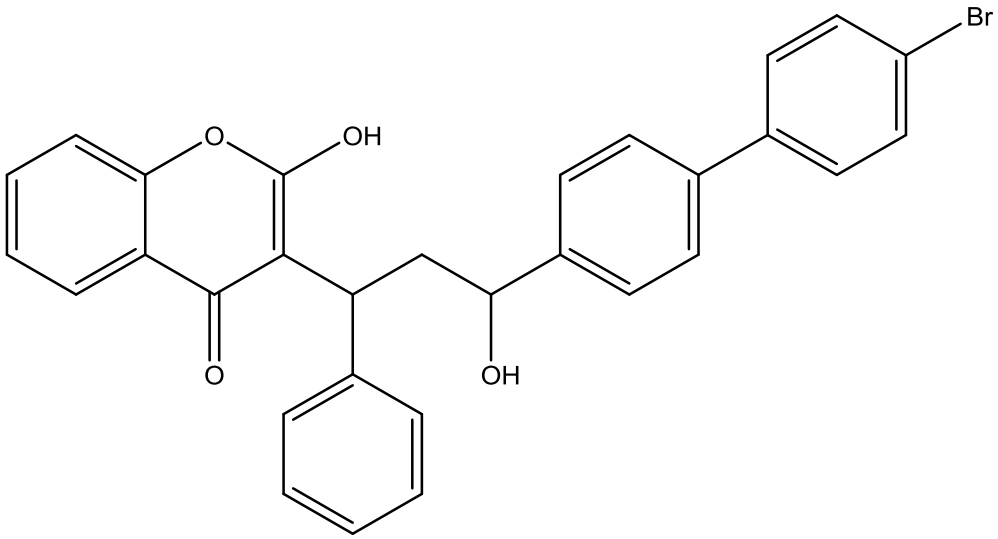
Sometimes poor GC transmission.

m/z	205	207	42	70	162	164	231	233
%	100	95	35	20	15	15	15	15

260,262 (5,5) – M^+
245,247 (3,3) – [M-15] due to loss of $CH_3$to $C_8H_{10}BrN_2O_2^+$ m/z 244.99257 (100%), 246.99052 (97%)
231,233 (15,15) – [M-29] due to loss of C_2H_5 to $C_7H_8BrN_2O_2^+$ m/z 230.9769 (100%), 232.9749 (97%)
205,207 (100,95) – [M-55] due to loss of C_4H_7 to $C_5H_6BrN_2O_2^+$, m/z 204.9607 (100%), 206.9641 (97%)
162,164 (15,15) – [M-98] due to loss of i-butyl isocyanate to $C_4H_5BrNO^+$ m/z 161.9555 (100%), 163.9534 (97%)
70 (20) – [M-190] $C_2H_4NCO^+$ m/z 70.0292
42 (35) – [M-217] NCO^+ m/z 41.9980

Cf. generally similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C314409&Mask=200#Mass-Spec
apart from low mass ions (m/z 41 and 69).

Bromadiolone **$C_{30}H_{23}BrO_4$** **M:526,528(0,0%)**
Theoretical molecular ion: m/z 526.0780 (100%), 528.0759 (97.3%)
Average MW: 527. 41



Anticoagulant rodenticide. As it is so toxic, formulated baits typically contain only 0.005% w/w active ingredient.

Acute oral LD50 for rat approx. 1 mg/kg (high toxicity).

Very poor GC transmission.

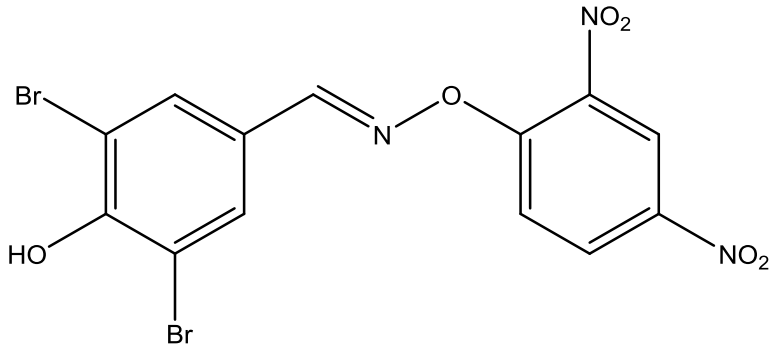
m/z	258	260	249	178	250	120	92	348
%	100	95	85	55	50	35	35	25

526,528 (0,0) – M^+

508,510 (3,3) – [M-18] due to loss of H_2O. $C_{30}H_{21}BrO_3^+$ m/z 508.06741 (100%), 510.06536 (97%),
346,348 (15,20) – [M-180], $C_{21}H_{15}Br^+$ m/z: 346.03571 (100%), 348.03367 (97%)
258,260 (100,95) – [M-268], $C_{14}H_{11}Br^+$ m/z 258.0044 (100%), 260.0024 (97%)
249 (85) – [M-277], $C_{16}H_9O_3^+$ m/z 249.0552
178 (55) – [M-348] due to loss of HBr from m/z 258 [$C_{14}H_{11}Br$] to $C_{14}H_{10}^+$

No NIST spectrum available.

Bromofenoxim **$C_{13}H_7Br_2N_3O_6$** **M:459,461,463(1,2,1%)**
Theoretical molecular ion: m/z 458.8702 (51%), 460.8681 (100%), 462.8661 (49%)
Average MW: 461.10



Phenoxy herbicide. Used for selective post-emergence, contact control of broadleaved weeds, especially in cereal crops. No longer approved for use in EU.

Acute oral LD50 for rat >1,100 mg/kg (moderate toxicity).

Rapidly degrades in soil. Metabolites include **bromoxynil** and 2,4-dinitrophenol.

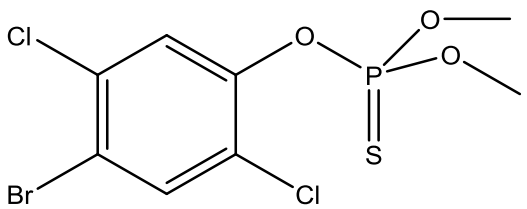
Poor transmission on GC.

m/z	277	184	88	279	275	63	53	91
%	100	75	70	55	50	45	40	35

459,461,463 (1,2,1) – M^+
275,277,279 (50,100,50) – [M-184] loss $C_7H_3NOBr_2^+$ m/z 274.8581 (51%), 276.8561 (100%), 278.8541 (49%)
184 (75) – [M-275] "dinitrophenol" $C_6H_4N_2O_5^+$ m/z 184.0120 (complementary ion to m/z 275,277, 279).

No NIST spectrum available.

Bromophos **$C_8H_8BrCl_2O_3PS$** **M:364,366,368(0,0,0%)**
Theoretical molecular ion: m/z 363.8492 (100%), 365.8472 (97%), 367.8442 (62%)
N.B. At low resolution the apparent M^+ isotope ratio is 60:100:49.
Average MW: 366.0



Organophosphorus insecticide and acaricide with contact and stomach action, effective against a wide range of pests (beetles, root maggots, aphids, moths etc.). No longer approved for use in EU.

Acute oral LD50 for rat approx. 1,600 mg/kg (moderate toxicity)

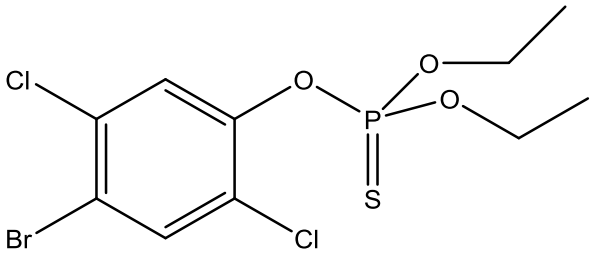
May be oxidised to bromophos oxon, $C_8H_8BrCl_2O_4P$, M^+ 348,350,352.

m/z	331	329	125	79	93	109	333	47
%	100	75	75	35	35	30	30	30

364,366 (0,0) – M^+ absent.
329,331,333 (75,100,30) – [M-35] loss of Cl to $C_8H_8BrClO_3PS^+$ m/z 328.8804 etc.
125 (75) – [M-237] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z124.9826
109 (30) – [M-255] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z109.0055
47 (30) – [M-317] PO^+ m/z 46.9687 (and/or O/S swap rearrangement ion CH_3S^+, m/z 46.9956)

Cf. similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2104963&Mask=200#Mass-Spec

Bromophos-ethyl **$C_{10}H_{12}BrCl_2O_3PS$** **M:392,394,396(0,0,0%)**
Theoretical molecular ion: m/z 391.8805 (100%), 393.8785 (98%), 395.8755 (63%)
N.B. At low resolution the apparent M^+ isotope ratio is 60:100:49.
Average MW: 394.04



m/z	97	359	29	303	357	301	125	242
%	100	50	50	40	40	30	25	25

Organophosphorus insecticide and acaricide (as bromophos).

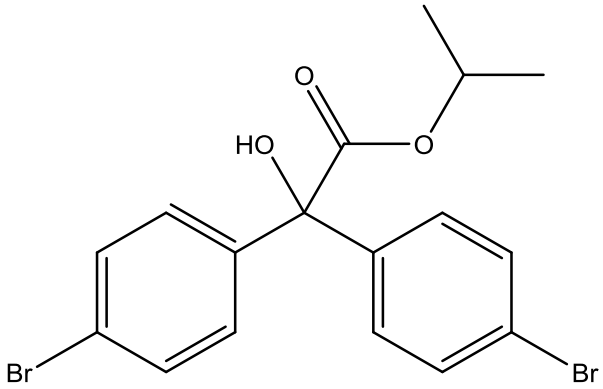
Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

May be oxidised to bromophos-ethyl oxon, $C_{10}H_{12}BrCl_2O_4P$, M^+ 376,378,380.

392,394 (0,0) – M^+ absent
357,359,361 (40,50,15) – [M-35] loss of Cl to $C_{10}H_{12}BrClO_3PS^+$ m/z 356.9111 (100%), 358.9097 (90%) etc.
329,331,333 (10,15,5) – [M-63] loss of Cl & C_2H_4 to $C_8H_8BrClO_3PS^+$ m/z 328.8804 (100%), 330.8783 (98%)
301,303,305 (10,15,5) - [M-91] loss of Cl & $2C_2H_4$ to $C_6H_4BrClO_3PS^+$ m/z 300.8491 (100%), 302.8470 (98%)
240,242,244 (15,25,10) – [M-152] bromodichlorophenol, $C_6H_3BrCl_2O$, m/z 239.8745 (100%), 241,8724 (98%)
125 (25) – [M-67] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (20) –[M-283] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z109.0055
97 (100) – [M-295] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C4824786&Mask=200#Mass-Spec

Bromopropylate **$C_{17}H_{16}Br_2O_3$** **M:426,428,430(0.5,1,0.5%)**
Theoretical molecular ion: m/z 425.9466 (51%), 427.9446 (100%), 429.9425 (49%)
Average MW: 428.12



Bridged diphenyl acaricide (cf. DDT) used to control mites on cotton and fruit and vegetable crops. Non-systemic with contact action and residual activity. No longer approved for use in EU.

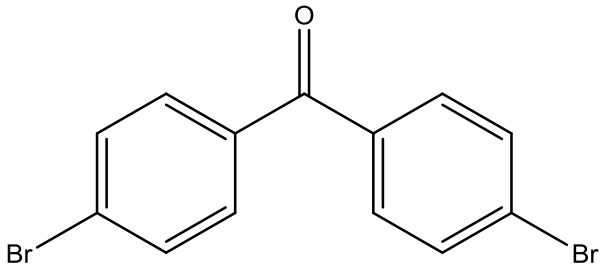
Acute oral LD50 for rat >5,000 mg/kg (Low).

m/z	341	183	185	339	343	155	157	76
%	100	50	50	50	50	15	15	15

426,428,430 (0.5,1,0.5) – M^+
339,341,343 (50,100,50) – [M-87] loss of $CO_2C_3H_7$ to $C_{13}H_{10}Br_2O^+$ m/z 338.9020 (51%), 340.9000 (100%), etc.
183,185 (50,50) – [M-243] $BrC_6H_4CO^+$ m/z 182.9446 (100), 183.9425 (98%)
155,157 (15,15) – [M-271] $BrC_6H_4^+$ m/z 154.9496 (100), 156.9476 (98%)
76 (15) – [M-419] $C_6H_4^+$ m/z 76.0313

Cf. similar but very weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C18181801&Mask=200#Mass-Spec

Bromopropylate related **$C_{14}H_8Br_2O$** **M:338,340,342(20,40,20%)**
4,4'-dibromobenzophenone
Theoretical molecular ion: m/z 337.8942 (51%), 339.8921 (100%), 341.8901 (49%)
Average MW: 340.01



GC degradation product.

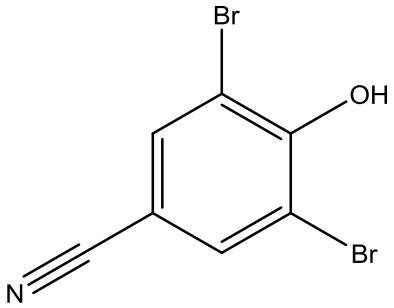
m/z	183	185	76	340	155	157	75	338
%	100	100	40	40	30	30	20	20

338,340,342 (20,40,20) – M^+
183,185 (50,50) – [M-155] $BrC_6H_4CO^+$ m/z 182.9446 (100), 183.9425 (98%)

155,157 (15,15) – [M-183] $BrC_6H_4^+$ m/z 154.9496 (100), 156.9476 (98%)
76 (15) – [M-419] $C_6H_4^+$ m/z 76.0313

No NIST spectrum available.

Bromoxynil **$C_7H_3Br_2NO$** **M:275,277,279(50,100,50%)**
Theoretical molecular ion: m/z 274.8581 (51%), 276.8561 (100%), 278.8541 (49%)
Average MW: 276.92



Nitrile herbicide. Used for post-emergence control of broadleaved weeds in cereals, maize etc.
Acute oral LD50 for rat approx 100 mg/kg (moderately toxic).

Degrades to 3,5-dibromo-4-hydroxybenzoic acid. Poor transmission on GC.

m/z	277	88	275	279	62	168	170	117
%	100	60	50	50	20	20	20	15

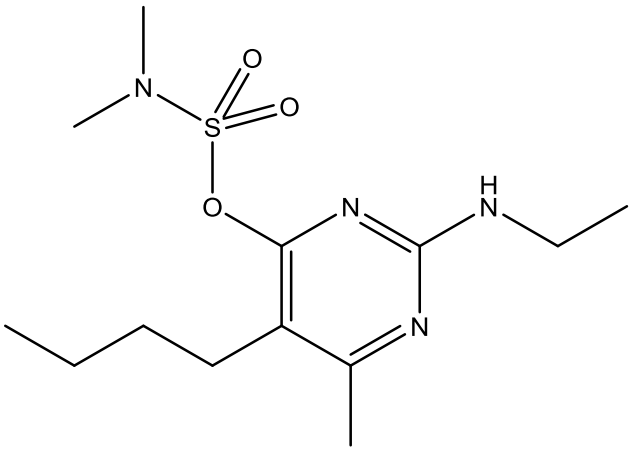
275,277,279 (50,100,50) – M^+
168,170 (20,20) – [M-109] due to loss of H_2COBr, to C_6HOBr^+ m/z 167.9211 (100%), 169.9190 (98%)
88 (60) – [M-187] possibly due to loss of HBr from m/z 168/170, to give the unexpected ion C_6O^+ m/z 87.9949 *
62 (20) – [M-213] $C_5H_2^+$ m/z 62.0157

* The tentative assignment of C_6O^+ is supported by its observation in C J Bennett et al. (2008), *Mechanistic studies on the decomposition of carbon suboxide (C_3O_2) in a cometary ice analog*. Planetary & Space Science, 56, 1181-1189.

Cf. similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1689845&Mask=200#Mass-Spec

Bupirimate **$C_{13}H_{24}N_4O_3S$** **M:316(35%)**

Theoretical molecular ion: m/z 316.1569 (100%), 317.1603 (14%), 318.1527 (4.5%)
Average MW: 316.42



Pyrimidine fungicide with systemic curative and protectant action against powdery mildew.

Acute oral LD50 for rat approx. 4000 mg/kg (low toxicity)

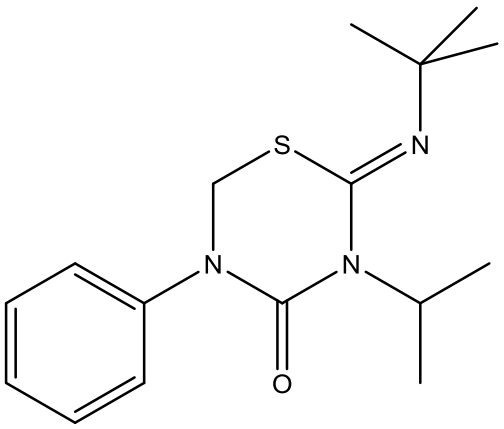
m/z	273	208	166	316	108	96	44	150
%	100	65	35	35	30	25	20	20

316 (35) – M^+
273 (100) – [M-43] loss of C_3H_7 to $C_{10}H_{17}N_4O_3S^+$ m/z 273.1021
208 (65) – [M-108] loss of $SO_2N(CH_3)_2$ to $C_{11}H_{18}N_3O^+$ m/z 208.1450
166 (35) – [M-150] loss of $SO_2N(CH_3)_2$ & C_3H_6 to $C_8H_{12}N_3O^+$ m/z 166.0980
108 (30) – [M-208] $SO_2N(CH_3)_2^+$ $C_2H_6NO_2S^+$ m/z 108.0119
96 (25) – [M-220] $C_6H_8O^+$ m/z 96.0575 and/or $C_5H_8N_2^+$ m/z 96.06875
44 (20) – [M-272] $NHCH_2CH_3^+$ $C_2H_6N^+$ m/z 44.0500

No NIST spectrum available. But cf. Similar spectrum at http://www.restek.com/compound/view/41483-43-6/Bupirimate

Buprofezin **$C_{16}H_{23}N_3OS$** **M:305(20%)**

Theoretical molecular ion: 305.1562 (100%), 306.1595 (17%), 307.1520 (4.5%)
Average MW: 305.44



Thiadiazine insecticide. Chitin biosynthesis/moulting inhibitor, for whitefly control. (Z)-isomer. Approved for use in EU.

Acute oral LD50 for rat >2,000 mg/kg.

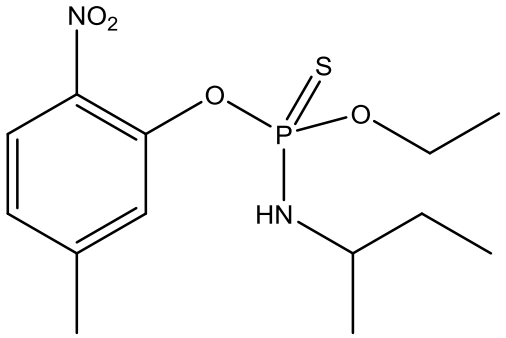
m/z	105	172	57	106	104	77	41	83
%	100	55	50	45	40	40	35	30

305 (20) – M^+
249 (10) – [M-56], loss of butene C_4H_8 to $C_{12}H_{15}N_3OS^+$ m/z 249.0936
190 (20) – [M-115] loss of SCN-$C(CH_3)_3$ to $C_{11}H_{14}N_2O^+$ m/z 190.1106
172 (55) – [M-133] perhaps loss of H_2O from m/z 190 to $C_{11}H_{12}N_2^+$ m/z172.10005
119 (20) – [M-186] $C_6H_5NCO^+$ m/z 119.0371
105 (100) – [M-200] $C_6H_5N{=}CH_2^+$ m/z 105.05785
57 (59) – [M-248] $C_4H_7^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C69327760&Mask=200#Mass-Spec

Butamifos **$C_{13}H_{21}N_2O_4PS$** **M:332(0%)**

Theoretical molecular ion: m/z 332.0960 (100%), 333.0993 (14%), 334.0918 (5%)
Average MW: 332.26



Organophosphorus herbicide, used to control annual and graminaceous weeds in beans, lawns, rice and vegetables. No longer approved for use in EU.

Acute oral LD50 for rat approx. 600 mg/kg (moderate toxicity).

May be oxidised to butamifos oxon, $C_{13}H_{21}N_2O_5P$, MW 316.

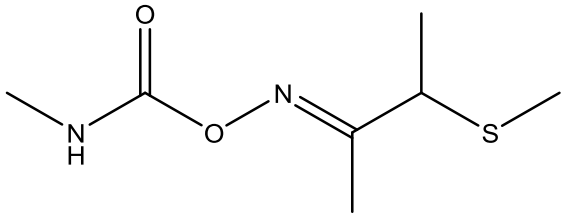
m/z	286	96	200	72	152	232	202	29
%	100	95	90	60	50	50	50	50

332 (0) – M^+ absent
286 (100) – [M-46] loss of NO_2 to $C_{13}H_{21}NO_2PS^+$ m/z 286.1031
260 (5) – [M-72] loss of $NHCH(CH_3)CH_2CH_3$ to $C_9H_{11}NO_4PS^+$ m/z 260.0146
258 (5) – [M-74] loss of NO_2 & C_2H_4 to $C_{11}H_{17}NO_2PS^+$ m/z 258.0718
232 (50) – [M-100] loss of $NHCH(CH_3)CH_2CH_3$+C_2H_4 to $C_7H_7NO_4PS^+$ m/z 231.9833
202 (50) – [M-130] loss of $NHCH(CH_3)CH_2CH_3$+C_2H_4+NO to $C_7H_7O_3PS^+$ m/z 201.9854
200 (90) – [M-132] $C_7H_7NO_4P^+$ m/z 200.0113
152 (5) – [M-180] $CH_3C_6H_3(NO_2)O^+$ $C_7H_6NO_3^+$ m/z 152.0348
96 (95) – [M-236] H_3NOPS^+ m/z 95.9673
72 (60) – [M-260] $NHCH(CH_3)CH_2CH_3^+$, $C_4H_{10}N^+$ m/z 72.08132

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C36335678&Mask=200#Mass-Spec

Butocarboxim **$C_7H_{14}N_2O_2S$** **M:190(0.5%)**

Theoretical molecular ion: m/z 190.07760 (100%), 191.08095 (7.6%), 192.07339 (4.5%)
Average MW: 190.26



Oxime carbamate insecticide and acaricide used to control a range of pests including aphids, thrips and mealybugs. Chemically, butocarboxim is an isomer of aldicarb.

Acute oral LD50 for rat approx. 150 mg/kg.

Rapidly metabolised to butocarboxim sulphoxide (MW 206) and sulphone (MW 222). Often poor GC transmission. May decompose on GC to the oxime described below, by loss of methyl isocyanate (CH_3NCO). This behaviour is unlike that of aldicarb which degrades further (by loss of water) to a nitrile.

m/z	87	41	74	55	44	144	42	75
%	100	75	60	60	55	55	55	50

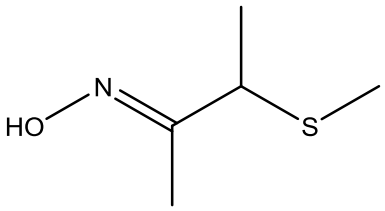
Assignments confirmed by accurate mass (Cardiff GCT)
190 (0.5) – M^+ very weak (not observed on GCT)
144 (55) – [M-46] loss of CH_2S to $C_6H_{12}N_2O_2^+$ m/z 144.0899
115 (5) – [M-75] $C_5H_9NS^+$ m/z 115.0456
100 (5) – [M-90] $C_4H_6NS^+$ m/z 100.0224
87 (100) – [M-103] $HON{=}C(CH_3)CH_2CH_3^+$ $C_4H_9NO^+$ m/z 87.0684
75 (70) – [M-115] $C_3H_7S^+$ m/z 75.0268
74 (75) – [M-116] $C_3H_6S^+$ m/z 74.0190
59 (100) – [M-131] $C_2H_3S^+$ m/z 58.9955
58 (50) – [M-132] $C_2H_2S^+$ m/z 57.9877
45 (15) – [M-145] CHS^+ m/z 44.9799

N.B. The EI mass spectral data reported here for butocarboxim are rather different from the NIST & Restek data, which both report a base peak at m/z 86 (100%) $C_6H_8NO^+$, and a weaker ion at m/z 108 (5%).
See http://webbook.nist.gov/cgi/cbook.cgi?ID=C34681102&Units=CAL&Mask=3F92
and http://www.restek.com/compound/view/34681-10-2/Butocarboxim

Butocarboxim related **$C_5H_{11}NOS$** **M:133(30%)**

3-(methylthio)butan-2-one oxime

Theoretical molecular ion: m/z 133.05613 (100%), 134.05949 (5.4%), 135.05193 (4.5%)
Average MW: 133.21



3-(methylthio)butan-2-one oxime

Oxime degradation product. Poor GC transmission.

m/z	87	57	42	41	55	133	71	75
%	100	75	55	40	35	30	25	25

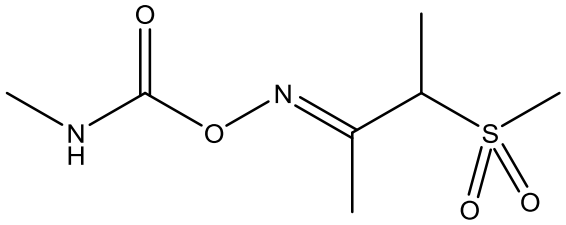
Assignments confirmed by accurate mass (Cardiff GCT)

133 (30) – M^+ $C_5H_{11}NOS^+$ m/z 133.0561
101 (5) – [M-32] loss of CH_3OH to $C_4H_7NS^+$ m/z 101.0299
87 (100) – [M-46] loss of SCH_2 to $C_4H_9NO^+$ m/z 87.0684
75 (90) – [M-58] $C_3H_7S^+$ m/z 75.0268
68 (15) – [M-65] $C_4H_6N^+$ m/z 68.0500
59 (90) – [M-74] $C_2H_3S^+$ m/z 58.9955
57 (75) – [M-76] loss of CH_3CHSCH_3 & H to $C_2H_3NO^+$ m/z 57.0215
55 (30) – [M-78] $C_4H_7^+$ m/z 55.0548
47 (45) – [M-86] CH_3S^+ m/z 46.9955
45 (45) – [M-88] CHS^+ m/z 44.9799

No NIST spectrum available.

Butoxycarboxim **$C_7H_{14}N_2O_4S$** **M:222(0%)**

Theoretical molecular ion: m/z 222.0674 (100%), 223.0708 (7.6%), 224.0632 (4.5%)
Average MW: 222.26



Very susceptible to GC degradation. Poor GC transmission.

m/z	108	80	69	41	65	149	86	134
%	100	70	60	60	35	25	25	20

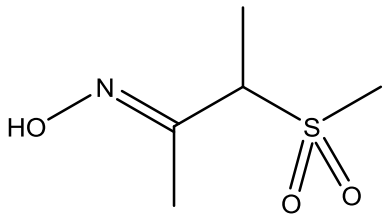
222 (0) – M^+ absent
149 (25) – [M-73] loss of CH_3NCOO to $C_5H_{11}NO_2S^+$ m/z 149.0511
134 (20) – [M-88] loss of CH_3NCOO & CH_3 to $C_4H_8NO_2S^+$ m/z 134.0276
108 (100) – [M-114] $CH_3CH_2SO_2CH_3^+$ = $C_3H_8O_2S$ m/z 108.0245
80 (70) – [M-142] CH_3SO_2H m/z 79.9932

No NIST spectrum available.

Butoxycarboxim related **$C_5H_{11}NO_3S$** **M:165(0%)**

3-(methylsulfonyl)butan-2-one oxime

Theoretical molecular ion: m/z 165.0460 (100%), 166.0493 (5.4%), 167.0418 (4.5%)
Average MW: 165.21



3-(methylsulfonyl)butan-2-one oxime

Oxime GC degradation product. Poor GC transmission.

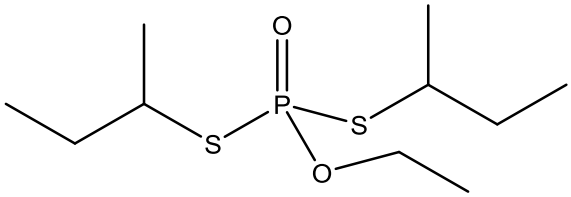
m/z	86	42	28	57	108	27	69	149
%	100	80	60	55	25	25	20	10

165 (0) – M^+ absent
149 (10) – [M-16] due to loss of O to $C_5H_{11}NO_2S^+$, m/z 149.0511(?? due to MS ion source reduction)
108 (25) – [M-57] $H+CH_3CHSO_2CH_3^+ = C_3H_8O_2S^+$ m/z 108.0245
86 (100) – [M-79] loss of SO_2CH_3 to $HON=CH(CH_3)CHCH_3^+$ or $C_4H_8NO^+$ m/z 86.0606

No NIST spectrum available. But see http://webbook.nist.gov/cgi/cbook.cgi?ID=C14357449&Units=SI&Mask=200#Mass-Spec for spectrum of isomer ($HO-N=CH.(CH_3)_2C.SO_2CH3$) - which exhibits m/z 86 (100%), 41 (80%), 28 (35%) and no ions above m/z 88 – and which bears several similar features.

Cadusafos **$C_{10}H_{23}O_2PS_2$** **M:270(15%)**

Theoretical molecular ion: m/z 270.0877 (100%)
Average MW: 270.39



Organophosphorus insecticide and nematicide. Broad spectrum activity. Two chiral centres.

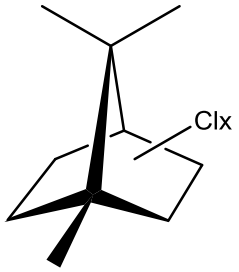
Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

m/z	159	158	97	88	57	127	125	213
%	100	80	50	40	40	35	30	20

270 (15) – M^+ $C_{10}H_{23}O_2PS_2^+$
213 (20) – [M-57] loss of $CH_3CH_2CH(CH_3)$ to $C_6H_{14}O_2PS_2^+$ m/z 213.0173
159 (100) – [M-111] loss of C_4H_8 & C_4H_7 to $(CH_3CH_2O)(HS)_2POH^+$ $C_2H_8O_2PS_2^+$ m/z 158.97033
158 (80) – [[M-112] loss of $2C_4H_8$ to $(CH_3CH_2O)(HS)_2PO^+$ $C_2H_7O_2PS_2^+$ m/z 157.9698
97 (50) – [M-173] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
88 (20) – [M-182] $C_4H_8S^+$ m/z 88.0347

Data from NIST spectrum: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95465999&Mask=200#Mass-Spec

Camphechlor (Toxaphene) **$C_{10}H_{10}Cl_8$ (etc.)** **Approx. MW 413.8**
Complex mixture (>500 components)
Average MW: 413.8



Main campheclor components - chlorobornanes

Obsolete, persistent, bioaccumulative and toxic organochlorine insecticide which comprises a complex mixture of polychlorinated camphenes, predominantly chlorobornanes (see Kimmel 2013). Over 1 million tons were produced.

Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

The most common production process is based on direct chlorination of crude camphene (camphene, α-terpinol and bornene etc.) until a chlorine content of 67 – 69 % is reached. The resulting mixture comprises 76% chlorinated bornanes, 18% chlorinated bornenes, 2% chlorinated bornadienes etc. According to the European Food Safety Authority (EFSA), camphechlor congeners CHB 26, 50 and 62, which accumulate in the food chain, can serve as indicators of camphechlor contamination.

Toxaphene is one of the “dirty dozen” organochlorine compounds/classes outlawed or restricted under the UN Stockholm Convention on Persistent Organic Pollutants, 2001. The others were aldrin, dieldrin, endrin, heptachlor, hexachlorobenzene, mirex, polychlorinated biphenyls (PCBs), DDT, polychlorinated dibenzo-p-dioxins ("dioxins") and polychlorinated dibenzofurans. Several other organohalogen compounds have since been added (e.g. isomers of HCH, chlordecone, endosulfan etc.). Camphechlor was banned in the US in 1990 and the EU in 1984.

Very unhelpful EI mass spectra for the trace analyst (Saleh 1983). Most congeners produce a large number of fragments, each of which is spread over its broad poly-chlorine isotope fingerprint, e.g.

m/z 243, 245, 247..
m/z 257, 259, 261..
m/z 269, 271, 273…
m/z 305, 307, 309..
m/z 327, 329, 331, 333 ..
m/z 377, 379, 381 …
m/z 441, 343, 345, 347, 349..

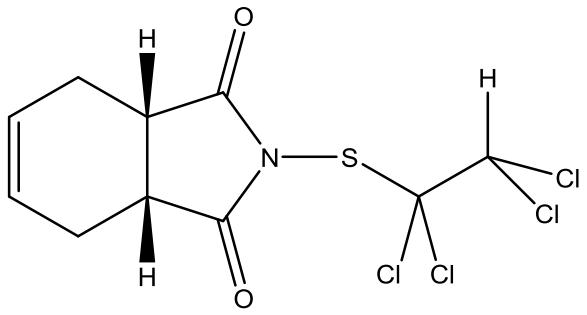
No NIST mass spectrum for “toxaphene” (and associated NIST WebBook entry has incorrect empirical formula: “C10H22Cl8 mw 425.906”). There are ten entries for C10H10Cl8, all octachloro-bornane isomers with GC data, but no MS data.

(see *Mass Spectrometry of Priority Pollutants*, Plenum Press, 1981, B S Middleditch et al., which gives the mass spectra of 5 toxaphene components.)

Sensitive trace determination of camphechlor residues requires extensive sample extract clean-up, followed by high resolution capillary GC and negative ion chemical ionisation MS. See US EPA recommendations in ***Method 8276 (Rev 1. Sept 2012)***. *Toxaphene and Toxaphene Congeners by Gas Chromatography/Negative Ion Chemical Ionization Mass Spectrometry (GC-NICI/MS),* www.epa.gov/osw/hazard/testmethods/pdfs/8276.pdf

Captafol **$C_{10}H_9Cl_4NO_2S$** **M:347,349,351(2,3,1%)**

Theoretical molecular ion: m/z 346.9108 (78%), 348.9079 (100%), 350.9049 (48%), 352.9020 (10%)
Average MW: 349.05



Phthalimide fungicide with broad spectrum action. Not approved for use in the EU. A suspect carcinogen and irritant, it has been banned under the Rotterdam Convention.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

Susceptible to GC degradation to 1,2,3,6-tetrahydrophthalimide. Transmission often best with OV-210 and other fluorosilicones.

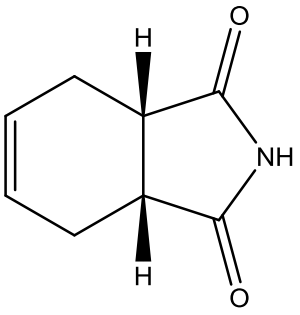
m/z	79	80	78	77	107	183	149	150
%	100	35	15	15	10	10	10	10

347,349,351 (2,3,1) – M^+
311,312,313,314,315,316 (4,3,5,4,3,2) – [M-36/35] loss of HCl/Cl to $C_{10}H_9Cl_3NO_2S^+$ m/z 311.9420 etc.
264,266 (3,2) – [M-83] loss of $CHCl_2$ to $C_9H_8Cl_2NO_2S^+$ m/z 263.9653 etc.
183 (10) – [M-164] loss of CCl_2CHCl_2 to $C_8H_9NO_2S^+$ m/z 183.0354
149 (10) – [M-198] $C_8H_7NO_2^+$ m/z 149.0477
79 (100) – [M-268] $C_6H_7^+$ m/z 79.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2425061&Mask=200#Mass-Spec

Captafol/captan related **$C_8H_9NO_2$** **M:151(85%)**
1,2,3,6-tetrahydrophthalimide

Theoretical molecular ion: m/z 151.0633 (100%), 152.0667 (9%)
Average MW: 151.17



1,2,3,6-tetrahydrophthalimide

Captafol and captan may decompose to 1,2,3,6-tetrahydrophthalimide:

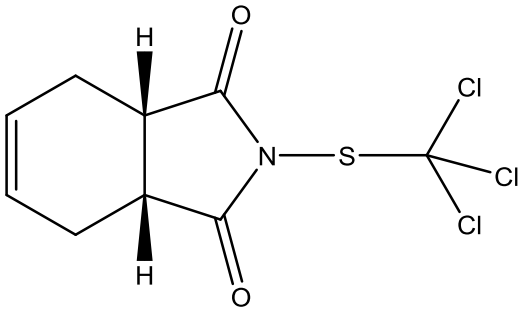
m/z	79	151	80	77	123	39	78	122
%	100	85	65	20	20	20	20	15

151 (85) – M^+
123 (20) – [M-28] loss of CO to $C_7H_9NO^+$ m/z 123.0684
79 (100) – [M-72] $C_6H_7^+$ m/z 79.0548

Cf. similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C85405&Units=SI&Mask=200#Mass-Spec

Captan **$C_9H_8Cl_3NO_2S$** **M:299,301,303(2,2,1%)**

Theoretical molecular ion: m/z 298.9341 (100%), 300.9312 (96%), 302.9282 (31%)
Average MW: 300.58



Phthalimide/dicarboximide fungicide. Widely used on edible and ornamental horticultural crops. Approved for use in EU.

Acute oral LD50 for rat >2,000 mg/kg (moderate toxicity).

Susceptible to GC degradation (transmission often best with OV-210 and other fluorosilicones). Captan may decompose on GC to 1,2,3,6-tetrahydrophthalimide (see "Captafol/captan related" entry).

Higher resolution (5,000), accurate mass SIR may be used to detect low residue levels in food extract using GC-MS, by monitoring $CSCl^+$ at m/z 78.941 (note "m/z 79" is mainly due to $C_6H_7^+$, m/z 79.055).

m/z	79	149	80	77	117	119	107	78
%	100	40	30	25	25	25	25	20

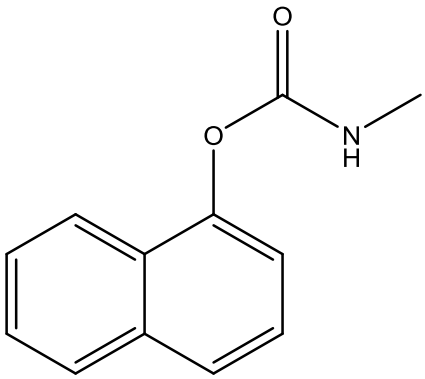
299,301,303 (2,2,1) – M^+

264,266 (10,5) – [M-35] loss of Cl to $C_9H_8Cl_2NO_2S^+$ m/z 263.9653 etc.
263, 265 (5,3) – [M-36] loss of HCl to $C_9H_7Cl_2NO_2S^+$ m/z 262.9575 etc.
182 (5) – [M-117] loss of CCl_3 to $C_8H_8NO_2S^+$ m/z 182.0276
149 (40) – [M-150] loss of HSCCl3 to $C_8H_7NO_2^+$ m/z 149.0477
79 (100) – [M-220] mixture of $C_6H_7^+$ m/z79.0548 and $CSCl^+$ m/z 78.9409 (confirmed by high resolution MS)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C133062&Mask=200

Carbaryl / Sevin **$C_{12}H_{11}NO_2$** **M:201(5%)**

Theoretical molecular ion: m/z 201.0790 (100%), 202.0823 (13%)
Average MW: 201.23



Carbamate insecticide and acaricide (also growth inhibitor plant growth regulator).
Used on maize, soya, cotton, fruit and vegetable crops. No longer approved for use in EU.

Acute oral LD50 for rat is approx. 500 mg/kg.

Susceptible to GC degradation to **1-naphthol**.

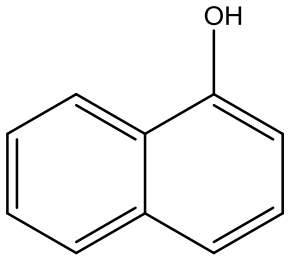
m/z	144	115	116	145	201	89	127	63
%	100	40	25	10	5	5	5	5

201 (5) – M^+
144 (100) – [M-57] loss of methyl isocyanate to naphthol, $C_{10}H_8O^+$ m/z 144.0575
127 (5) – [M-74] $C_{10}H_7^+$ m/z 127.0548
115 (40) – [M-86] loss of CHO from m/z 144 to $C_9H_7^+$ m/z 115.0548
89 (5) – [M-112] $C_7H_5^+$ m/z 89.0391

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C63252&Mask=200#Mass-Spec

Carbaryl related **$C_{10}H_8O$** **M:144(100%)**
1-naphthol

Theoretical molecular ion: m/z 144.0575 (100%)
Average MW: 144.17



1-naphthol

Carbaryl may decompose to 1-naphthol

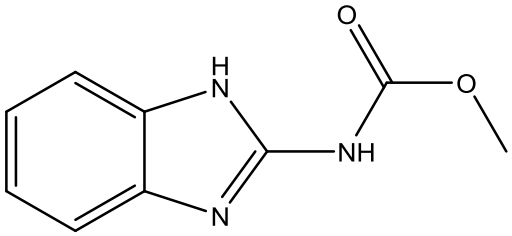
m/z	144	115	116	89	72	145	63	58
%	100	65	40	10	10	10	10	10

144 (100) – M^+
127 (5) – [M-17] $C_{10}H_7^+$ m/z 127.0548
115 (40) – [M-29] loss of CHO from m/z 144 to $C_9H_7^+$ m/z 115.0548
89 (5) – [M-58] $C_7H_5^+$ m/z 89.0391

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C90153&Units=SI&Mask=200#Mass-Spec although the minor ion at m/z 127 is weaker, at 1%.

Carbendazim **$C_9H_9N_3O_2$** **M:191(20%)**

Theoretical molecular ion: 191.0695 (100%), 192.0728 (10%)
Average MW: 191.19



Broad spectrum benzimidazole fungicide. Carbendazim is also a metabolite of **benomyl**. Widely used on arable crops, fruit and vegetables, and ornamentals. Post-harvest treatment agent. Approved for use in EU.

Acute oral LD50 for rat is > 15,000 mg/kg.

Carbendazim is not amenable to GC, but may be determined by LC-MS.

m/z	159	104	191	131	31	160	77	105
%	100	25	20	15	15	15	10	10

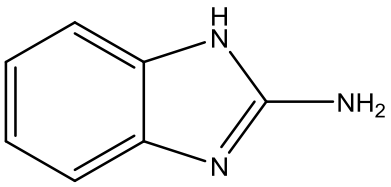
191 (20) – M+
159 (100) – [M-32] loss of CH_3OH to $C_8H_5N_3O^+$ m/z 159.0433
131 (15) – [M-60] loss of CH_3OH & C=O to $C_7H_5N_3^+$ m/z 131.0484
104 (25) – [M-87] loss of CH_3OH & C=O & HCN to $C_6H_4N_2^+$ m/z 104.0375

No NIST spectrum available.

Carbendazim related **$C_7H_7N_3$** **M:133(100%)**

2-aminobenzimidazole

Theoretical molecular ion: m/z 133.0640 (100%), 134.0674 (8%)
Average MW: 133.15



2-aminobenzimidazole

Carbendazim decomposes to 2-aminobenzimidazole on GC analysis. For efficient conversion, the injector must be hot (300°C) and contain a dense plug of glass wool (to increase analyte residence time). Sometimes poor GC transmission/peak shape is observed for the 2-aminobenzimidazole product.

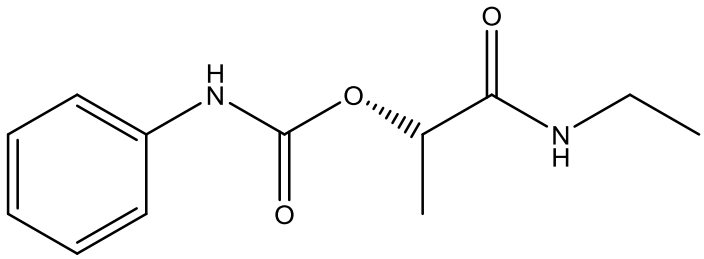
m/z	133	134	105	106	79	132	78	90
%	100	20	20	15	10	5	5	5

133 (100) – M^+
105 (20) – [M-28] loss of H_2CN to $C_6H_5N_2^+$ m/z 105.0453

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C934327&Units=SI&Mask=200#Mass-Spec
Listed under "1H-benzimidazol-2-amine"

Carbetamide **$C_{12}H_{16}N_2O_3$** **M:236(5%)**

Theoretical molecular ion: m/z 236.1161 (100%), 237.1195 (13%)
Average MW: 236.27



Carbanilate herbicide, used pre- and post-emergence on a range of field crops to control annual grasses and some broadleaved weeds. Sold as (R)-isomer (illustrated).

Moderate toxicity to mammals. Acute oral toxicity for rat is approx. 2,000 mg/kg.

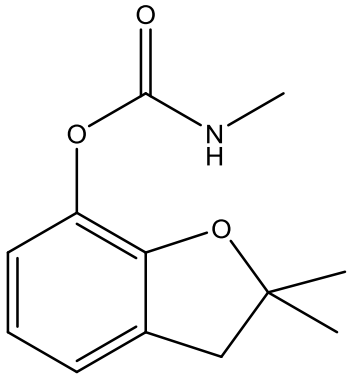
m/z	119	44	45	29	72	91	73	120
%	100	35	35	30	25	25	25	20

236 (5) – M^+
119 (100) – [M-117] C_6H_5NCO, phenyl isocyanate, $C_7H_5NO^+$ m/z 119.0371
72 (25) – [M-164] $CH_3CH_2NHCO^+$, $C_3H_6NO^+$ m/z 72.0449
44 (35) – [M-192] $CH_3CH_2NH^+$ $C_2H_6N^+$ m/z 44.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C16118493&Mask=200

Carbofuran **$C_{12}H_{15}NO_3$** **M:221(10%)**

Theoretical molecular ion: m/z 221.1052 (100%), 222.1086 (13%)
Average MW: 221.26



Very toxic carbamate insecticide. Broad spectrum activity against insects, mites, and nematodes on contact or after ingestion. It is used against soil and foliar pests of field, fruit, vegetable, and forest crops. Banned in EU and Canada.

Acute oral LD50 for rat is approx. 10 mg/kg. Sometimes poor GC transmission.

m/z	164	149	122	123	221	165	131	91
%	100	45	10	10	10	10	10	5

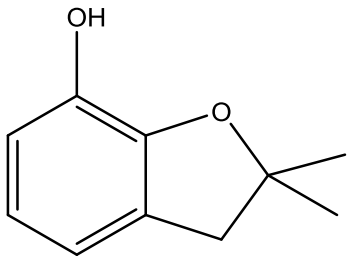
221 (10) – M^+
164 (100) – [M-57] due to loss of methyl isocyanate CH_3NCO to $C_{10}H_{12}O_2^+$ m/z 164.0837
149 (45) - [M-72] $C_9H_9O_2^+$ m/z 149.0603

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1563662&Mask=200#Mass-Spec

Carbofuran related **$C_{10}H_{12}O_2$** **M:164(100%)**

2,2-dimethyl-2,3-dihydro-benzofuranol

Theoretical molecular ion: m/z 164.0837 (100%), 165.0871 (11%)
Average MW: 164.20



2,2-dimethyl-2,3-dihydro-benzofuranol

Degradation product sometimes observed on GC (due to loss of methyl isocyanate).

m/z	164	149	131	103	122	77	123	121
%	100	80	40	40	40	35	35	35

164 (100) – M^+
149 (45) - [M-15] $C_9H_9O_2^+$ m/z 149.0603

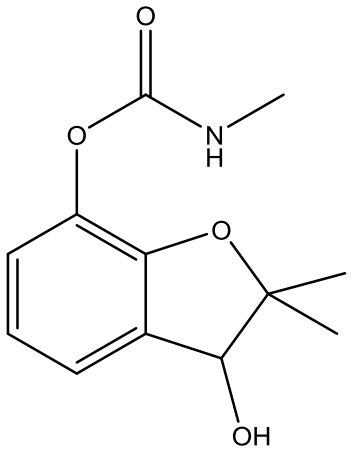
122 (40) – [M-42] loss of C_3H_6 to $C_7H_6O_2^+$ m/z 122.03678

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1563388&Mask=200#Mass-Spec
listed under "7-Benzofuranol, 2,3-dihydro-2,2-dimethyl-"

Carbofuran related **$C_{12}H_{15}NO_4$** **M:237(2%)**

3-hydroxy-carbofuran

Theoretical molecular ion: 237.1001 (100%)
Average MW: 237.25



3-hydroxy-carbofuran

An oxidative metabolite of carbofuran included in carbofuran MRLs. Poor GC transmission..

m/z	137	180	147	151	162	57	161	39
%	100	45	25	20	20	15	10	10

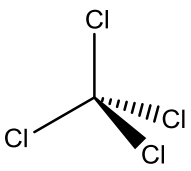
237 (2) – M^+
180 (100) – [M-57] due to loss of methyl isocyanate CH_3NCO to $C_{10}H_{12}O_3^+$ m/z 180.07865
137 (100) – [M-100] $C_7H_5O_3^+$ m/z 137.0239 *

* m/z 137 has been proposed as characteristic fragment of oxidised degradation products at C3 position of carbofuran (Jongki Hong 1999).

** See also (noisy, weak) spectrum of 3-furanone oxidative analogue at
http://webbook.nist.gov/cgi/cbook.cgi?ID=C17781167&Units=SI&Mask=200#Mass-Spec
with main ions at m/z 137, 110, 135, 178.

Carbon tetrachloride **CCl_4** **M:152,154,156(0,0,0%)**

Theoretical molecular ion: m/z 151.8754 (78%), 153.8725 (100%), 155.8695 (47.9%)
Average MW: 153.81



Fumigant insecticide for use in stored grain. Banned in US in 1970.

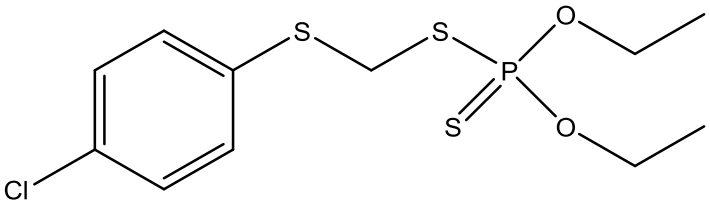
Acute oral rat LD50 approx. 2,000 mg/kg (moderate toxicity).

m/z	117	119	121	82	47	84	35	49
%	100	95	35	30	25	20	15	10

152,154 (0,0) – M^+ absent
117,119,121 (100,95,45) – [M-35] CCl_3^+ m/z 116.9066 etc.
82,84 (30,20) – [M-70] CCl_2^+ m/z 81.9377

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C56235&Mask=200#Mass-Spec

Carbophenothion / Trithion **$C_{11}H_{16}ClO_2PS_3$** **M:342,344(45,15%)**
Theoretical molecular ion: m/z 341.9739 (100%), 343.97091 (32%)
Average MW: 342.85



Organophosphorus insecticide. Used on citrus fruits and cotton to control aphids and spider mites. Now restricted due to toxicity concerns. No longer approved for use in EU.

Acute oral LD50 for rat approx. 10 mg/kg (high toxicity).

Cf. dimethyl homologue. See **Methyl Trithion**

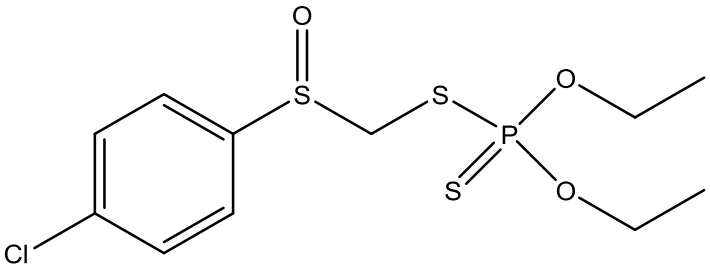
Carbophenothion contains a P=S and a thioether group, both of which may be oxidised: P=S to P=O (oxon); and thioether to sulphoxide and sulphone (see below).
KI (SE-30) = 22.2

m/z	157	121	153	342	159	199	125	97
%	100	50	45	45	40	40	40	40

342,344 (45,15) – M^+
296,298 (5,2) – [M-46] loss of CH_3CH_2OH to $C_9H_{10}ClOPS_3^+$ m/z 295.9320 etc.
199 (40) – [M-143] $(CH_3CH_2O)_2PS.SCH_2^+$ $C_5H_{12}O_2PS_2^+$ m/z 199.0026
157,159 (100,40) – [M-185] $ClC_6H_4SCH_2^+$ $C_7H_6ClS^+$ m/z 156.9879 etc.
153 (20) – [M-189] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
121 (50) – [M-221] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C786196&Mask=200 though relative abundances are different, and low abundance ions (<2-5%) at high mass (> m/z 200) are absent.

Carbophenothion sulphoxide **$C_{11}H_{16}ClO_3PS_3$** **M:358(0%)**
Theoretical molecular ion: 357.9688 (100%), 359.9658 (32%)
Average MW: 358.85



Carbophenothion oxidative metabolite. KI (SE-30) = 24.5

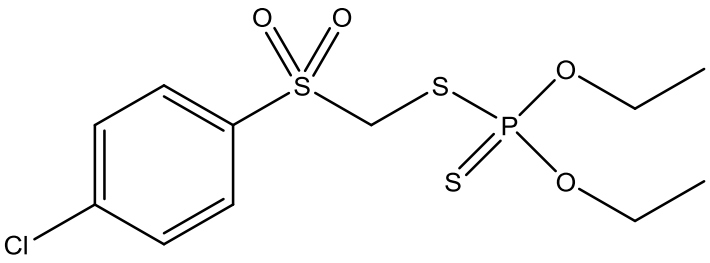
m/z	97	153	199	125	109	171	65	45
%	100	80	70	70	30	20	20	20

358 (0) – M^+ absent
342,344 (3,1) – [M-16] loss of O (due to reduction in ion source?) to m/z 341.9739 etc.
199 (100) – [M-159] $(CH_3CH_2O)_2PS.SCH_2^+$ $C_5H_{12}O_2PS_2^+$ m/z 199.0026
171 (20) – [M-187] $(CH_3CH_2O)(HO)PS.SCH_2^+$ $C_3H_8O_2PS_2^+$ m/z 170.9703
153 (80) – [M-205] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
143 (15) – [M-215] $(HO)_2PS.SCH_2^+$ $CH_4O_2PS_2^+$ m/z 142.9390
125 (70) – [M-233] $(CH_3CH_2O)(HO)PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (100) – [M-261] $(HO)_2PS^+$ $C_2H_6O_2PS^+$ m/z 96.9513
65 (20) – [M-293] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
45 (20) – [M-313] $CH_3CH_2O^+$ $C_2H_5O^+$ m/z 45.0340

N.B. No significant ions confirming presence of the sulphoxide group (e.g. $ClC_6H_4SO^+$ at m/z 158.9671 or $ClC_6H_4SOCH_2^+$ at 172.9828)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C17297404&Mask=200

Carbophenothion sulphone **$C_{11}H_{16}ClO_4PS_3$** **M:374,376(3,1%)**
Theoretical molecular ion:
Average MW:



Carbophenothion oxidative metabolite

KI (SE-30) = 24.5

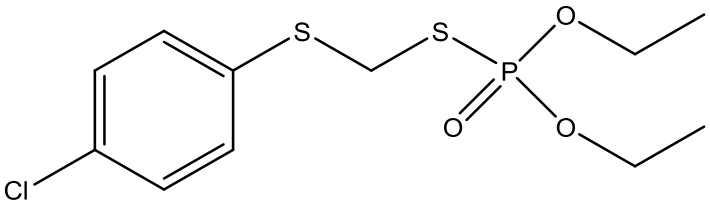
m/z	153	97	199	125	159	65	171	45
%	100	80	70	70	25	25	15	15

374,376 (3,1)) – M^+ absent
215 (5) – [M-159] rearrangement and loss of SOC_6H_4Cl to $(CH_3CH_2O)_2PS.SCH_2O^+$ $C_5H_{12}O_3PS_2^+$ m/z 214.9966
199 (70) – [M-175] $(CH_3CH_2O)_2PS.SCH_2^+$ $C_5H_{12}O_2PS_2^+$ m/z 199.0026
175,177 (10,5) – [M-199] due to $^+SO_2C_6H_4Cl$ m/z 174.9621 etc.

159,161 (25,10) – [M-215] due to $ClC_6H_4SO^+$ $C_6H_4ClOS^+$ m/z 158.9671 etc. (rearrangement)
153 (80) – [M-221] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (70) – [M-249] $(CH_3CH_2O)(HO)PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (100) – [M-277] $(HO)_2PS^+$ $C_2H_6O_2PS^+$ m/z 96.9513

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C16662854&Mask=200#Mass-Spec

Carbophenothion oxon **$C_{11}H_{16}ClO_3PS_2$** **M:326,328(55,23%)**
"Carbophenoxon"
Theoretical molecular ion: 325.9967 (100%), 327.99375 (32%)
Average MW: 326.79



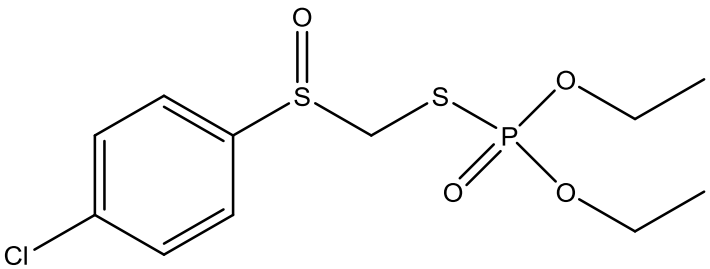
Carbophenothion oxidative metabolite

m/z	183	109	326	139	157	111	155	75
%	100	95	55	53	44	44	42	40

326,328 (55,23) – M^+
183 (100) – [M-143] loss of ClC_6H_4SO to $(CH_3CH_2O)_2P{=}O.SCH_2^+$ $C_5H_{12}O_3PS^+$ m/z 183.0245
157,159 (44,10) – [M-185] $ClC_6H_4SCH_2^+$ $C_7H_6ClS^+$ m/z 156.9879 etc.
155 (42) – [M-171] $(CH_3CH_2O)(HO)P{=}O.SCH_2^+$ $C_3H_8O_3PS^+$ m/z 154.9932
139 (53) - [M-187] $(CH_3CH_2O)(HO)P.SCH_2^+$ $C_3H_8OPS^+$ m/z 138.9983
137 (25) – [M-189] $(CH_3CH_2O)_2P{=}O^+$ $C_4H_{10}O_3P^+$ m/z 137.0368
111 (44) - [M-215] $(HO)_2P.SCH_2^+$ CH_4OPS^+ m/z 110.9670
109 (95) - [M-217] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
81 (30) – [M-245] $(HO)_2P{=}O^+$ $H_2O_3P^+$ m/z 80.9742
75 (30) – [M-251] $C_6H_3^+$ m/z 75.0235

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C7173844&Mask=200

Carbophenothion oxon sulphoxide **$C_{11}H_{16}ClO_4PS_2$** **M:342,344(0,0%)**
Theoretical molecular ion: 341.9916 (100%), 343.9887 (32%)
Average MW: 342.79



Carbophenothion oxidative metabolite

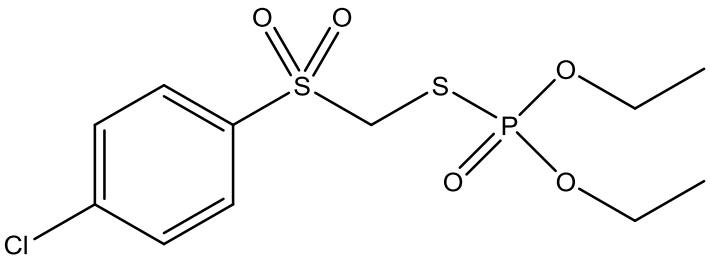
m/z	109	183	139	81	137	75	155	127
%	100	61	32	31	29	27	21	15

342,344 (0,0) – M^+ absent
183 (61) – [M-159] $(CH_3CH_2O)_2P{=}O.SCH_2^+$ $C_5H_{12}O_3PS^+$ m/z 183.0245
155 (21) – [M-187] $(CH_3CH_2O)(HO)P{=}O.SCH_2^+$ $C_3H_8O_3PS^+$ m/z 154.9932
139 (32) – [M-203] $(CH_3CH_2O)(HO)P.SCH_2^+$ $C_3H_8OPS^+$ m/z 138.9983
137 (29) – [M-205] $(CH_3CH_2O)_2P{=}O^+$ $C_4H_{10}O_3P^+$ m/z 137.0368
127 (15) – [M-15] $(HO)_2P{=}O.SCH_2^+$ $CH_4O_3PS^+$ m/z 126.9619
109 (100) – [M-233] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
81 (30) – [M-261] $(HO)_2P{=}O^+$ $H_2O_3P^+$ m/z 80.9742
75 (30) – [M-267] $C_6H_3^+$ m/z 75.0235

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C16662865&Units=SI&Mask=200#Mass-Spec listed as "Carbophenoxon sulfoxide", which exhibits m/z 343 (2%) due to $(M+H)^+$ (auto-CI?), and m/z 326 from in source reduction, or contamination with sulphide.

Carbophenothion oxon sulphone $C_{11}H_{16}ClO_5PS_2$ M:358,356(0,0%)

Theoretical molecular ion: 357.9865 (100%), 359.9836 (32%)
Average MW: 358.79



Carbophenothion oxidative metabolite

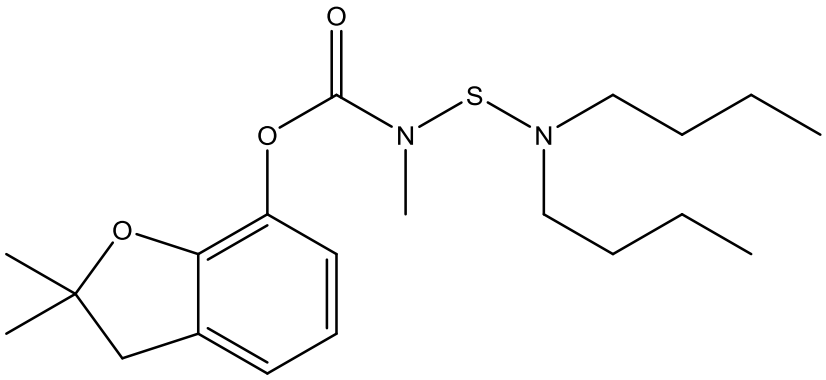
m/z	183	109	139	137	75	155	127	184
%	100	45	30	23	19	18	9	7

358,360 (0,0) – M^+
183 (100) [M-175] $(CH_3CH_2O)_2P{=}O.SCH_2^+$ $C_5H_{12}O_3PS^+$ m/z 183.0245
155 (18) – [M-203] $(CH_3CH_2O)(HO)P{=}O.SCH_2^+$ $C_3H_8O_3PS^+$ m/z 154.9932
139 (30) – [M-219] $(CH_3CH_2O)(HO)P.SCH_2^+$ $C_3H_8OPS^+$ m/z 138.9983
137 (23) – [M-221] $(CH_3CH_2O)_2P{=}O^+$ $C_4H_{10}O_3P^+$ m/z 137.0368
127 (9) – [M-231] $(HO)_2P{=}O.SCH_2^+$ $CH_4O_3PS^+$ m/z 126.9619
109 (45) – [M-249] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
75 (19) – [M-283] $C_6H_3^+$ m/z 75.0235

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C16662876&Units=SI&Mask=200#Mass-Spec listed as "Carbophenoxon sulfone", which exhibits weak m/z 359 (0.3%) due to (M+H)+ (auto-CI).

Carbosulfan **$C_{20}H_{32}N_2O_3S$** **M:380(1%)**

Theoretical molecular ion: m/z 380.2134 (100%), 381.2167 (22%), 382.2092 (4.5%)
Average MW: 380.55



Carbamate insecticide. Used for control of soil dwelling and foliar pests. No longer approved for use in EU (withdrawn in 2007).

Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

Rapidly metabolised to **carbofuran**.

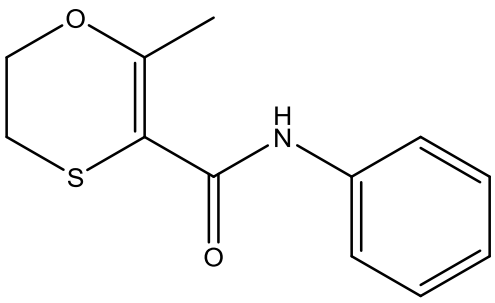
m/z	160	118	163	164	57	84	135	149
%	100	95	50	50	30	20	20	20

380 (1) – M^+
323 (10) – [M-57] loss of $C_4H_9^+$ to $C_{16}H_{23}N_2O_2S^+$ m/z 323.1429
163 (50) – [M-217] loss of $CON(CH_3)SN(C_4H_9)_2$ to $C_{10}H_{11}O_2^+$ m/z 163.0759
160 (100) – [M-220] $SN(C_4H_9)_2^+$, $C_8H_{18}NS^+$ m/z 160.1160
135 (20) – [M-245] $C_9H_{11}O^+$ m/z 135.0910
118 (95) – [M-262] $HSN(C_4H_9)(CH_2)^+$ $C_5H_{12}NS^+$ m/z 118.06905
57 (30) – [M-323] $C_4H_9^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C55285148&Mask=200

Carboxin **$C_{12}H_{13}NO_2S$** **M:235(40%)**

Theoretical molecular ion: m/z m/z: 235.0667 (100%), 236.07005 (13%), 237.0625 (4.5%)
Average MW: 235.30



Anilide (oxathiin) systemic fungicide. Used to control for bunts and smuts, normally as a seed treatment. Inhibits mitochondrial function. Approved for use in EU.

Acute oral LD50 for rat approx 2,500 mg/kg (low toxicity).

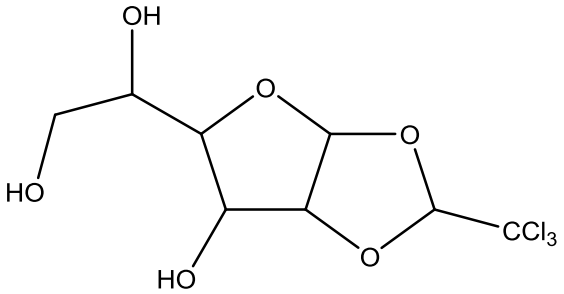
Carboxin sulphoxide and sulphone are its oxidative metabolites.

m/z	143	43	87	235	77	115	91	132
%	100	55	50	40	10	10	10	5

235 (40) – M^+
143 (100) – [M-92] loss of NHC_6H_5 to $C_6H_7O_2S^+$ m/z 143.0167
115 (10) – [M-120] $C_5H_7OS^+$ m/z 115.0218
87 (50) – [M-148] $C_3H_3OS^+$ m/z 86.9905
43 (55) – [M-192] $NHCO^+$ m/z 43.0058

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C5234684&Mask=200

Chloralose / α-chloralose **$C_8H_{11}Cl_3O_6$** **308,310,312 (0,0,0%)**
Theoretical molecular ion: m/z 307.9621 (100%), 309.9592 (96%), 311.9562 (31%)
Average MW: 309.52



Avicide, bird repellent and rodenticide. Not approved for use in the EU. Sometimes used illegally to poison wildlife.

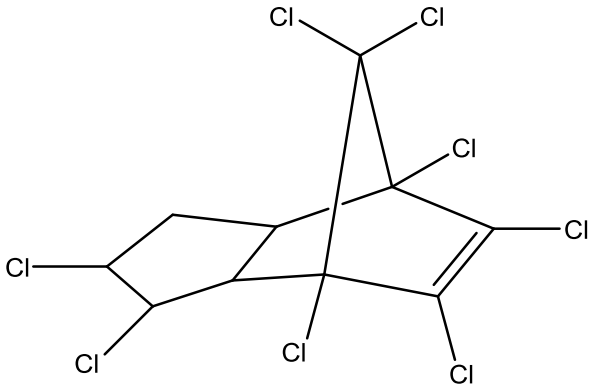
Acute oral LD50 for rat approx 400 mg/kg (moderate toxicity).

Two main isomers present: alpha and beta.
Not directly amenable to GC analysis, but may be analysed following
- trimethylsilylation (Odam 1984)
- acetylation (Savin 2003) or
- hydrolysis and detection of liberated chloral, CCl_3CHO (Kintz 1999)

Chloralose may be sensitively detected directly using LC-negative electrospray MS, by monitoring its characteristic $(M-H)^-$ ions at m/z 308, 309, 310 and their transitions to m/z 161 and 189 (Hunter 2004).

No NIST MS spectrum available.

Chlordane $C_{10}H_6Cl_8$ **M:406,408,410,412(2,4,5,2%)**
Theoretical molecular ion: m/z 405.7978 (45%), 407.7948 (57%), 409.7919 (100%), 411.7889 (76%), 413.7860 (24%)
Average MW: 409.76



Obsolete, banned organochlorine insecticide. Approx 70,000 tonnes produced since 1946, of which an estimated 25-50% still exists in the environment (Dearth 1991).

Acute oral LD50 for rat approx 500 mg/kg (moderate toxicity).

Technical chlordane is a complex mixture. Nominally "octachloro-dicyclopentadiene", manufactured by chlorination of the Diels-Alder reaction product of hexachloro-cyclopentadiene and cyclopentadiene.

Chlordane was commercially introduced as a non-systemic, contact and ingested insecticide in 1947. Technical chlordane is a mixture, which consists of at least 147 compounds and the composition varies with the manufacturing process. It contained 43-75 % cis- and trans - chlordane and lesser amounts of heptachlor, cis- and trans-nonachlor and chlordenes. After 1970, a more refined formulation containing >95 % of cis- and trans-chlordane was also produced. Chlordane was used for agricultural purposes, mainly for soil and seed treatment and wood protection, the latter being applied mostly in the USA. It has been banned for use in the European Union since 1981 and most other countries worldwide.
See http://www.atsdr.cdc.gov/toxprofiles/tp31.pdf#page=23&zoom=auto,-73,769

The two major components are (ca. 70%) endo-cis-/alpha- chlordane and (ca. 25%) endo-trans-/gamma- chlordane, which have similar mass spectra:
KI (SE-30) = 21.0 (alpha), 20.5 (gamma).

See also **oxychlordane**, an oxidative metabolite of chlordane.

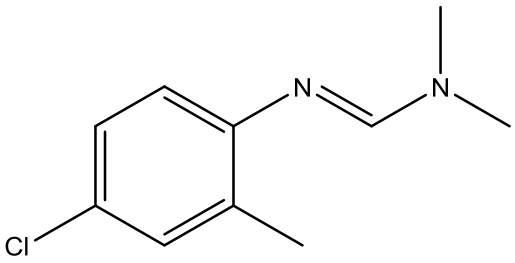
m/z	373	375	377	371	237	272	100	379
%	100	95	50	45	25	20	20	20

406,408,410,412 (2,5,5,2) – M^+
371,373,375,377 (45,100,95,50) – [M-35/36] loss of Cl to $C_{10}H_6Cl_7^+$ m/z 370.8289 etc.
270,272,274 (15,20,15) – [M-136] loss of $C_5H_6Cl_2$ to $C_5Cl_6^+$ m/z 269.8131 etc.
235,237,239 (15,25,15) – [M-171] loss of $C_5H_6Cl_3$ to $C_5Cl_5^+$ m/z 234.8443 etc.

Cf. similar mass spectra for
chlordane at http://webbook.nist.gov/cgi/cbook.cgi?ID=C57749&Mask=200 and separate isomers:
cis-chlordane http://webbook.nist.gov/cgi/cbook.cgi?ID=C5103719&Units=SI&Mask=200#Mass-Spec
trans-chlordane http://webbook.nist.gov/cgi/cbook.cgi?ID=C5103742&Units=SI&Mask=200#Mass-Spec

Chlordimeform **$C_{10}H_{13}ClN_2$** **M:196,198(85,25%)**

Theoretical molecular ion: m/z 196.0767 (100%), 198.0738 (32%)
Average MW: 196.68



Acaricide. Used on a wide variety of fruit, vegetable and cotton crops to control mites, ticks and some Lepidoptera. It has also been used to control livestock external parasites and stem borers in rice. No longer approved for use in EU.

Acute oral LD50 for rat approx. 160 mg/kg (moderate toxicity). Metabolised to 4-chlorotoluidine, a suspected carcinogen.

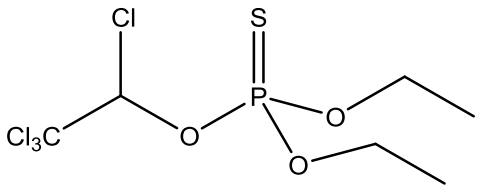
m/z	44	196	181	117	152	42	154	198
%	100	85	50	50	40	30	30	25

196,198 (85,25) – M^+
181,183 (50,30) – [M-15] loss of CH_3 to $C_9H_{10}ClN_2^+$ m/z 181.0533 etc.
154 (30) – [M-42] loss of $(CH_3)CHN$ to $C_8H_9ClN^+$ m/z 154.0424
152 (40) – [M-44] loss of $(CH_3)_2N$ to $C_8H_7ClN^+$ m/z 152.0267
117 (50) – [M-79] loss of $(CH_3)_2N$ & Cl to $C_8H_7N^+$ m/z 117.0579
44 (100) – [M-152] $(CH_3)_2N^+$ $C_2H_6N^+$ m/z 44.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C6164983&Mask=200#Mass-Spec

Chlorethoxyfos **$C_6H_{11}Cl_4O_3PS$** **M:334,336,338(5,8,3%)**

Theoretical molecular ion: m/z 333.8921 (78%), 335.8891 (100%), 337.8862 (48%)
Average MW: 335.98



Organophosphorus insecticide. Chiral molecule. An insecticide used to control soil pests including corn rootworm, cutworms and wireworms. Not approved for use in EU.

Acute oral LD50 for rat approx. 1.8 mg/kg (high toxicity).

m/z	153	97	299	301	125	166	263	115
%	100	85	50	50	40	30	30	25

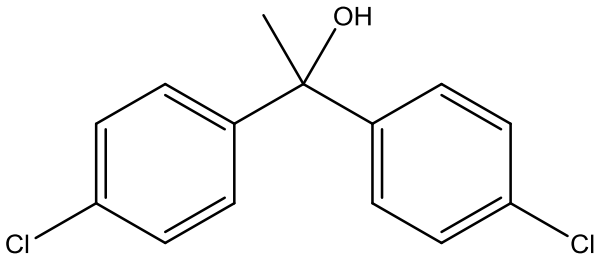
334,336,338 (5,8,4) – M^+
299,301,303 (50,50,10) – [M-35] loss of Cl to $C_6H_{11}Cl_3O_3PS^+$ m/z 298.9232 etc.
271,273,275 (10,10,3) – [M-63] loss of Cl & C_2H_4 to $C_4H_7Cl_3O_3PS^+$ m/z 270.8919 etc.
263,265,267 (10,7,2) – [M-71] loss of HCl_2 to $C_6H_{10}Cl_2O_3PS^+$ m/z 262.9465 etc.

243,245,247 (10,12,3) – [M-91] loss of Cl & $2C_2H_4$ to $C_2H_3Cl_3O_3PS^+$ m/z 242.8606 etc.
153 (100) – [M-181] $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (40) – [M-209] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (85) – [M-207] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
65 (7) – [M-269] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

No NIST spectrum. Data from Peter Kuklenyik (2009).

Chlorfenethol **$C_{14}H_{12}Cl_2O$** **M:266,268(15,5%)**

Theoretical molecular ion: m/z
Average MW: 267.15



Obsolete organochlorine acaricide ("Dimite"). Degrades (-H_2O) to DDNU.

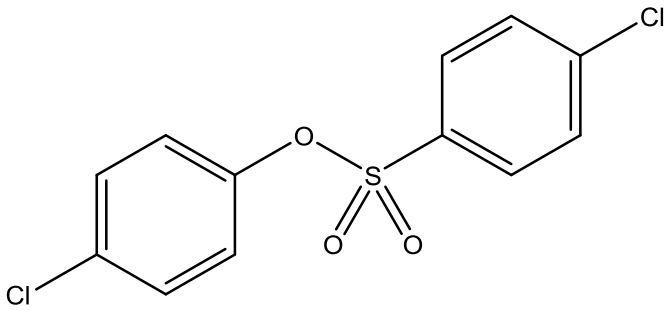
m/z	139	251	43	253	111	141	75	266
%	100	95	90	60	40	35	30	15

266,268(15,5) – M^+
251,253 (95,60) – [M-15] loss of CH_3 to "dichlorobenzophenone+H", $C_{13}H_9Cl_2O^+$ m/z 251.00305 etc.
139,141 (100,35) – [M-127] $ClC_6H_4CO^+$ m/z 138.9951 etc.
111,113 (40,15) – [M-155] $ClC_6H_4^+$ m/z 111.0002 etc.
75 (30) – [M-191] $C_6H_3^+$ m/z 75.0235
43 (90) – [M-223] CH_3CO^+ $C_2H_3O^+$ m/z 43.0184

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C80068&Mask=200#Mass-Spec

Chlorfenson / Ovex **$C_{12}H_8Cl_2O_3S$** **M:302,304(25,15%)**

Theoretical molecular ion: m/z 301.9571 (100%), 303.9542 (65%), 305.9512 (10%)
Average MW: 303.16



Bridged diphenyl organochlorine acaricide. Not approved for use in EU.

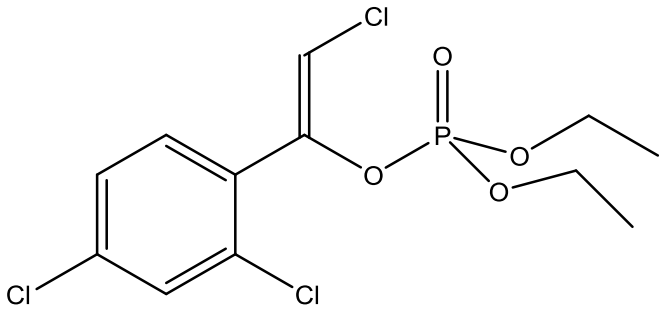
Acute oral LD50 for rat >2,000 mg/kg (moderate toxicity).

m/z	175	111	177	113	302	75	304	127
%	100	95	40	30	25	25	15	20

302,304 (25,15) – M^+
175,177 (100,40) – [M-127] $ClC_6H_4SO_2^+$ m/z 174.9621 etc.
127,129 (20,50 – [M-175] $ClC_6H_4O^+$ m/z 126.9951 etc.
111,113 (95,30) – [M-191] $ClC_6H_4^+$ m/z 111.0002
99,101 (20,5) – [M-203] $C_5H_4Cl^+$ m/z 99.0002
75 (25) – [M-227] $C_6H_3^+$ m/z 75.0235
63 (15) – [M-239] $C_5H_3^+$ m/z 63.0235

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C80331&Mask=200#Mass-Spec

Chlorfenvinphos **$C_{12}H_{14}Cl_3O_4P$** **M:358,360(1,1%)**
Theoretical molecular ion: m/z 357.9695 (100%), 359.96658 (96%), 361.9636 (31%)
Average MW: 359.57



Chlorfenvinphos-(Z) isomer (90%)

Organophosphorus insecticide. Applied to soil to control root-flies, rootworms and other soil pests. Also used as a sheep dip. No longer approved for use in EU.

Acute oral LD50 for rat approx. 12 mg/kg (high toxicity).

Technical chlorfenvinphos comprises 90% (Z)-isomer and 10% (E)-isomer, with indistinguishable mass spectra. The more abundant (Z)-isomer has a longer GC retention time.

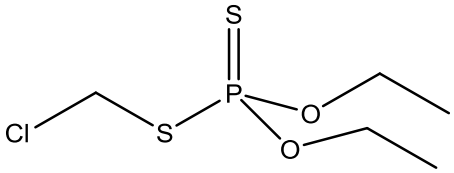
m/z	267	323	269	81	325	109	29	295
%	100	70	65	60	45	45	45	25

358,360 (1,1) – M^+
323,325,327 (70,50,10) – [M-35] loss of Cl to $C_{12}H_{14}Cl_2O_4P^+$ m/z 323.0007 etc.
295,297 (25,15) – [M-63] loss of Cl & C_2H_4 to $C_{10}H_{10}Cl_2O_4P^+$ m/z 294.9694 etc.
267,269 (100,65) – [M-91] loss of Cl & $2C_2H_4$ to $C_8H_6Cl_2O_4P^+$ m/z 266.9381 etc.
194,196,198 ((15,15,10) – [M-164] rearrangement $Cl_2C_6H_3CH_2Cl^+$ $C_7H_5Cl_3^+$ m/z 193.9457 etc.
170,172 (25,15) – [M-188] dichlorophenyl acetylene $Cl_2C_6H_3CCH^+$ $C_8H_4Cl_2^+$ m/z 169.9690 etc.
159,161 (15,5) – [M-199] $C_7H_5Cl_2^+$ m/z 158.9768 etc.
123,125 (30,10) – [M-235] $ClC_6H_3CH^+$ $C_7H_4Cl^+$ m/z 123.0002 etc.
109 (45) – [M-249] $(CH_3CH_2O)(HO)PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
81 (60) – [M-277] $(HO)_2PO^+$ $H_2O_3P^+$ m/z 80.9742

Cf. similar spectra at
http://webbook.nist.gov/cgi/cbook.cgi?ID=C18708877&Mask=200#Mass-Spec ((Z)/cis- isomer)
and
http://webbook.nist.gov/cgi/cbook.cgi?ID=C18708866&Mask=200#Mass-Spec ((E)/trans- isomer)

Chlormephos $C_5H_{12}ClO_2PS_2$ **M:234,236(30,10%)**

Theoretical molecular ion: m/z 233.9705 (100%), 235.9675 (32%)
Average MW: 234.69



Organophosphorus thiophosphate insecticide, used to control soil dwelling pests including wireworms, millipedes and symphylids.

Acute oral LD50 for rat approx. 10 mg/kg (high toxicity).

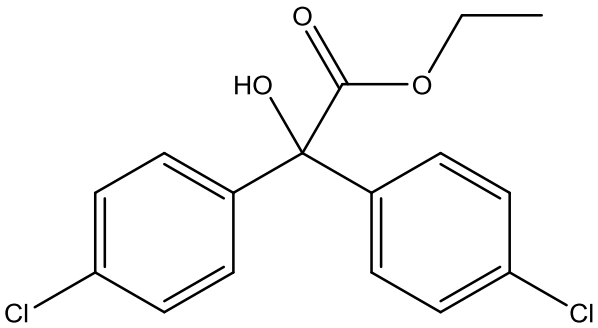
m/z	97	121	154	65	29	93	234	47
%	100	90	50	50	50	35	30	25

234, 236 (30,10) – M^+
154 (50) – [M-80] loss of SCHCl to $(CH_3CH_2O)_2(HS)P^+$ m/z $C_4H_{11}O_2PS^+$ m/z 154.017
125 (10) – [M-109] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121 (90) – [M-113] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
97 (100) – [M-137] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
65 (50) – [M-169] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
47,49 (25,10) – [M-187] CCl^+ m/z 46.9689

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C24934916&Mask=200

Chlorobenzilate $C_{16}H_{14}Cl_2O_3$ **M:324,326(1,0.5%)**

Theoretical molecular ion: m/z
Average MW: 325.19



Bridged diphenyl acaricide (DDT family). Used to control mites on top fruit, walnuts and some other crops. Now classed a persistent organic pollutant and not approved for use in EU.

Acute oral LD50 for rat > 2,00 mg/kg (low toxicity).

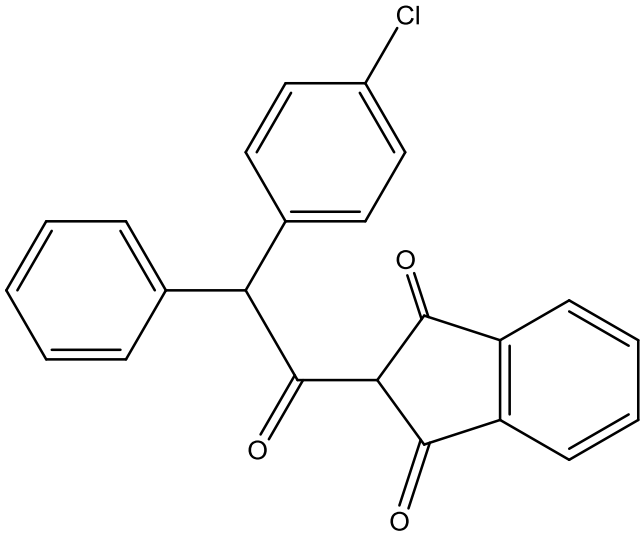
m/z	251	139	253	111	141	235	165	255
%	100	85	60	30	25	25	10	10

324,326 (1,0.5) – M^+ weak
308,310 (3,2) – [M-16] reduction of alcohol to $C_{16}H_{14}Cl_2O_2^+$ m/z 308.0371 etc.
251,253 (100,60) – [M-73] $(ClC_6H_4)_2COH^+$ "dichlorobenzophenone+H" $C_{13}H_9OCl_2^+$ m/z 251.00305
235,237 (25,10) – [M-89] $(ClC_6H_4)_2CH^+$ $C_{13}H_9Cl_2^+$ m/z 235.0081 etc. (characteristic DDT ion)
139,141 (85,25) – [M-185] Cl-C_6H_4-CO^+ $C_7H_4ClO^+$ m/z 138.9951 etc.
111,113 (30,10) – [M-213] Cl-$C_6H_4^+$ $C_6H_4Cl^+$ m/z 111.0002 etc

Cf. similar but weak spectrum (lacking high mass ions and m/z 235,237) at
http://webbook.nist.gov/cgi/cbook.cgi?ID=C510156&Units=CAL&Mask=1A8F#Mass-Spec

Chlorophacinone **$C_{23}H_{15}ClO_3$** **M:374,376(15,5%)**

Theoretical molecular ion: m/z 374.0710 (100%), 376.0680 (32%)
Average MW: 374.82



Anticoagulant rodenticide. Approved for use in EU.

Acute oral LD50 for rat approx. 3 mg/kg (high toxicity).

Poor GC transmission.

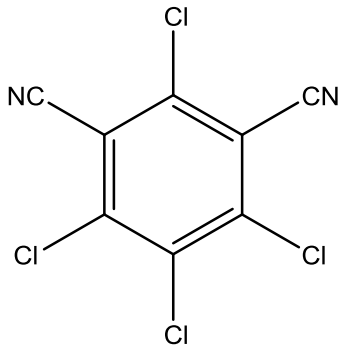
m/z	173	374	165	174	89	166	201	105
%	100	15	15	10	10	10	10	5

374,376 (15,5) – M^+
201,203 (10,3) – [M-173] $C_6H_5CHC_6H_4Cl^+$ $C_{13}H_{10}Cl^+$ m/z 201.0471 etc.
173 (100) – [M-201] $C_6H_4.C_3HO_2.CO^+$ $C_{10}H_5O_3^+$ m/z 173.0239
165 (15) – [M-209] $C_6H_5CC_6H_4^+$ $C_{13}H_9^+$ m/z 165.07043

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3691358&Mask=200#Mass-Spec

Chlorothalonil **$C_8Cl_4N_2$** **M:264,266,268(80,100,50%)**

Theoretical molecular ion: m/z 263.8816 (77%), 265.8786 (100%), 267.8757 (49%)
Average MW: 265.91



Aromatic fungicide. It has a broad spectrum of activity and is approved for use in the EU. It is widely used. It has a low mammalian toxicity but is a recognised irritant.

Acute oral LD50 for rat > 5,000 mg/kg (low toxicity).

Technical chlorothalonil (2,4,5,6-tetrachloro-1,3-dicyanobenzene) may contain low levels (ca. 1%) of an isomeric compound (very similar mass spectrum, slightly shorter GC RT – probably 1,4-dicyano isomer as less polar).

m/z	266	264	268	109	124	229	270	194
%	100	80	50	20	15	10	10	10

264,266,268,270 (80,100,50,10) – M^+
229,231 (10,10) – [M-35] loss of Cl to $C_8Cl_3N_2^+$ m/z 228.9127 etc.
194 (10) – [M-70] loss of 2Cl to $C_8Cl_2N_2^+$ m/z 193.9439 etc.
124 (20) [M-140] loss of 4Cl to $C_8N_2^+$ m/z 124.00615
109,111 (20,7) – [M-155] loss of 3Cl & C_3N to C_5ClN^+ m/z 108.9719 etc.

Cf. similar spectrum at Restek http://www.restek.com/compound/view/1897-45-6/Chlorothalonil

Chlorothalonil related **C_7Cl_5N** **M:273,275,277,279(65,100,65,20%)**

Pentachlorocyanobenzene

Theoretical molecular ion: m/z 272.8473 (62%), 274.8444 (100%), 276.8414 (65%)
Average MW: 275.35

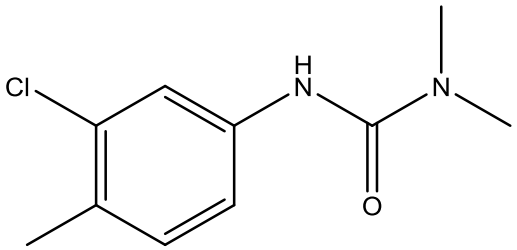
Pentachlorocyanobenzene. A minor (~1%) contaminant of technical chlorothalonil, with shorter GC retention time.

m/z	275	273	277	133	240	279	238	203
%	100	65	65	25	20	20	15	15

273,275,277 (65,100,65) – M^+
238,240,242 (15,15) – [M-35] loss of Cl to C_7ClN^+ m/z 237.8785 etc.
203,205 (15,15) – [M-70] loss of 2Cl to $C_7Cl_3N^+$ m/z 202.9096 etc.
133,135 (25,10) – [M-140] loss of 4Cl to C_7ClN^+ m/z 132.9719 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C20925853&Units=CAL&Mask=200#Mass-Spec

Chlorotoluron / Chlortoluron $C_{10}H_{13}ClN_2O$ **M:212,214(10,3%)**
Theoretical molecular ion: m/z 212.0717 (100%), 214.069 (32%)
Average MW: 212.68



Phenylurea herbicide. Commonly used to control broad-leaved weeds and grasses.

Acute oral LD50 for rat >10,000 mg/kg (low toxicity).

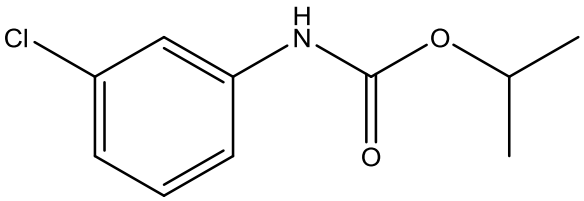
Not amenable to GC analysis.

m/z	72	44	212	45	77	132	167	104
%	100	20	10	10	10	5	5	5

212,214 (10,3) – M^+
167,169 (5,2) – [M-45] loss of $(CH_3)_2NH$ to isocyanate $C_8H_6NOCl^+$ m/z 167.0138 etc.
132 (5) – [M-80] loss of Cl & $(CH_3)_2NH$ to $C_8H_6NO^+$ m/z 132.0449
72 (100) – [M-140] dimethyl isocyanate $(CH_3)_2NCO^+$ $C_3H_6NO^+$ m/z 72.0449

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C15545489&Mask=200

Chlorpropham $C_{10}H_{12}ClNO_2$ **M:213,215(15,5%)**
Theoretical molecular ion: m/z 213.0557 (100%), 215.0527 (32%)
Average MW: 213.66



Phenylurea herbicide. Residual action. Also used as potato sprout suppressant.

Acute oral LD50 for rat approx. 4,200 mg/kg (low toxicity).

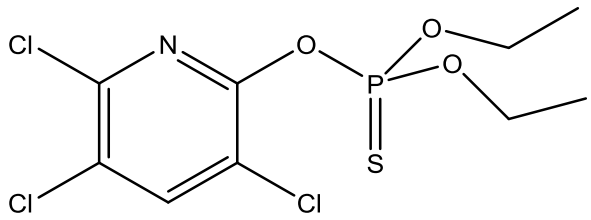
May degrade on GC to 3-chlorophenyl isocyanate (see **diflubenzuron** related).

m/z	43	127	213	171	129	154	41	27
%	100	50	15	15	15	15	15	10

213,215 (15,5) – M^+
171,173 (15,5) – [M-42] loss of C_3H_6 to $C_7H_6ClNO_2^+$ m/z 171.0087
154,156 (15,5) – [M-59] loss of OC_3H_6 to $ClC_6H_4NHCO^+$, $C_7H_5ClNO^+$ m/z 154.0060 etc.
127,129 (50,15) – [M-86] $ClC_6H_4NH_2^+$ $C_6H_6ClN^+$ m/z 127.0189
43 (100) – [M-170] $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C101213&Mask=200

Chlorpyrifos **$C_9H_{11}Cl_3NO_3PS$** **M:349,351,353(2,2,1%)**
Theoretical molecular ion: m/z 348.9263 (100%), 350.9233 (96%), 352.9204 (31%)
Average MW: 350.57



Organophosphorus thiophosphate insecticide and acaricide, used on cotton, corn, almonds, and fruit trees including oranges, bananas and apples.

Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

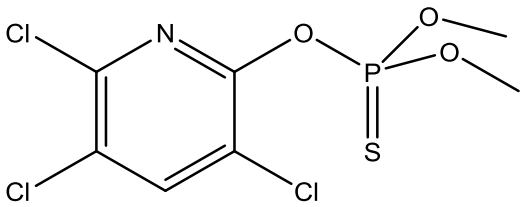
The metabolite 3,5,6-trichloropyridinol (also associated with **triclopyr**) is of toxicological concern regarding human male reproductive health.

m/z	97	197	199	314	316	125	258	286
%	100	80	80	60	50	40	30	30

Assignments confirmed by accurate mass (Cardiff GCT)
349,351,353 (2,2,1) – M^+ $C_9H_{11}Cl_3NO_3PS^+$ m/z 348.9263 etc.
314,316,318 (60,50,10) – [M-35] loss of Cl to $C_9H_{11}Cl_2NO_3PS^+$ m/z 313.9574 etc.
286,88 (30,20) – [M-63] loss of Cl & C_2H_4 to $C_7H_7Cl_2NO_3PS^+$ m/z285.9261etc.
258,260 (30,30) – [M-91] loss of Cl & $2C_2H_4$ to $C_5H_3Cl_2NO_3PS^+$ m/z 257.8948 etc.
197,199,201 (80,80,20) – [M-152] trichloropyridinol $Cl_3(C_5HN)OH^+$ $C_5H_2Cl_3NO^+$ m/z 196.9202 etc.
153 (5) – [M-196] $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (40) – [M-224] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (100) – [M-252] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
65 (15) – [M-258]] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
47 (30) – [M-274] PO^+ m/z 46.9687
29 (20) – [M-320] $C_2H_5^+$ m/z 29.0391

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2921882&Mask=200

Chlorpyrifos-methyl **$C_7H_7Cl_3NO_3PS$** **M:321,323,325(5,5,2%)**
Theoretical molecular ion: m/z 320.8950 (100%), 322.8920 (96%), 324.8891 (31%)
Average MW: 322.52



Organophosphorus thiophosphate insecticide and acaricide, used to control soil and foliage pests including *Coleoptera, Diptera* and *Lepidoptera*.

Acute oral LD50 for rat approx. 3,000 mg/kg (low toxicity).

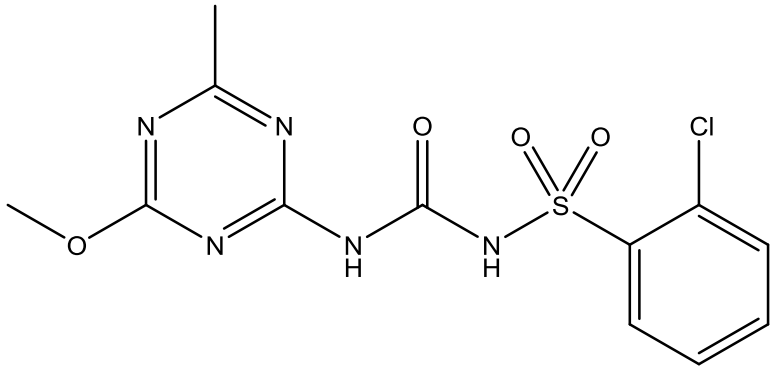
The metabolite 3,5,6-trichloropyridinol (also associated with triclopyr) is of toxicological concern regarding human male reproductive health.

m/z	125	286	288	79	47	93	109	290
%	100	90	60	35	30	25	20	15

321,323 (5,5,2) – M^+
286,288,290 (90,60,15) – [M-35] loss of Cl to $C_7H_7Cl_2NO_3PS^+$ m/z
197,199,201 (10,10,5) – [M-124] trichloropyridinol $Cl_3(C_5HN)OH^+$ $C_5H_2Cl_3NO^+$ m/z 196.9202 etc.
125 (100) – [M-196] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (20) – [M-212] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (25) – [M-228] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (35) – [M-242] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (15) – [M-258] PS^+ m/z 62.9458
47 (30) – [M-274] PO^+ m/z 46.9687 and/or CH_3S^+ m/z 46.99555

Cf. Similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C5598130&Mask=200

Chlorsulfuron **$C_{12}H_{12}ClN_5O_4S$** **M:357(0%)**
Theoretical molecular ion: m/z 357.02985 (100%), 359.0269 (32%)
Average MW: 357.78



Triazinylsulphonylurea herbicide. Used to control broad-leaved weeds and grasses. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

Not amenable to GC.

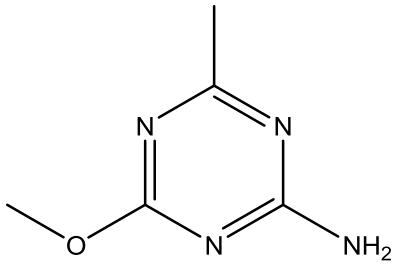
m/z	111	175	69	75	140	42	110	112
%	100	55	55	50	40	40	40	35

357,359 (0,0) – M^+ absent
258 (10) – [M-99] loss of $CH_3O.CNC(CH_3)NH$ to $NCNCONHSO_2C_6H_4Cl^+$ $C_8H_5ClN_3O_3S^+$ m/z 257.9740
217,219 (25,20) – [M-140] $OCN\text{-}SO_2\text{-}C_6H_4Cl^+$ $C_7H_4ClNO_3S^+$ m/z 216.9600 etc.
175,177 (55,20) – [M-182] $SO_2C_6H_4Cl^+$ $C_6H_4ClO_2S^+$ m/z 174.9621 etc.
140 (40) – [M-217] $(CH_3O)(CH_3)C_3N_3.NH_2^+$ $C_5H_8N_4O^+$ m/z 140.0698
111,113 (100,35) – [M-246] $C_6H_4Cl^+$ m/z 111.00015 etc.
110 (40) – [M-247] "140-30" (see chlorsulfuron related i) below) $C_4H_6N_4^+$ m/z 110.0593
75 (50) – [M-283] $C_6H_3^+$ m/z 75.0235
69 (55) – [M-288] $(CH3)C{=}NCNH_2^+$ $C_3H_5N_2^+$ m/z 69.0453

Cf. some similar ions in spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C64902723&Mask=200 but different relative abundances.

Chlorsulfuron related, (i) **$C_5H_8N_4O$** **M:140(75%)**

2-amino-4-methoxy-6-methyl-1,3,5-triazine
Theoretical molecular ion: m/z 140.0698 (100%), 141.0732 (5.4%),
Average MW: 140.15



2 amino-4-methoxy-6-methyl-1,3,5-triazine

Degradation product of chlorsulfuron (and several other sulfonylurea herbicides).

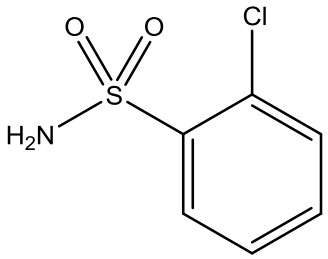
m/z	69	140	110	42	58	139	43	68
%	100	75	70	55	25	20	20	15

140 (75) – M^+
110 (70) – [M-30] loss of CH_2O to $C_4H_6N_4^+$ m/z 110.0593
69 (100) – [M-71] $CH3.C{=}NC.NH_2^+$ $C_3H_5N_2^+$ m/z 69.0453

No NIST spectrum available.

Chlorsulfuron related, (ii) **$C_6H_6ClNO_2S$** **M:191,193(55,15%)**

2-chlorobenzenesulphonamide
Theoretical molecular ion: m/z
Average MW: 191.63



2 chlorobenzenesulphonamide

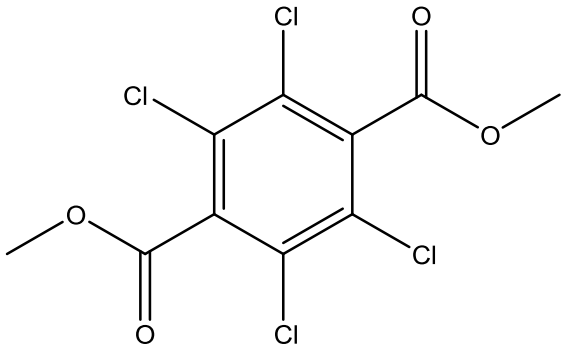
Chlorsulfuron degradation product.

m/z	111	75	128	191	113	175	50	92
%	100	75	55	55	30	25	25	20

191,193 (55,15) – M^+
175,177 (25,10) – [M-16] loss of NH_2 to $SO_2C_6H_4Cl^+$ m/z 174.9621 etc.
128 (55) – [M-63] loss of Cl & CO to $C_5H_6NOS^+$ m/z 128.0170
111,113 (100,30) – [M-80] loss of NH_2SO_2 to $C_6H_4Cl^+$ m/z 111.00015 etc
75 (75) – [M-116] $C_6H_3^+$ m/z 75.0235
50 (25) – [M-141] $C_4H_2^+$ m/z 50.0157

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C6961826&Units=SI&Mask=200#Mass-Spec

Chlorthal-dimethyl / DCPA **$C_{10}H_6Cl_4O_4$** **M:330,332,334(20,30,15%)**
Theoretical molecular ion: m/z 329.9020 (78%), 331.8991 (100%), 333.8961 (48%), 335.8932 (10%)
Average MW: 331.95



Dimethyl tetrachloroterephthalate (DCPA). Phthalic acid herbicide. Residual action for pre-emergent control of annual grasses and some annual broad-leaved weeds. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

m/z	301	299	303	332	330	334	221	223
%	100	80	45	30	20	15	15	10

330,332,334 (20,30,15) – M^+
299,301,303 (80,100,45) – [M-31] loss of CH_3O to $C_9H_3Cl_4O_3^+$ m/z 298.8836 etc.
221,223 (15,10) – [M-109] loss of CH_3CO & OCH_3 & Cl to $C_7Cl_3O_2^+$ m/z 220.8964 etc.

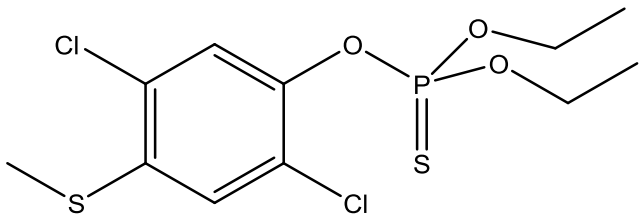
Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1861321&Mask=200#Mass-Spec
listed under "DCPA", with some ^{13}C isotope peaks missing because of insufficient MS resolution.

Chlorthiophos - mixture of three isomers
See *The Pesticide Manual* (2012) (bcpcdata.com/_assets/files/PM16-supplementary-BCPC.pdf):
I O-2,5-dichloro-4-methylthiophenyl O,O-diethyl phosphorothioate - main component, ~73% w/w
II O-4,5-dichloro-2-methylthiophenyl O,O-diethyl phosphorothioate - small quantities, ~13% w/w
III O-2,4-dichloro-5-methylthiophenyl O,O-diethyl phosphorothioate - minor component, ~14% w/w

With typical GC elution order: II, III and I

NIST WebBook includes major isomer, but no MS data.

Chlorthiophos I **$C_{11}H_{15}Cl_2O_3PS_2$** **M:360,362,364(44,33,8%)**
Theoretical molecular ion: m/z 359.9577 (100%), 361.9548 (64%), 363.9518 (10%)
Average MW: 361.23



Organophosphorus insecticide and acaricide, used to control ants and mites. No longer approved for use in EU. Acute oral LD50 for rat approx. 10 mg/kg. Highly toxic.

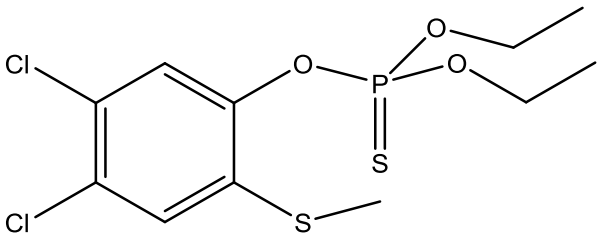
m/z	269	97	325	297	360	271	109	125
%	100	99	79	51	44	43	42	35

360,362,364 (44,33,8) - M^+
325,327,329 (79,43,4) – [M-35] loss of Cl to $C_{11}H_{15}ClO_3PS_2^+$ m/z 324.9998 etc.
297, 299 (51,15) – [M-63] loss of Cl & C_2H_4 to $C_9H_{11}ClO_3PS_2^+$ m/z 296.9676 etc.
269,271 (100,43) – [M-91] loss of Cl & $2C_2H_4$ to$C_7H_7ClO_3PS_2$+ m/z 268.9263 etc.
125 (35) – [M-235] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (42) – [M-251] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P$+ m/z 109.0055
97 (99) – [M-263] $(HO)_2P{=}S^+$ m/z 96.9513

No NIST spectrum available.

Chlorthiophos II **$C_{11}H_{15}Cl_2O_3PS_2$** **M:360,362,364(43,32,7%)**
Theoretical molecular ion: m/z 359.9577 (100%), 361.9548 (64%), 363.9518 (10%)
Average MW: 361.23

The mass spectrum of chlorthiophos II is very different to those of I and III because of *ortho*-effect of the methylthio (CH_3S-) group.

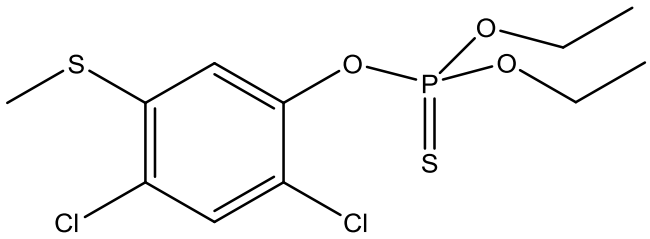


m/z	222	97	224	257	45	360	289	259
%	100	97	77	61	45	43	41	40

360,362,364 (43,32,7) – M^+
289 (41) – [M-71] loss of HCl_2 to $C_{11}H_{14}O_3PS_2^+$ m/z 289.0122
257,259,261 (61,40) – [M-103] loss of CH_3S & $2C_2H_4$ to $C_6H_4Cl_2O_3PS^+$ m/z 256.8996 etc.
222,224,226 (100,77,10) – [M-128] perhaps due to O/S rearrangement and loss of $(CH_3CH_2O)_2P{=}O$ (notional m/z 137) to bicyclic ion $Cl_2C_6H_2{:}S_2CH_2^+$ $C_7H_4Cl_2S_2^+$ m/z 221.913 (100%), 223.9102 (74%), 225.9073 (17%).
[At nominal mass resolution, the observed isotope abundances are consistent with theoretical values of m/z 222 (100%), 224 (74%), 226 17%)]
97 (97) – [M-263] $(HO)_2P{=}S^+$ m/z 96.9513
45 (45) – $CH_3CH_2O^+$ m/z 45.0340

No NIST spectrum available.

Chlorthiophos III **$C_{11}H_{15}Cl_2O_3PS_2$** **M:360,362,364(13,10,2%)**
Theoretical molecular ion: m/z 359.9577 (100%), 361.9548 (64%), 363.9518 (10%)
Average MW: 361.23

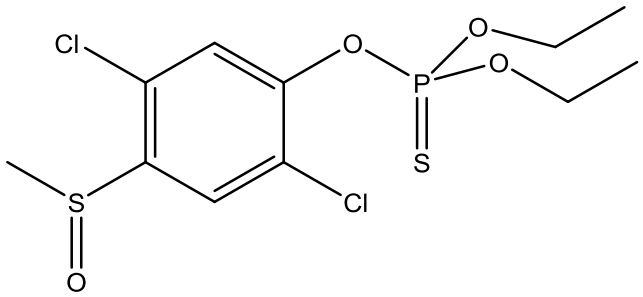


m/z	269	325	97	271	297	327	65	299
%	100	81	55	42	37	34	18	15

360,362,364 (13,10,2) – M^+
325,327 (81,34) – [M-35] loss of Cl to $C_{11}H_{15}ClO_3PS_2^+$ m/z 324.9998 etc.
297, 299 (37,15) – [M-63] loss of Cl & C_2H_4 to $C_9H_{11}ClO_3PS_2^+$ m/z 296.9676 etc.
269,271 (100,42) – [M-91] loss of Cl & $2C_2H_4$ to $C_7H_7ClO_3PS_2^+$ m/z 268.9263 etc.
97 (99) – [M-263] $(HO)_2P{=}S^+$ m/z 96.9513
65 (18) – [M-295] $(HO)_2P^+$ m/z 64.9792

No NIST spectrum available.

Chlorthiophos I sulphoxide **$C_{11}H_{15}Cl_2O_4PS_2$** **M: 376,378,380(0.2,0.2,0.1%)**
Theoretical molecular ion: m/z 375.9526 (100%), 377.9497 (64%), 379.94674 (10%)
Average MW: 377.23



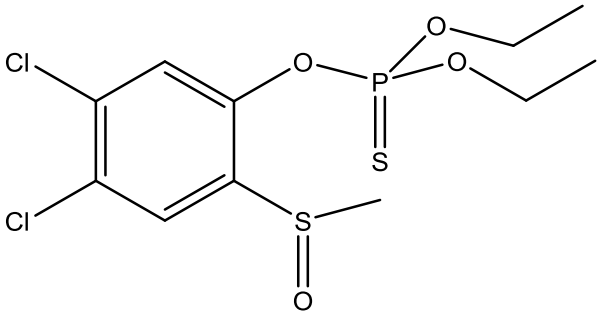
m/z	97	341	125	285	343	109	153	313
%	100	85	56	53	36	33	32	32

376,378,380 (0.2,0.2,0.1) – M^+
341, 343 (85,36) – [M-35] loss of Cl to $C_{11}H_{15}ClO_4PS_2^+$ m/z 340.9838 etc.
313,315 (32,10) – [M-63] loss of Cl & C_2H_4 to $C_9H_{11}ClO_4PS_2^+$ m/z 312.95250 etc.
(not loss of CH_3SO to m/z 312.96219 – incorrect isotope ratios)
285 (53) – [M-91] loss of Cl & $2C_2H_4$ to $C_7H_7ClO_4PS_2^+$ m/z 285.9212 etc.
125 (56) – [M-251] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (33) – [M-267] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (100) – [M-279] $(HO)_2P{=}S^+$ m/z 96.9513

No NIST spectrum available.

Chlorthiophos II sulphoxide **$C_{11}H_{15}Cl_2O_4PS_2$** **M: 376,378,380(0,0,0%)**
Theoretical molecular ion: m/z 375.9526 (100%), 377.9497 (64%), 379.94674 (10%)

Average MW: 377.23

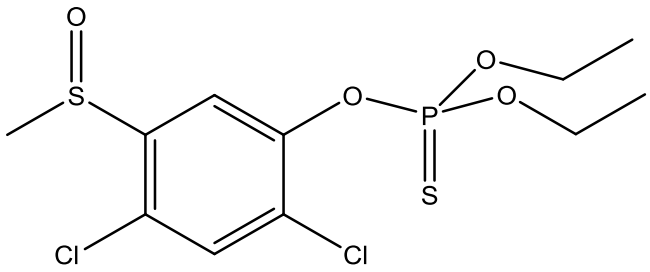


m/z	257	259	97	313	222	45	224	315
%	100	66	64	42	35	33	29	27

376,378,380 (0,0,0) – M^+ absent
313,315,317 (42,27,8) – [M-63] loss of CH_3SO to m/z 312.96219 etc.
(Note elevated m/z 317, confirming ion not due to loss of Cl & C_2H_4)
257,259,261 (100,66, 15) – [M-119] loss of CH_3SO & $2C_2H_4$ to $C_6H_4Cl_2O_3PS^+$ m/z 256.8996 etc.
222,224 (35,29) – [M-154] $C_7H_4Cl_2S_2^+$ m/z 221.913 etc.
97 (64) – [M-279] $(HO)_2P{=}S^+$ m/z 96.9513
45 (33) – [M-331] $CH_3CH_2O^+$ m/z 45.0340

No NIST spectrum available.

Chlorthiophos III sulphoxide $C_{11}H_{15}Cl_2O_4PS_2$ M: 376,378,380(1.0,0.8,0.2%)
Theoretical molecular ion: m/z 375.9526 (100%), 377.9497 (64%), 379.94674 (10%)
Average MW: 377.23

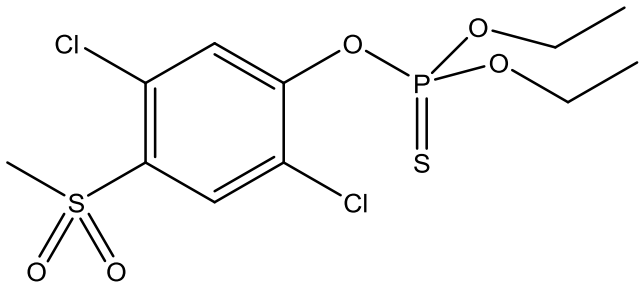


m/z	97	341	269	325	271	343	285	297
%	100	86	80	58	40	37	36	34

376,378,30 (1.0,0.8,0.2) – M^+
341,343 (86,37) – [M-35] loss of Cl to $C_{11}H_{15}ClO_4PS_2^+$ m/z 340.9838 etc.
325,327 (58,15) – [M-51] loss of Cl & O to $C_{11}H_{15}ClO_3PS_2^+$ m/z 324.9889 etc. (!)
285,287 (36,10) – [M-91] loss of Cl & $2C_2H_4$ to $C_7H_7ClO_4PS_2^+$ m/z 285.9212 etc.
269, 271 (80,40) – [M-107] loss of Cl & $2C_2H_4$ & O to $C_7H_7ClO_3PS_2^+$ m/z 268.9263 etc.
97 (100) – [M-279] $(HO)_2P{=}S^+$ m/z 96.9513

No NIST spectrum available.

Chlorthiophos I sulphone **$C_{11}H_{15}Cl_2O_5PS_2$** **M:392,394,396(0,0,0%)**
Theoretical molecular ion: m/z 391.9476 (100%), 393.9446 (64%), 395.94166 (10%)
Average MW: 393.23

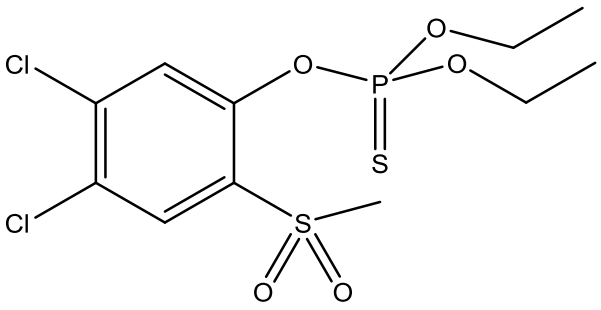


m/z	301	97	357	303	329	359	125	65
%	100	85	79	44	41	35	31	18

392,394,396 (0,0,0) – M^+
357,359 (79,35) - [M-35] loss of Cl to $C_{11}H_{15}ClO_5PS_2^+$ m/z 356.9787 etc.
329,331 (41,13) – [M-63] loss of Cl & C_2H_4 to $C_9H_{11}ClO_5PS_2^+$ m/z 328.9474 etc.
301,303 (100,44) – [M-91] loss of Cl & $2C_2H_4$ to $C_7H_7ClO_5PS_2^+$ m/z 300.9161 etc.
125 (31) – [M-267] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (100) – [M-295] $(HO)_2P{=}S^+$ m/z 96.9513
65 (18) – [M-327] $(HO)_2P^+$ m/z 64.9792

No NIST spectrum available.

Chlorthiophos II sulphone **$C_{11}H_{15}Cl_2O_5PS_2$** **M:392,394,396(0,0,0%)**
Theoretical molecular ion: m/z 391.9476 (100%), 393.9446 (64%), 395.94166 (10%)
Average MW: 393.23

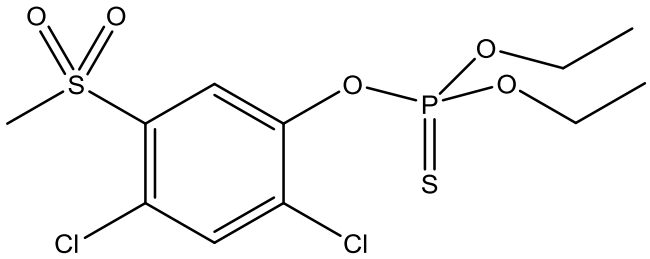


m/z	257	259	97	313	315	285	287	179
%	100	64	49	43	35	25	22	22

392,394,396 (0,0,0) – M^+ absent
313,315,317 (43,35,8) – [M-79] loss of CH_3SO_2 to $C_{10}H_{12}Cl_2O_3PS^+$ m/z 312.96219 etc.
285,287 (25,22) – [M-107]] loss of CH_3SO_2 & C_2H_4 to $C_8H_8Cl_2O_3PS^+$ m/z 284.9309 etc.
257,259,261 (100,64,15) – [M-135] loss of CH_3SO_2 & $2C_2H_4$ to $C_6H_4Cl_2O_3PS^+$ m/z 256.8996 etc.
179 (22) – [M-213]
97 (100) – [M-295] $(HO)_2P{=}S^+$ m/z 96.9513

No NIST spectrum available.

Chlorthiophos III sulphone **$C_{11}H_{15}Cl_2O_5PS_2$** **M:392,394,396(4,3,1%)**
Theoretical molecular ion: m/z 391.9476 (100%), 393.9446 (64%), 395.94166 (10%)
Average MW: 393.23

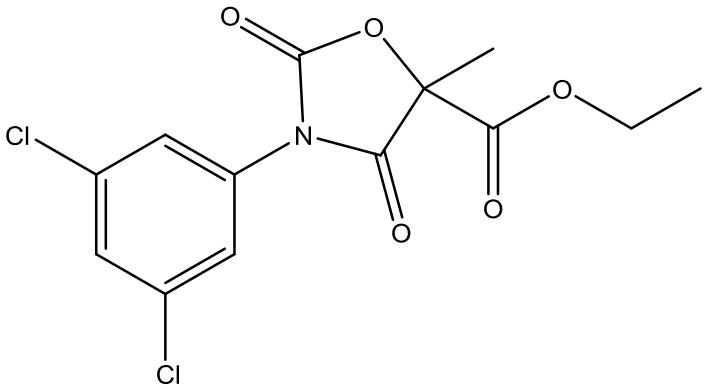


m/z	97	357	301	125	109	329	359	240
%	100	81	60	49	46	39	35	32

392,394,396 (4,3,1) – M^+
357,359 (81,35) – [M-35] loss of Cl to $C_{11}H_{15}ClO_5PS_2^+$ m/z 356.9787 etc.
329,331 (39,10) – [M-63] loss of Cl & C_2H_4 to $C_9H_{11}ClO_5PS_2^+$ m/z 328.9474 etc.
301,303 (60,20) – [M-91] loss of Cl & $2C_2H_4$ to $C_7H_7ClO_5PS_2^+$ m/z 300.9161 etc.
240,242 (32,20) – [M-152] phenol $(CH_3SO_2)Cl_2(C_6H_2)OH^+$ $C_7H_6Cl_2O_3S^+$ m/z 239.9415 etc.
125 (49) – [M-267] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (46) – [M-283] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (100) – [M-295] $(HO)_2P{=}S^+$ m/z 96.9513

No NIST spectrum available.

Chlozolinate **$C_{13}H_{11}Cl_2NO_5$** **M:331,333,335(25,15,5%)**
Theoretical molecular ion: m/z 331.0014 (100%), 332.9985 (64%), 334.9955 (10%)
Average MW: 332.13



Dicarboximide fungicide. No longer approved for use in EU. Used as a foliar spray against *Botrytis, Sclerotinia* and *Monilia spp*. No longer approved for use.

Acute oral LD50 for rat >4,500 mg/kg (low toxicity).

Chiral molecule. The metabolite 3,5-dichloroaniline is toxicologically significant (see "iprodione related (ii)").

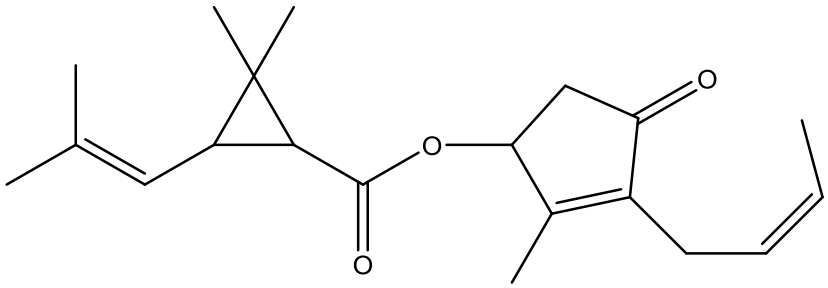
m/z	43	29	259	188	331	187	261	186
%	100	70	30	30	25	25	20	20

331,333,335 (25,15,5) – M^+
259,261,263 (30,20,5) – [M-72] loss of CH_2CH_2OCO to $C_{10}H_7Cl_2NO_3^+$ m/z 258.9803 etc.
187,189 (25,20) [M-144] dichlorophenyl isocyanate, $C_7H_3Cl_2NO^+$ m/z 186.9592 etc.
186,188 (20,30) [M-145] dichlorophenyl isocyanate-H, $C_7H_2Cl_2NO^+$ m/z 185.95135 etc.
43 (100) – [M-288] CH_3CO^+ $C_2H_3O^+$ m/z 43.0184 (rearrangement?)
29 (70) – [M-302] $C_2H_5^+$ m/z 29.03913

No NIST spectrum available.

Cinerin I **$C_{20}H_{28}O_3$** **M:316(1%)**

Theoretical molecular ion: m/z 316.2038 (100%), 317.2072 (22%)
Average MW: 316.44



(Z)–(S)-cinerolone (1R)-trans-chrysanthemate

A natural pyrethrin (see also jasmolin I and II and pyrethrin I and II). A non-persistent insecticide extracted from *Pyrethrum*, comprised of several different compounds. Used to control a variety of pests on crops, in domestic and public health situations.

Acute oral LD50 for rat (as pyrethrins) approx 1,000 mg/kg (moderate toxicity).

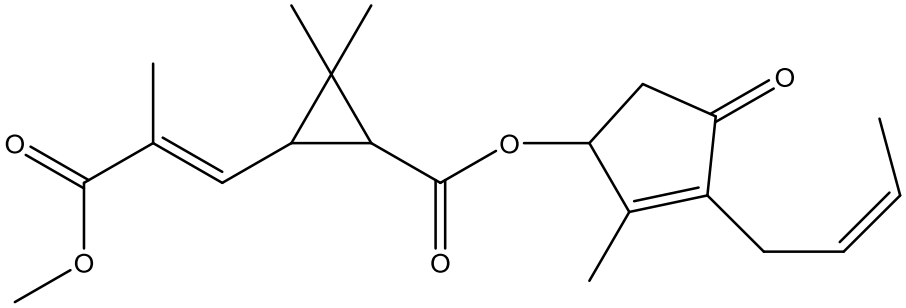
m/z	123	150	121	93	81	43	107	168
%	100	30	30	25	25	20	20	10

316 (1) – M^+ weak
168 (10) – [M-150] $(CH_3)_2C{=}CH.C_3H_2(CH_3)_2.COOH^+$ $C_{10}H_{16}O_2^+$ m/z 168.1150
150 (30) – [M-166] $C_{10}H_{14}O^+$ m/z 150.1045
123 (100) – [M-193] $(CH_3)_2C{=}CH.C_3H_2(CH_3)_2^+$ $C_9H_{15}^+$ m/z 123.1174

Cf. Similar (weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C25402066&Mask=200

Cinerin II **$C_{21}H_{28}O_5$** **M:360(1%)**

Theoretical molecular ion: m/z 360.1937 (100%), 361.1970 (23%)
Average MW: 360.45



(Z)–(S)-cinerolone (1R)-trans-pyrethrate

A natural pyrethrin (see also jasmolin I and II and pyrethrin I and II).

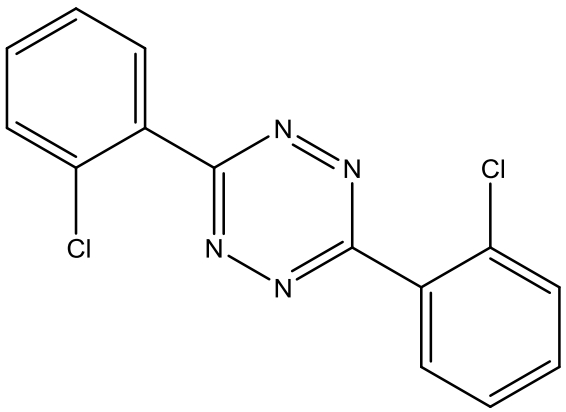
m/z	107	121	149	167	93	150	135	91
%	100	80	70	50	50	30	20	20

360 (1) – M^+ weak
167 (50) – [M-193] $CH_3OOC.(CH_3)C{=}CH.C_3H_2(CH_3)_2^+$ $C_{10}H_{15}O_2^+$ m/z 167.1072
149 (70) – [M-211] $C_5H_3(CH_3)(O).CH_2CH{=}CHCH_3^+$ $C_{10}H_{13}O^+$ m/z 149.0966
121 (80) – [M-39] $C_9H_{13}^+$ m/z 121.1017
107 (100) – [M-253] $C_8H_{11}^+$ m/z 107.0861

No NIST spectrum available.

Clofentezine **$C_{14}H_8Cl_2N_4$** **M:302,304(5,3%)**

Theoretical molecular ion: m/z 302.0126 (100%), 304.0097 (64%)
Average MW: 303.1



Tetrazine acaricide, with selective ovicidal action for use in a range of crops including fruit and ornamentals.

Acute oral LD50 for rat >5,200 mg/kg (low toxicity).

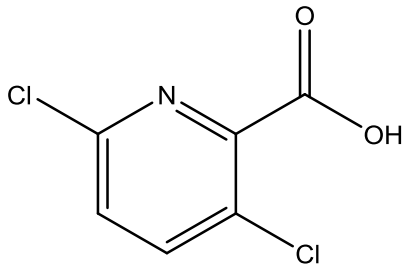
m/z	137	102	75	139	77	138	103	302
%	100	50	30	30	15	10	5	5

302,304 (5,3) – M^+

137,139 (100,30) – [M-165] Cl-C_6H_4-CN^+ $C_7H_4ClN^+$ m/z 137.0032 etc.
102 (100) – [M-200] C_6H_4CN+ $C_7H_4N^+$ m/z 102.0344
75 (30) – [M-227] $C_6H_3^+$ m/z 75.0235

No NIST spectrum available.

Clopyralid, acid **$C_6H_3Cl_2NO_2$** **M:191,193,195(10,7,2%)**
Theoretical molecular ion: m/z 190.9545 (100%), 192.9511 (64%), 194.9482 (10%)
Average MW: 192.00



Clopyralid, 3,6-dichloropicolinic acid

Herbicide. Used for post-emergence control of many broad-leaved weeds in a range of crops. Approved for use in EU.

Acute oral LD50 for rat >2,500 mg/kg (low toxicity). Irritant.

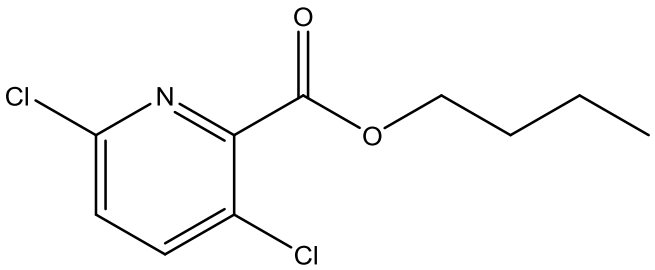
Poor GC transmission if underivatised.

m/z	147	149	112	76	110	75	50	85
%	100	65	50	45	25	20	20	15

191,193,195 (10,7,2) – M^+
147,149 (100,65) – [M-44] loss of CO2 to $C_5H_3Cl_2N+$ m/z 146.9643 etc.
112 (50) – [M-79] loss of CO_2 & Cl to $C_5H_3ClN^+$ m/z 111.9954 etc.

No NIST spectrum available. But **Clopyralid methyl** spectrum ("Methyl 3,6-dichloropyridine-2-carboxylate") is available, at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1532247&Mask=200 with main ions at m/z 147, 149, 110,112 and M^+ at m/z 206, 208.

Clopyralid, n-butyl **$C_{10}H_{11}Cl_2NO_2$** **M:247,249(2,1%)**
Theoretical molecular ion: m/z 247.0167 (100%), 249.0137 (64%), 251.0108 (10%),
Average MW: 248.10



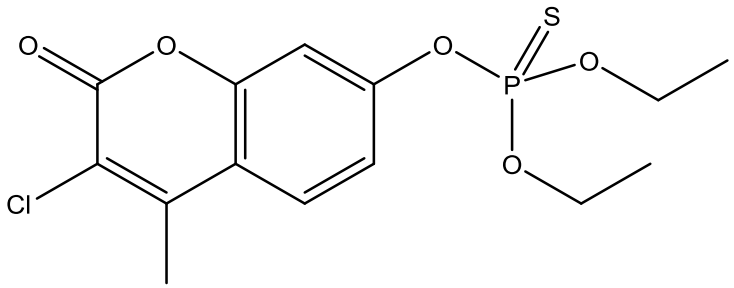
Herbicide.

m/z	174	176	147	146	56	41	148	192
%	100	65	55	50	50	50	30	30

247,249 (2,1) – M^+ weak
174,176 (100,65) – [M-73] loss of OC_4H_9 to $C_6H_2Cl_2NO^+$ m/z 173.9513 etc.
147,149 (55,30) – [M-100] loss of $COOC_4H_8$ to $C_5H_3Cl_2N^+$ m/z 146.9643 etc.
146,148 (50,30) – [M-101] loss of $COOC_4H_9$ to $C_5H_2Cl_2N^+$ m/z 145.9564 etc.

No NIST spectrum available.

Coumaphos **$C_{14}H_{16}ClO_5PS$** **M:362,364(100,35%)**
Theoretical molecular ion: m/z 362.0145 (1000%), 364.0115 (32%)
Average MW: 362.76



Organophosphorus veterinary insecticide & acaricide. Used for control of a wide variety of livestock insects including cattle grubs, screw-worms, lice, scabies, flies, and ticks.

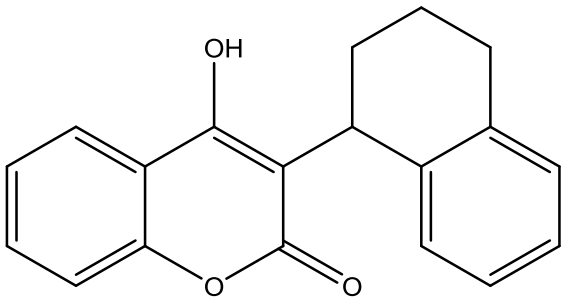
Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

m/z	362	109	97	226	210	29	125	364
%	100	95	90	70	50	50	35	35

362,364 (100,35) – M^+
226,228 (70,20) – [M-136] loss of $(C_2H_5O)(C_2H_4O)PO$ to $C_{10}H_7ClOS^+$ m/z 225.9855 [O/S swap]
210, 212 (50,15) – [M-152] loss of $(C_2H_5O)(C_2H_4O)PS$ to $C_{10}H_7ClO_3^+$ m/z 209.9906
125 (35) – [M-237] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (100) – [M-253] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (90) – [M-265] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C56724&Mask=200

Coumatetralyl **$C_{19}H_{16}O_3$** **M:292(100%)**
Theoretical molecular ion: m/z 292.1099 (100%), 293.1133 (21%)
Average MW: 292.33



Anticoagulant rodenticide. Not approved for use in EU.

Acute oral LD50 for rat approx. 10 mg/kg (high toxicity).

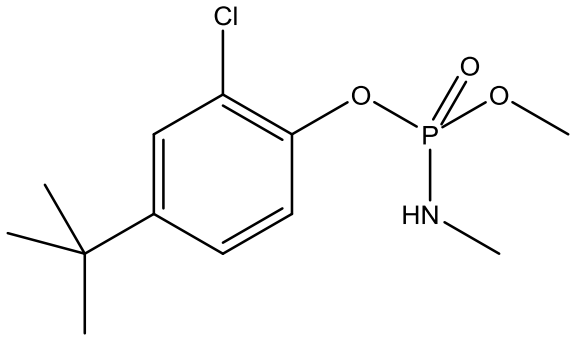
Poor GC transmission.

m/z	292	188	130	121	129	115	91	175
%	100	70	55	55	25	25	15	15

292 (100) – M^+
188 (70) – [M-104] $C_9H_4O_2(OH)\text{-}CH{=}CH_2^+$ $C_{11}H_8O_3^+$ m/z 188.0473
130 (5) – [M-162] $C_{10}H_{10}^+$ m/z 130.0783
121 (55) – [M-171] $C_7H_5O_2^+$ m/z 121.0290

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C5836293&Mask=200#Mass-Spec
Listed as "2H-1-Benzopyran-2-one, 4-hydroxy-3-(1,2,3,4-tetrahydro-1-naphthalenyl)-"

Crufomate **$C_{12}H_{19}ClNO_3P$** **M:291,293(20,7%)**
Theoretical molecular ion: m/z 291.0791 (100%), 293.0762 (32%)
Average MW: 291.71



Organophosphorus phosphoramidate insecticide. Previously used to control grubs, lice, and horn fly on cattle. No longer approved in the EU.

Acute oral LD50 for rat approx 900 mg/kg (moderate toxicity).

Chiral molecule.

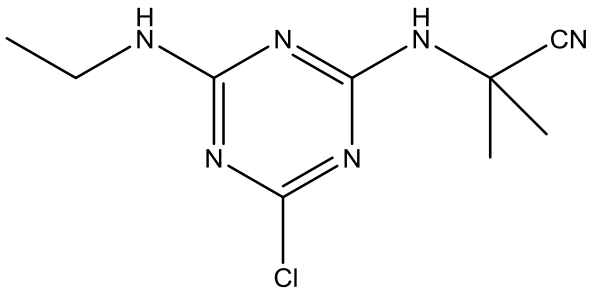
m/z	256	108	276	169	182	278	41	171
%	100	95	80	65	60	25	25	25

291,293 (20,7) – M^+
276,278 (80,5) – [M-15] loss of CH_3 to $C_{11}H_{16}ClNO_3P^+$ m/z 276.0556
256 (100) – [M-35] loss of Cl to $C_{12}H_{19}NO_3P^+$ m/z 256.1103
182 (60) – [M-109] $C_{10}H_{11}ClO^+$ m/z 182.0498 etc.
169,171 (65,25) – [M-122] $C_9H_{10}ClO^+$ m/z 169.0420 etc.
108 (95) – [M-183] $(CH_3O)(CH_3NH)P{=}O^+$ $C_2H_7NO_2P^+$ m/z 108.0214

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C299865&Mask=200

Cyanazine **$C_9H_{13}ClN_6$** **M:240,242(65,20%)**

Theoretical molecular ion: m/z 240.0890 (100%), 242.0861 (32%)
Average MW: 240.70



Chlorotriazine herbicide. A pre-emergence herbicide used for general weed control, including grasses and broad-leaved weeds, in a range of crops.

Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

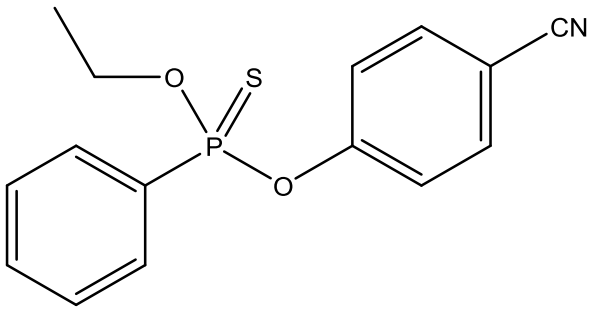
m/z	212	44	225	68	173	198	240	172
%	100	100	90	85	75	65	65	65

240,242 (65,20) – M^+
225,227 (90,30) – [M-15] loss of CH_3 to $C_8H_{10}ClN_6^+$ m/z 225.0656 etc.
212,214 (100,35) – [M-28] loss of C_2H_4 to $C_7H_9ClN_6^+$ m/z 212.0577 etc
173,175 (75,25) – [M-67] loss of $(CH_3)(CH2)C.CN$ to $C_5H_8ClN_5^+$ m/z 173.0468 etc.
68 (85) – [M-172] $(CH_3)_2C(CN)^+$ $C_4H_6N^+$ m/z 68.0990
44 (100) – [M-196] $CH_3CH_2NH^+$ $C_2H_6N^+$ m/z 44.0500

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C21725462&Mask=200 which shares many prominent ions, but with different abundances to those reported here.

Cyanofenphos **$C_{15}H_{14}NO_2PS$** **M:303(15%)**

Theoretical molecular ion: m/z 303.0483 (100%), 304.0516 (16%)
Average MW: 303.32



Organophosphorus phenylphosphonothioate insecticide. Used mainly for the control of insects affecting livestock, such as blow flies, lice and ticks.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

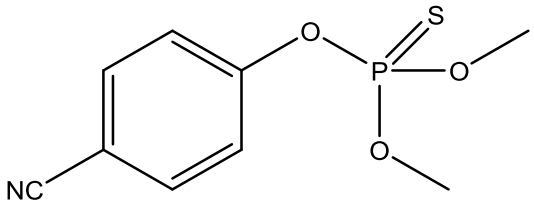
Chiral molecule.

m/z	157	169	141	185	77	63	47	303
%	100	55	35	35	25	25	15	15

303 (15) – M^+
185 (35) – [M-118] loss of OC_6H_4CN to $C_8H_{10}OPS^+$ m/z 185.0190
169 (55) – [M-134] loss of SC_6H_4CN to $C_8H_{10}O_2P^+$ m/z 169.0418 [O/S swap]
157 (100) – [M-146] loss of OC_6H_4CN & C_2H_4 to $C_6H_6OPS^+$ m/z 185.0190
141 (35) – [M-162] loss of SC_6H_4CN & C_2H_4 to $C_6H_6O_2P^+$ m/z 141.0105
77 (25) – [M-226] $C_6H_5^+$ m/z 77.0391

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C13067931&Mask=200

Cyanophos **$C_9H_{10}NO_3P_S$** **M:243(50%)**
Theoretical molecular ion: m/z 243.0119 (100%), 244.0153 (10%), 245.0077 (4.5%)
Average MW: 243.22



Organophosphorus insecticide. Used to control aphids and other insects in fruit and vegetables.

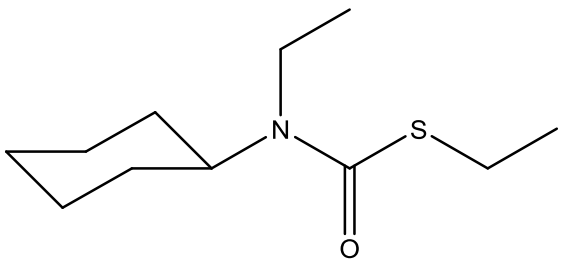
Acute oral LD50 or rat approx 600 mg/kg (moderate toxicity).

m/z	109	125	243	79	47	93	63	102
%	100	60	50	30	30	15	15	10

243 (50) – M+
125 (60) – [M-118] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (100) – [M-134] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055 [O/S swap]
102 (10) – [M-141] $CN\text{-}C_6H_4^+$ $C_7H_4N^+$ m/z 102.0344
79 (30) – [M-164] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (15) – [M-180] PS^+ m/z 68.9458
47 (30) –[M-196] PO^+ m/z 46.9687 and/or CH_3S^+ m/z 46.9956

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C2636262&Mask=200

Cycloate **$C_{11}H_{21}NOS$** **M:215(5%)**
Theoretical molecular ion: m/z 215.1344 (100%), 216.1377 (12%), 217.1302 (4.5%)
Average MW: 215.36



Thiocarbamate herbicide. Used to control annual grass weeds and some broad-leaved weeds. Not approved for use in EU.

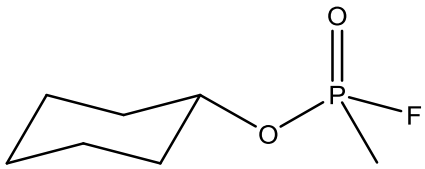
Acute oral LD50 or rat approx >2,000 mg/kg (moderate toxicity).

m/z	83	154	55	41	72	215	186	27
%	100	55	40	15	15	5	5	5

215 (5) – M^+
154 (55) – [M-61] loss of CH_3CH_2S to $C_9H_{16}NO^+$ m/z 154.1232
83 (100) – [M-132] cyclohexyl moiety $C_6H_{11}^+$ m/z 83.0861

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1134232&Mask=200#Mass-Spec

Cyclosarin / GF nerve agent **$C_7H_{14}FO_2P$** **M:180(0%)**
Theoretical molecular ion: m/z 180.0715 (100.0%), 181.0749 (7.6%)
Average MW: 180.16



Cyclosarin, O-cyclohexyl methylphosphonofluoridate

Organophosphorus chemical warfare agent, first developed in Germany during WWII.

Acute oral LD50 for rat **<0.1 mg/kg** (very high toxicity).

Approximately 1mg is enough to kill a human.

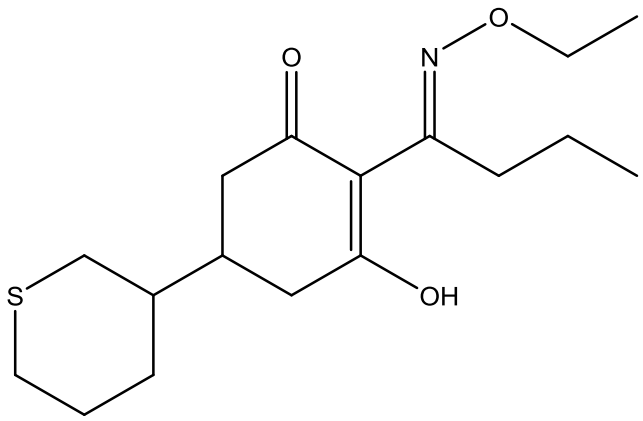
m/z	99	67	54	41	39	82	81	55
%	100	20	15	10	5	5	5	5

180 (0) – M^+ absent
137 (2) – [M-43] loss of C_3H_7 to $C_3H_4O(CH_3)FP{=}O^+$ $C_4H_7FO_2P^+$ m/z 137.0168
125 (1) – [M-55] loss of C_4H_7 to $C_2H_4O(CH_3)FP{=}O^+$ $C_3H_7FO_2P^+$ m/z 125.0168
99 (100) – [M-81] loss of C_6H_9 to $CH_3(HO)_2FP^+$ $CH_5FO_2P^+$ m/z 99.0011
82 (10) – [M-98] cyclohexene $C_6H_{10}^+$ m/z 82.0783 and/or $CH_3(HO)FP^+$ CH_4FOP^+ m/z 81.9984
81 (10) – [M-99] $C_6H_{10}^+$ m/z 81.0704
67 (20) – [M-113] $C_5H_7^+$ (as in cyclohexanol spectrum) m/z 67.0548 (or $FPOH^+$ m/z 66.9749?)
54 (15) – [M-126] $C_4H_6^+$ m/z 54.0470

Data from NIST spectrum http://webbook.nist.gov/cgi/cbook.cgi?ID=C329997&Units=SI&Mask=200#Mass-Spec
N.B. listed under "*Cyclohexyl methylphosphonofluoridate*" rather than cyclosarin.

Cycloxydim $C_{17}H_{27}NO_3S$ **M:325(1%)**

Theoretical molecular ion: m/z 325.171 (100%), 326.1745 (18%), 327.1670 (4.5%)
Average MW: 325.47



Systemic cyclohexene oxime herbicide. Approved for use in the EU as post-emergence foliar applied grass herbicide.

Acute oral LD50 for rat approx 4,000 mg/kg (low toxicity). Irritant.

Poor GC transmission.

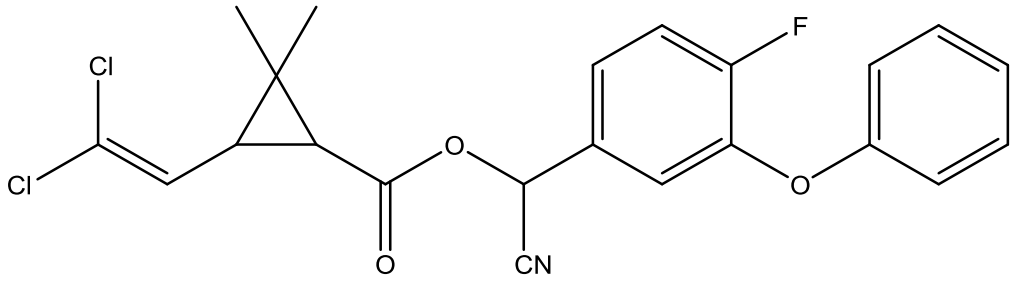
m/z	178	280	41	101	136	150	179	67
%	100	45	35	30	20	20	15	15

325 (1) – M^+
280 (45) – [M-45] loss of $OCH_2CH_3$to $C_{15}H_{22}NOS^+$ m/z 280.1371
178 (100) – [M-147] loss of OCH_2CH_3 & $C_5H_{10}S$ to $C_{10}H_{12}NO^+$ m/z 178.0868

No NIST spectrum available.

Cyfluthrin $C_{22}H_{18}Cl_2FNO_3$ **M:433,435(2,1%)**

Theoretical molecular ion: m/z 433.0648 (100%), 435.0618 (64%), 437.059 (10%)
Average MW: 434.29



Synthetic pyrethroid insecticide. Used to control a range of pests including *Lepidoptera, Coleoptera* and *Hemiptera*. Approved for use in EU.

Acute oral LD50 for rat approx 800 mg/kg (medium toxicity).

May be resolved into four peaks on capillary GC (roughly 2:2:1:1).

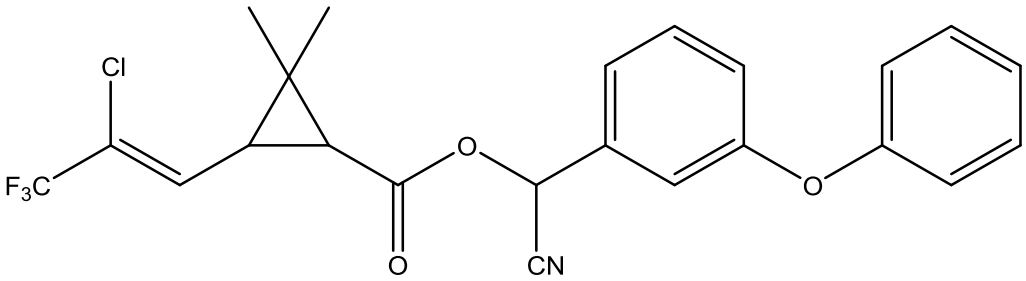
m/z	163	165	226	206	77	199	91	127
%	100	65	55	45	35	30	30	25

433,435 (2,1) – M^+
226 (55) – [M-207] $^+C(CN)C_6H_3F\text{-}O\text{-}C_6H_5$ $C_{14}H_9FNO^+$ m/z 226.0668
163,165 (100,65) – [M-270] $Cl_2C{=}C\text{-}C_3H_3(CH_3)_2^+$ $C_7H_9Cl_2^+$ m/z 163.0081 etc.

Cf. fairly similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C68359375&Mask=200#Mass-Spec but with different relative intensities.

Cyhalothrin **$C_{23}H_{19}ClF_3NO_3$** **M:449,451(8,3%)**

Theoretical molecular ion: m/z 449.1006 (100%), 451.0976 (32%)
Average MW: 449.85



Synthetic pyrethroid insecticide and acaricide, used to control animal ectoparasites. Not approved for use in EU.

Acute oral LD50 for rat approx. 140 mg/kg (moderate toxicity).

Diastereomers may be resolved into two peaks on capillary GC (roughly 1:7).

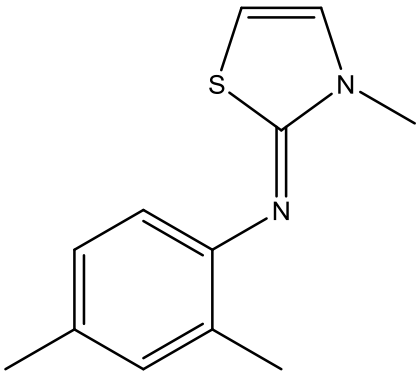
m/z	181	197	208	209	199	77	141	180
%	100	85	85	45	25	25	25	20

449,451 (8,3) – M^+
208 (85) – [M-241] $^+C(CN)C_6H_4\text{-}O\text{-}C_6H_5$ $C_{14}H_{10}NO^+$ m/z 208.0762
197,199 (85,25) – [M-252] $(CF3)ClC{=}C\text{-}C_3H_3(CH_3)_2^+$ $C_7H_9Cl_2^+$ m/z 163.0081 etc.
181 (100) – [M-268] $C_{13}H_9O^+$ m/z 181.0653

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C91465086&Mask=200#Mass-Spec

Cymiazole **$C_{12}H_{14}N_2S$** **M:218(100%)**

Theoretical molecular ion: m/z 218.0878 (100%), 219.0911 (13%), 220.0836 (4.5%)
Average MW: 218.32



An acaricide. Used for the control of mites and ticks especially those resistant to organochlorines, organophosphates and carbamates. Not approved for use in EU.

Acute oral LD50 for rat approx. 700 mg/kg (moderate toxicity).

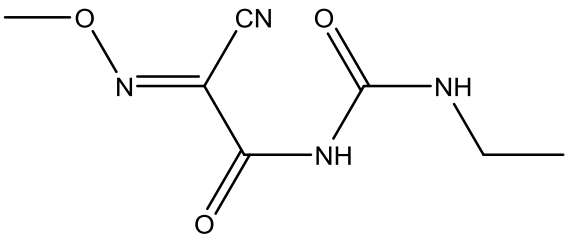
m/z	218	119	144	185	77	183	219	220
%	100	20	15	10	10	5	5	5

218 (100) – M^+
185 (10) –[M-33] loss of SH to $C_{12}H_{13}N_2^+$ m/z 185.01079
119 (20) – [M-99] $(CH_3)_2C_6H_3.N^+$ $C_8H_9N^+$ m/z 119.0735

No NIST spectrum available.

Cymoxanil **$C_7H_{10}N_4O_3$** **M:198(1%)**

Theoretical molecular ion: m/z 198.0753 (100%), 199.07865 (7.6%)
Average MW: 198.13



Fungicide. Used to control *Peronosporales* on a range of crops including vines, hops and potatoes. Approved for use in EU.

Acute oral LD50 for rat approx.760 mg/kg (moderate toxicity).

m/z	44	30	29	70	111	167	128	183
%	100	90	40	30	30	20	15	10

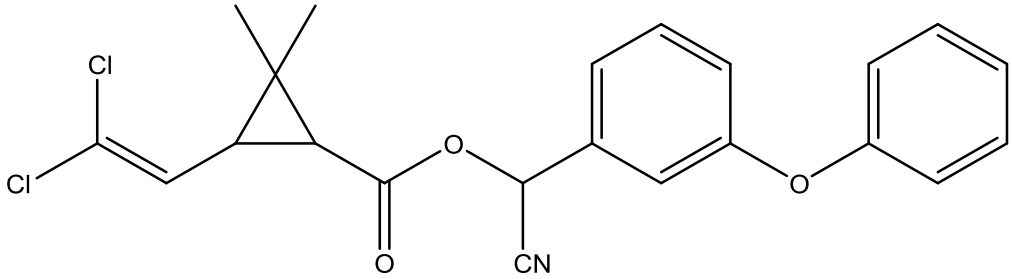
198 (1) – M+
183 (10) – [M-15] loss of CH_3 to $C_6H_7N_4O_3^+$ m/z 183.0518
167 (20) – [M-31] loss of CH_3O to $C_6H_7N_4O_2^+$ m/z 167.0569

44 (100) – [M-154] $NHCH_2CH_3^+$ C_2H_6N+ m/z 44.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C57966957&Mask=200#Mass-Spec

Cypermethrin **$C_{22}H_{19}Cl_2N0_3$** **M:415,417(2,1%)**

Theoretical molecular ion: m/z 415.0742 (100%), 417.07125 (64%), 418.07460 (15%)
Average MW: 416.30



Synthetic pyrethroid insecticide. Approved for use in EU.

Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

May be resolved into several (up to 4 roughly equal) peaks on capillary GC.

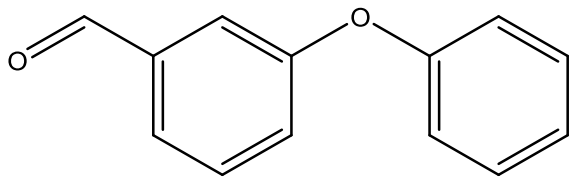
m/z	163	165	181	77	91	208	209	127
%	100	60	50	30	30	25	20	20

415,417 (2,1) – M+
208,209 (25,20) – [M-207] $^+C(CN)C_6H_4$-O-C_6H_5 $C_{14}H_{10}NO^+$ m/z 208.0762
163,165 (100,65) – [M-252] Cl_2C=C-$C_3H_3(CH_3)_2^+$ $C_7H_9Cl_2^+$ m/z 163.0081

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C52315078&Mask=200#Mass-Spec

Cypermethrin (etc.) related **$C_{13}H_{10}O_2$** **M:198(100%)**
3-phenoxy-benzaldehyde

Theoretical molecular ion: m/z 198.0681 (100%), 199.0714 (14%)
Average MW: 198.22



3-phenoxy-benzaldehyde

A degradation product of cypermethrin and several other synthetic pyrethroids.

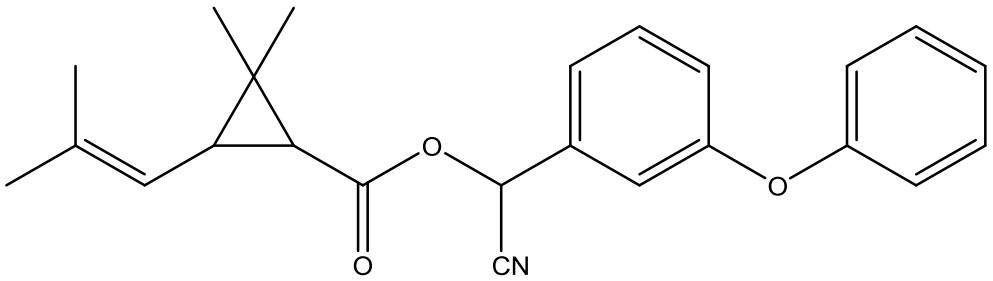
m/z	198	51	77	169	197	141	181	115
%	100	45	40	40	40	35	20	15

198 (100) – M^+

No NIST spectrum available.

Cyphenothrin **$C_{24}H_{25}NO_3$** **M:375(5%)**

Theoretical molecular ion: m/z 375.1834 (100%), 376.1868 (26%)
Average MW: 375.18



Synthetic pyrethroid insecticide. Used to control flies, midges, cockroaches and other pests in domestic, public health and industrial situations. Not approved for use in EU.

Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

May be resolved into three peaks on capillary GC (ca 1:5:10).

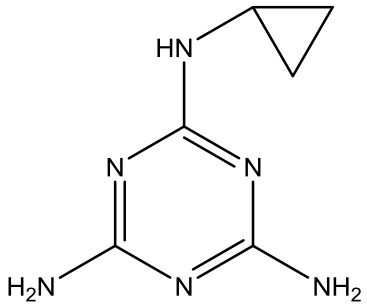
m/z	123	209	181	77	43	80	198	141
%	100	50	30	30	25	25	20	20

375 (5) – M^+
123 (100) – [M-252] $(CH_3)_2C{=}C\text{-}C_3H_3(CH_3)_2^+$ $C_9H_{15}^+$ m/z 123.1174
209 (50) – [M-166] $CH_2(CN)C_6H_4\text{-}O\text{-}C_6H_5^+$ $C_{14}H_{11}NO^+$ m/z 209.0841

No NIST spectrum available.

Cyromazine **$C_6H_{10}N_6$** **M:166(45%)**

Theoretical molecular ion: m/z 166.09670 (100%), 167.1001 (6.5%),
Average MW: 166.19



Triazine growth regulator acaricide and insecticide. Used as insect larvicide used mainly to control Diptera larvae and flies on livestock and other insect pests in the field and greenhouse.

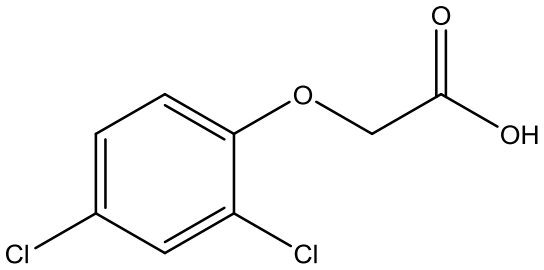
Acute oral LD50 for rat approx. 3,000 mg/kg (low toxicity).

m/z	151	43	69	68	166	109	165	56
%	100	95	60	50	45	40	30	30

166 (45) – M^+
151 (100) – [M-15] loss of NH to $C_6H_9N_5^+$ m/z 151.0858
[or loss of CH_3 by rearrangement?]
109 (40) – [M-57] loss of $NH_2C_3H_5$ to $C_3H_3N_5^+$ m/z 109.0388
43 (95) – [M-123] $C_3H_7^+$ m/z 43.0548 and/or $C_2H_5N^+$ m/z 43.04220 (?)

Cf. Similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C66215278&Mask=200

2,4-D acid **$C_8H_6Cl_2O_3$** **M:220,222(65,45%)**
Theoretical molecular ion: m/z 219.9694 (100%), 221.9665 (64%), 223.9635 (10%)
Average MW: 221.04



Chlorophenoxy herbicide. Selective, systemic action, used to control weeds in cereals and grass. Approved for use in EU.

Acute oral LD50 for rat >300 mg/kg (moderate toxicity).

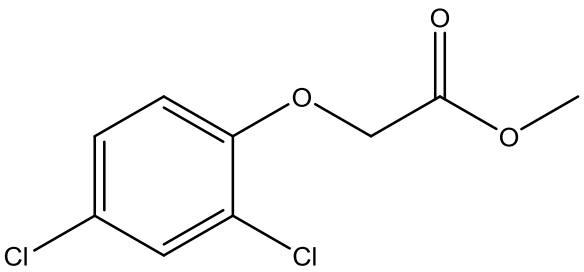
Poor transmission on GC unless derivatised.

m/z	162	164	220	222	161	163	175	133
%	100	65	65	45	40	35	30	30

220,222 (65,45) – M^+
162,164 (100,65) – [M-58] "dichlorophenol" $C_6H_4Cl_2O^+$ m/z 161.9639 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C94757&Mask=200

2,4-D methyl **$C_9H_8Cl_2O_3$** **M:234,236(65,40%)**
Theoretical molecular ion: m/z 233.9851 (100%), 235.9821 (64%), 237.9792 (10%)
Average MW: 235.06



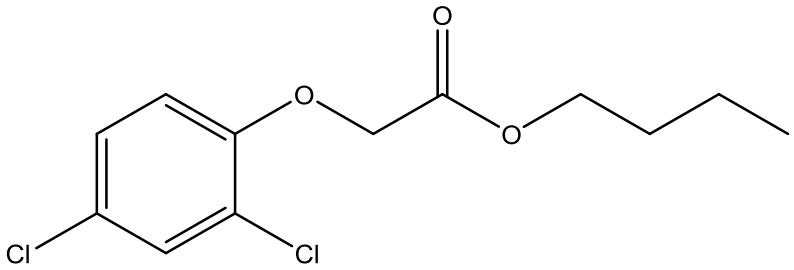
m/z	199	175	234	45	177	236	161	201
%	100	65	65	45	40	35	30	30

234,236 (65,40) – M^+
199,201 (100,30) – [M-35] loss of Cl to $C_9H_8ClO_3^+$ m/z 199.0162 etc.
175,177 (65,40) – [M-59] loss of COOCH3 to $C_7H_5Cl_2O^+$ m/z 174.97175 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1928387&Mask=200#Mass-Spec

2,4-D n-butyl **$C_{12}H_{14}Cl_2O_3$** **M:276,278(30,20%)**

Theoretical molecular ion: m/z 276.0320 (100%), 278.0291 (64%), 280.0261 (10%)
Average MW: 277.14



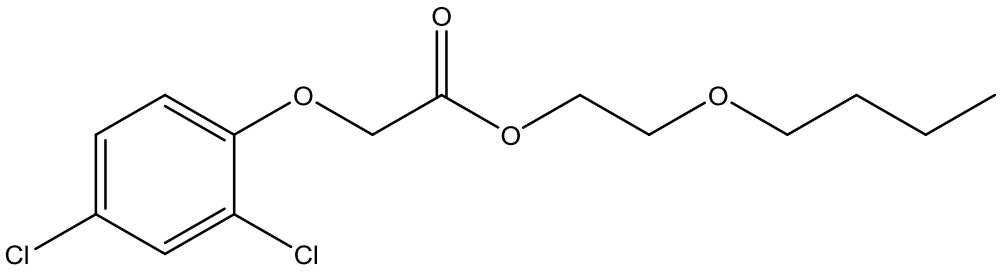
m/z	57	185	41	29	276	175	162	278
%	100	50	45	40	30	25	25	20

276,278 (30,20) - M+
185,187 (50,15) – [M-91] loss of Cl & C_4H_8 to $C_8H_6ClO_3^+$ m/z 185.00055 etc.

Cf. similar, but noisy, spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C94804&Units=SI&Mask=200#Mass-Spec listed as "Acetic acid, (2,4-dichlorophenoxy)-, butyl ester"

2,4-D butoxyethyl **$C_{14}H_{18}Cl_2O_4$** **M:320,322(8,5%)**

Theoretical molecular ion: m/z 320.0582 (100%), 322.0553 (64%), 324.0523 (10%)
Average MW: 321.19



Sometimes called 2,4-D-butotyl or 2,4-D-BOE.

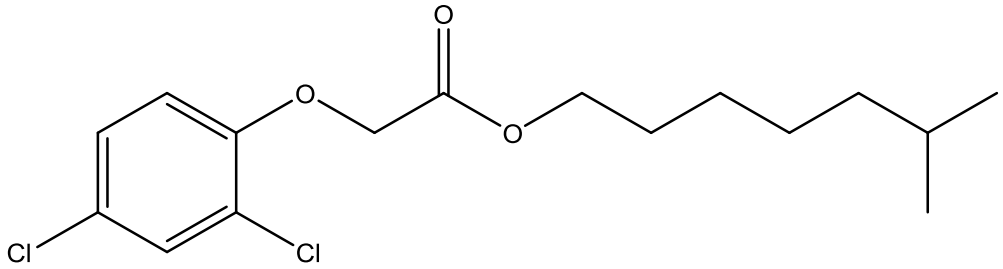
m/z	57	56	41	220	29	85	175	222
%	100	40	25	20	20	15	15	15

320,322 (8,5) – M^+
247,249 (5,3) – [M-73] loss of C_4H_9O to $C_{10}H_9Cl_2O_3^+$ m/z 246.9929 etc.
220,222 (20,15) – [M-100] loss of $C_6H_{12}O$ to $C_8H_6Cl_2O_3^+$ (free acid) m/z 219.9694 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1929733&Units=SI&Mask=200#Mass-Spec

2,4-D i-octyl **$C_{16}H_{22}Cl_2O_3$** **M:332,334(20,15%)**

Theoretical molecular ion: m/z 332.0946 (100%), 334.0916 (64%), 335.0950 (11%)
Average MW: 333.25



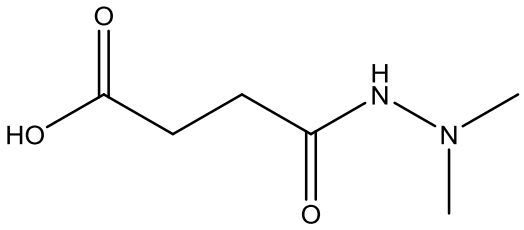
m/z	57	71	43	220	70	41	222	332
%	100	65	65	50	40	35	25	20

332,334 (20,15) – M^+
220,222 (50,250 – [M-112] $C_8H_6Cl_2O_3^+$ (free acid) m/z 219.9694 etc.

No NIST spectrum available.

Daminozide "Alar" **$C_6H_{12}N_2O_3$** **M:160(5%)**

Theoretical molecular ion: m/z 160.0848 (100%), 161.0882 (6%)
Average MW: 160.17



Hydrazide plant growth regulator, for use in certain ornamentals. Approved for use in EU and US. Acute oral LD50 for rat >5,000 mg/kg (low toxicity). Irritant.

Very poor GC transmission. GC analysis may be performed following methylation or conversion (by dehydration) to a cyclic (**daminozide lactam**) derivative (reaction catalysed by acetic anhydride)

Daminozide may be metabolised to "unsymmetrical dimethyl hydrazine" UDMH [NH_2-$N(CH_3)_2$], which is of toxicological concern (see below). This may be determined more conveniently by GC-MS following conversion to e.g. **UDMH benzaldehyde imine** (below).

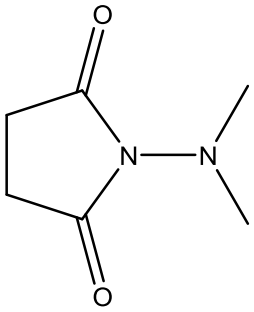
m/z	59	43	60	42	100	44	118	142
%	100	50	45	20	20	15	10	10

160 (5) – M^+
59 (100) – [M-101] $(CH_3)_2N.NH^+$ (m/z 59.0609) and/or CH_2COOH (m/z 59.0133)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1596845&Mask=200

Daminozide lactam $C_6H_{10}N_2O_2$ **M:142(10%)**

Theoretical molecular ion: m/z 142.0742 (100%), 143.0776 (6.5%)
Average MW: 142.16



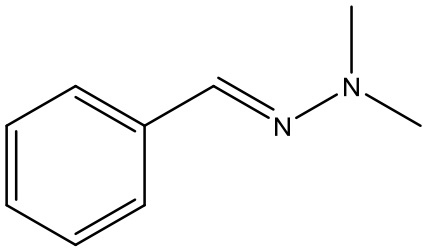
m/z	43	59	42	100	142	44	72	55
%	100	40	30	25	10	10	10	10

No NIST spectrum available.

Daminozide UDMH derivative $C_9H_{12}N_2$ **M:148(100%)**

UDMH benzaldehyde imine

Theoretical molecular ion: m/z 148.1001 (100%), 149.1034 (9.7%)
Average MW: 148.21



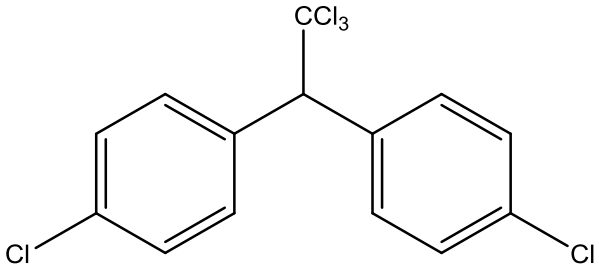
A toxicologically important degradation product of daminozide is 1,1-dimethylhydrazine (sometimes called "unsymmetrical dimethylhydrazine" UDMH ($C_2H_8N_2$, mw 60). It is more convenient to determine this by GC after derivatisation, e.g. as the benzaldehyde condensation product (imine):

m/z	148	77	133	147	118	92	104	122
%	100	30	20	20	20	15	15	15

No NIST spectrum available.

DDT **$C_{14}H_9Cl_5$** **M:352,354,356(1,2,1%)**

Theoretical molecular ion: m/z 351.91469 (62.6%), 353.91174 (100%), 355.90879 (44.7%), 357.90584 (14.3%)
Average MW: 354.48



Organochlorine insecticide and acaricide. DDT is banned for agricultural use in most countries, but is still used for public health purposes, e.g. mosquito control.

A mosquito was heard to complain,
That chemists were poisoning his brain.
The cause of his sorrow,
Was para-dichloro
Diphenyltrichloroethane.

Acute oral LD50 for rat >100 mg/kg (moderate toxicity).

Technical DDT comprises mainly the p,p'- isomer, but contains low levels (1-5%) of the o,p'-isomer, which has a very similar mass spectrum and a shorter GC retention time. DDT may undergo reductive degradation to **TDE (DDD)** in "active" GC injectors and columns.

DDT has several metabolites, see **DDA, DDE, DDMU, DDMS, DDNU, DDOH, TDE,** etc.

For residues purposes, "total DDT" is usually defined as *p,p'*-DDT plus its main isomer (*o,p'*-DDT) and two degradation products *p,p'*-TDE and *p,p'*-DDE:
N.B. Note the rather similar GC-MS characteristics of o,p'-DDT and p,p'-TDE.
KI (SE-30) = 23.0 (cf o,p'-DDT = 22.3)

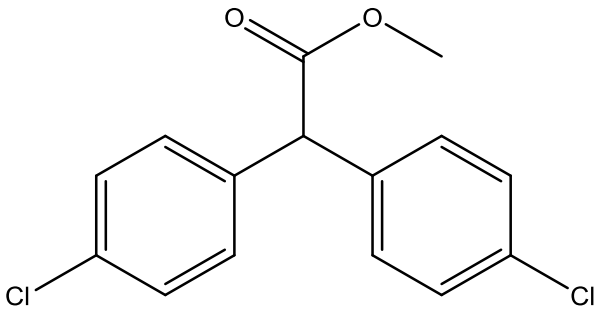
m/z	235	237	165	236	199	239	200	246
%	100	65	40	15	15	10	10	10

352,354,356 (1,2,1) – M^+ very weak
316,317,318,319 (1,1,2,1) – [M-36] loss of HCl to C14H8Cl4+
281,282,283,284 (1,3,1,3) – [M-71] loss of HCl2 to C14H8Cl3+ m/z
246,248 (6,4)- [M-106] loss of HCl3to C14H8Cl2+ m/z
235,237 (100,65) – [M-117] loss of CCl_3 to $(ClC_6H_4)_2CH^+$ $C_{13}H_9Cl_2^+$ m/z 235.0081 (100%), 237.0052 (64%)
165 (40) – [M-187] $C_{13}H_9^+$ m/z 165.0704

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C50293&Mask=200

DDT metabolites/degradation products:

DDA, methyl ester **$C_{15}H_{12}Cl_2O_2$** **M:294,296(15,10%)**
Theoretical molecular ion: m/z 294.0214 (100%), 296.0185 (64%), 295.0248 (16%),
Average MW: 295.16

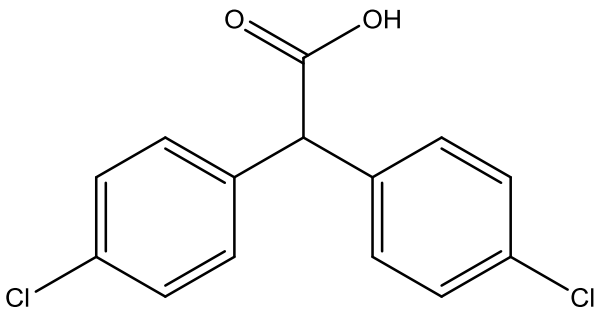


Methyl ester of **DDT** acid metabolite.

m/z	235	237	165	294	199	200	296	72
%	100	65	30	15	10	10	10	5

No NIST spectrum available.

DDA **$C_{14}H_{10}Cl_2O_2$** **M:280,282(10,7%)**
Theoretical molecular ion: m/z 280.0058 (100%), 282.0028 (64%), 281.0091 (15%)
Average MW: 281.13

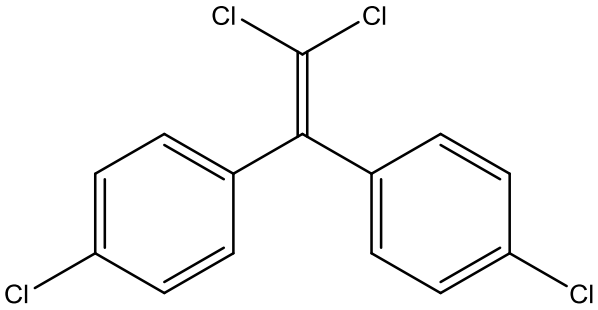


DDT metabolite. Poor GC transmission.

m/z	235	237	165	236	280	201	199	282
%	100	65	30	10	10	10	10	5

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C83056&Units=SI&Mask=200#Mass-Spec

DDE **$C_{14}H_8Cl_4$** **M:316,318,320 (60,80,40%)**
Theoretical molecular ion: m/z 317.9351 (100%), 315.9380 (78%), 319.9321 (24%)
Average MW: 318.02



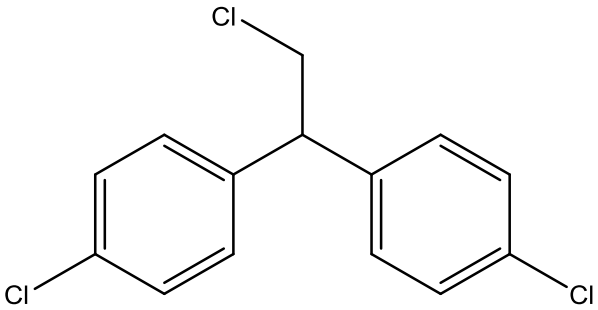
DDT metabolite. KI (SE-30) = 21.0

m/z	246	318	248	316	176	320	210	247
%	100	80	65	60	45	40	20	15

316,318,320 (60,80,40) – M^+
281,282,283,284,285,286 (8,5,8,6,3,2) – [M-35] loss of Cl to $C_{14}H_8Cl_3^+$ m/z 280.9692 etc.
246,248,250 (100,65,10) – [M-70] loss of Cl_2 to $C_{14}H_8Cl_2^+$ m/z 246.0003 etc.

Cf. similar (weak) NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C72559&Units=SI&Mask=200#Mass-Spec

DDMS **$C_{14}H_{11}Cl_3$** **M:284,286,288(5,5,2%)**
Theoretical molecular ion: m/z 283.9926 (100%), 285.9897 (96%), 287.9867 (31%)
Average MW: 285.59

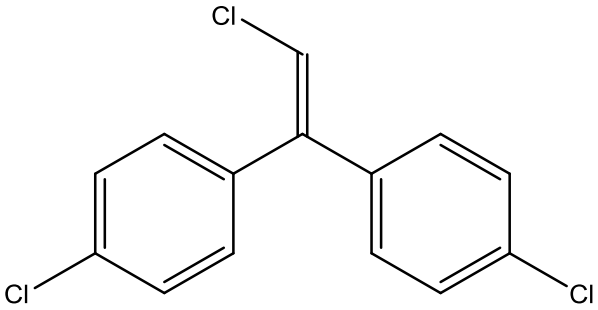


Reductive metabolite of **DDT**.

m/z	235	237	165	236	284	286	199	200
%	100	65	30	15	5	5	5	5

Cf. Similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2642800&Units=SI&Mask=200#Mass-Spec

DDMU ("TDE-olefin") **$C_{14}H_9Cl_3$** **M:282,284,286(80,80,30%)**
Theoretical molecular ion: m/z 281.9770 (100%), 283.9740 (96%), 285.9711 (31%)
Average MW: 283.58



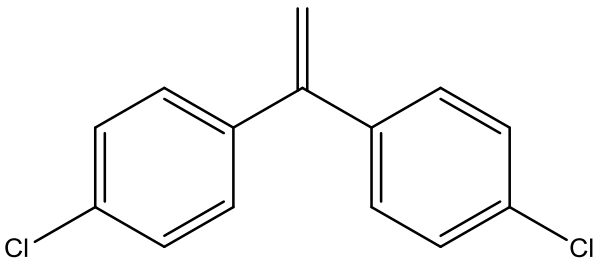
DDT metabolite.

m/z	212	282	284	176	214	247	286	88
%	100	80	80	45	45	30	30	25

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1022226&Units=SI&Mask=200#Mass-Spec

DDNU **$C_{14}H_{10}Cl_2$** **M:248,250(80,50%)**

Theoretical molecular ion: m/z 248.01596 (100%), 250.0130 (64%), 249.0193 (15%),
Average MW: 249.13



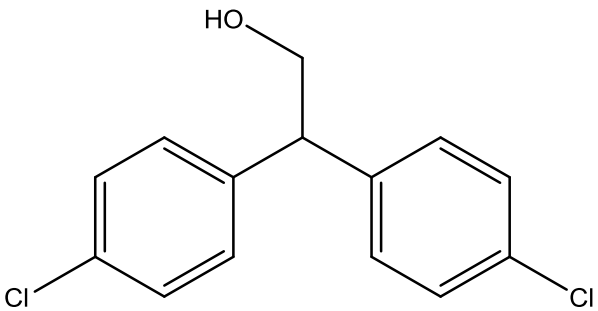
DDT metabolite, and potential dehydration product of **chlorfenethol**.

m/z	178	248	250	213	88	177	176	106
%	100	80	60	40	30	20	20	20

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2642811&Units=SI&Mask=200#Mass-Spec

DDOH **$C_{14}H_{12}Cl_2O$** **M:266,268(5,2%)**

Theoretical molecular ion: m/z 266.0265 (100%), 268.0236 (64%), 267.0299 (15%)
Average MW: 267.15



DDT metabolite. Poor GC transmission.

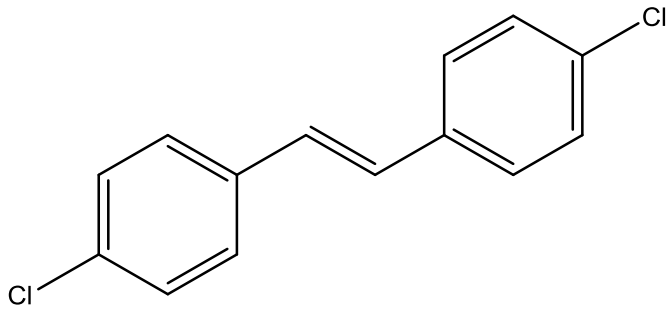
m/z	235	237	165	200	199	236	266	239
%	100	65	30	15	10	10	5	5

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2642822&Units=SI&Mask=200#Mass-Spec

DDE isomer **$C_{14}H_8Cl_4$** **M:316,318,320(40,55,25%)**

***Aspergillus niger* metabolite**

Theoretical molecular ion: m/z 317.9351 (100%), 315.9380 (78%), 319.9321 (24%)
Average MW: 318.02



DDT metabolite produced by *Aspergillus niger*.

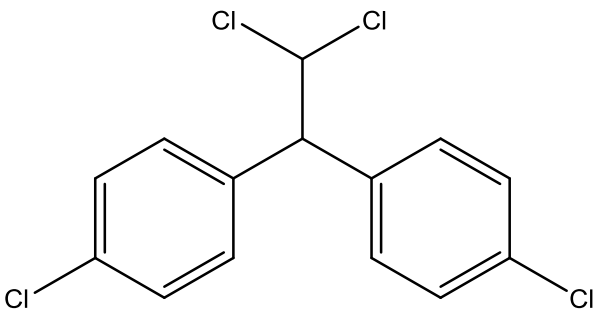
An isomer of p,p'-DDE, with very similar mass spectrum but longer GC RT.

m/z	246	248	318	316	320	176	281	283
%	100	65	55	40	25	25	15	15

No NIST spectrum available

TDE (DDD) **$C_{14}H_{10}Cl_4$** **M:318,320,322 (1,2,1%)**

Theoretical molecular ion: m/z 317.9537 (78%), 319.9507 (100%), 321.9478 (48%)
Average MW: 320.03



A metabolite of **DDT**.

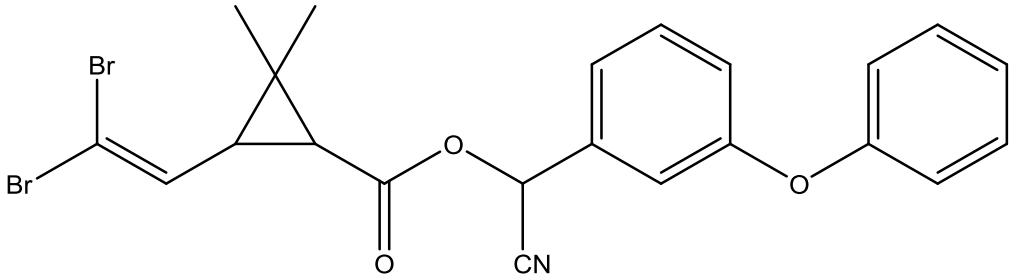
May be produced by degradation of DDT in "active" GC systems. KI (SE-30) = 22.0

m/z	235	237	165	236	199	239	200	212
%	100	65	35	15	15	10	10	10

318,320,322 (1,2,1) – M^+ very weak
282,283,284,285 (2,1,2,1) – [M-36] loss of HCl to C14H9Cl3+ m/z
246,248 (1,2) – [M-72] loss of H2Cl2 loss of 2HCl to C14H8Cl2 m/z
235,237 (100,65) – [M-83] loss of $CHCl_2$ to $(ClC_6H_4)_2CH^+$ $C_{13}H_9Cl_2^+$ m/z 235.0081 etc.
165 (40) – [M-187] $C_{13}H_9^+$ m/z 165.0704

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C72548&Units=SI&Mask=200#Mass-Spec

Deltamethrin **$C_{22}H_{19}Br_2NO_3$** **M:503,505,507(1,2,1%)**
Theoretical molecular ion: m/z 502.9732 (51%), 504.9711 (100%), 506.9691 (49%)
Average MW: 505.21



Synthetic pyrethroid insecticide and veterinary treatment Very widely used. It is highly toxic to humans and other mammals and is a neurotoxin. It is relatively non-toxic to birds and earthworms, although it presents a high risk to most aquatic organisms and honeybees.

Approved for use in the EU, Australia and the USA.

Acute oral LD50 for rat approx. 90 mg/kg (high toxicity).

One peak on capillary GC (unlike many other pyrethroids).

m/z	253	181	251	255	208	93	77	172
%	100	85	50	50	45	40	30	30

503,505,507 (1,2,1) – M^+
251,253,255 (50,100,50) – [M-252] $Br_2C{=}CHC_3H_3(CH_3)_2^+$ $C_7H_9Br_2^+$ m/z 250.9071 etc.
208 (45) – [M-295] $CH(CN)C_6H_4OC_6H_5^+$ $C_{14}H_{10}NO^+$ m/z 208.0762
181 (85) – [M-322] $C_7H_4OC_6H_5^+$ $C_{13}H_9O^+$ m/z 181.0653
172,174 (30,30) – [M-331] $BrC{=}CH(C_3H_3(CH_3)_2^+$ $C_7H_9Br^+$ m/z 171.9888 etc.
93 (40) – [M-410] $C_6H_5O^+$ m/z 93.0340

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C52918635&Mask=200

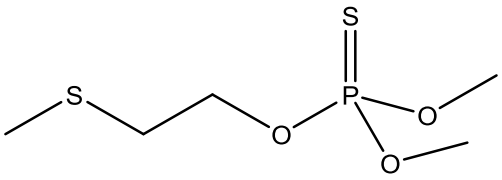
Demephion – a mixture of **demephion-O** and **demephion-S**

Organophosphorus insecticide. Acute oral LD50 for rat approx. 20 mg/kg (high toxicity)

Both isomers are rapidly metabolised to sulphoxide and sulphone.

Demephion-O **$C_5H_{13}O_3PS_2$** **M:216(0.5%)**

Theoretical molecular ion: m/z 216.0044 (100%), 218.0002 (9.0%), 217.0077 (5.4%),
Average MW: 216.25



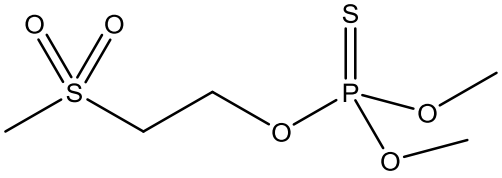
m/z	74	75	143	41	76	125	47	109
%	100	33	9	7	6	5	4	3

216 (0.5) – M^+ weak
143 (9) – [M-75] $(CH_3O)_2(HS)(HO)P^+$ $C_2H_8O_3PS^+$ m/z 142.9932
125 (5) – [M-91] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (3) – [M-107] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055 [O/S swap]
75 (33) – [M-141] $CH_3SCH_2CH_2^+$ $C_3H_7S^+$ m/z 75.0269
74 (100) – [M-142] $CH_3SCH{=}CH_2^+$ $C_3H_6S^+$ m/z 74.0190
47 (4) – [M-169] CH_3S^+ m/z 46.9956

No NIST spectrum available.

Demephion-O sulphone **$C_5H_{13}O_5PS_2$** **M:248(1%)**

Theoretical molecular ion: m/z 247.9942 (100%), 248.9976 (5.4%), 249.9900 (9%)
Average MW: 248.25



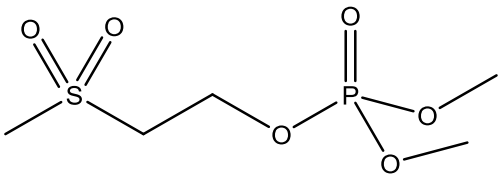
m/z	125	169	79	109	111	63	47	107
%	100	65	43	18	11	11	11	11

248 (1) – M^+ weak
169 (65) – [M-79] loss of CH_3SO_2 to $C_4H_{10}O_3PS^+$ m/z 169.0088
125 (100) – [M-123] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
107 (11) – [M-241] $CH_3SO_2CH_2CH_2^+$ $C_3H_7O_2S^+$ m/z 107.0167
79 (43) – [M-169] $CH_3SO_2^+$ $CH_3O_2S^+$ m/z 78.9854

No NIST spectrum available.

Demephion-O oxon sulphone **$C_5H_{13}O_6PS$** **M:232(0%)**

Theoretical molecular ion: m/z 232.0171 (100%), 233.0204 (5.4%), 234.0128 (4.5%)
Average MW: 232.19



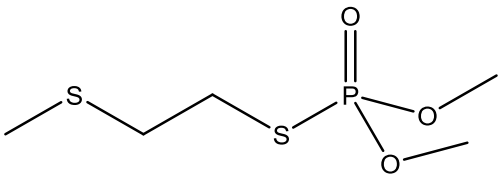
m/z	153	109	127	79	96	95	154	63
%	100	82	64	15	10	9	7	7

232 (0) – M^+ absent
153 (100) – [M-79] loss of CH_3SO_2 to $C_4H_{10}O_4P^+$ m/z 153.0317
109 (82) – [M-123] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (15) – [M-153] $CH_3SO_2^+$ $CH_3O_2S^+$ m/z 78.9854
and/or $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

No NIST spectrum available.

Demephion-S **$C_5H_{13}O_3PS_2$** **M:216(3%)**

Theoretical molecular ion: m/z 216.0044 (100%), 217.0077 (5.4%), 218.0002 (9.0%)
Average MW: 216.25



Demephion-S is rapidly metabolised to sulphoxide and sulphone.

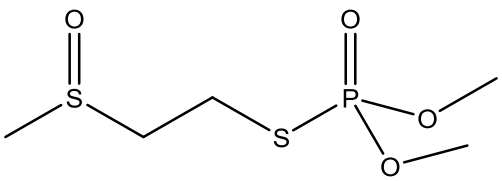
m/z	74	142	112	75	109	41	76	79
%	100	15	13	12	10	9	8	7

216 (3) – M^+
142 (15) – [M-74] $(CH_3O)_2(HO)PS^+$ $C_2H_7O_3PS^+$ m/z 141.9854
112 (13) – [M-104] $(CH_3O)(HO)(HS)P^+$ CH_5OPS^+ m/z 111.9748
109 (100) – [M-107] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (7) – [M-137] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
74 (100) – [M-142] $CH_3SCH{=}CH_2^+$ $C_3H_6S^+$ m/z 74.0190

No NIST spectrum available.

Demephion-S sulphoxide **$C_5H_{13}O_4PS_2$** **M:232(0%)**

Theoretical molecular ion: m/z 231.9993 (100%), 233.0026 (5.4%), 233.9951 (9.0%)
Average MW: 232.25



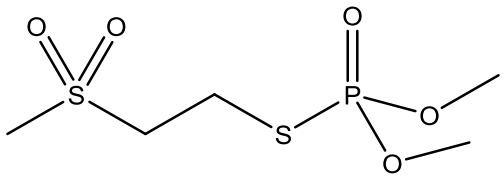
Prone to degradation on GC. (Spectrum from direct insertion MS)

m/z	169	109	125	74	91	171	142	110
%	100	69	42	10	7	6	5	5

232 (0) – M^+ absent
169 (100) – [M-61] loss of CH_3SO to $C_4H_{10}O_3PS^+$ m/z 169.0088
125 (42) – [M-107] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (82) – [M-121] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055

No NIST spectrum available.

Demephion-S sulphone **$C_5H_{13}O_5PS_2$** **M:248(0.5%)**
Theoretical molecular ion: m/z 247.9942 (100%), 248.9976 (5.4%), 249.9900 (9.0%)
Average MW: 248.25



m/z	169	109	125	168	110	142	170	127
%	100	52	48	32	21	20	10	8

248 (0.5) – M^+ weak
169 (100) – [M-79] loss of CH_3SO_2 to $C_4H_{10}O_3PS^+$ m/z 169.0088
125 (48) – [M-123] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (82) – [M-139] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055

No NIST spectrum available.

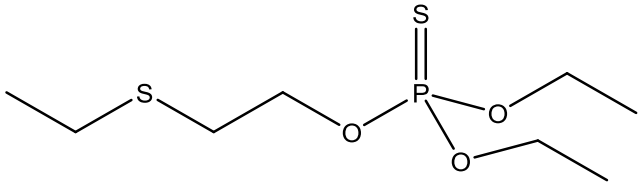
Demeton – a mixture of **demeton-O** and **demeton-S**

Organophosphorus thiophosphate insecticide. Not approved for use in EU.

Acute oral LD50 for rat approx. 2 mg/kg (high toxicity). Neurotoxic.

Both demeton isomers are rapidly metabolised to sulphoxide and sulphone.

Demeton-O **$C_8H_{19}O_3PS_2$** **M:258(0.3%)**
Theoretical molecular ion: m/z 258.0513 (100%), 259.0547 (8.7%), 260.0471 (9.0%)
Average MW: 258.33



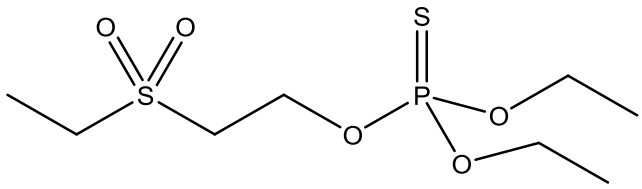
m/z	88	89	60	61	29	171	115	59
%	100	53	39	27	12	10	9	8

258 (0.3) – M^+ weak
171 (10) – [M-87] $(CH_3CH_2O)_2(HO)(HS)P^+$ $C_4H_{12}O_3PS^+$ m/z 171.0245
88 (100) – [M-170] $CH_3CH_2SCH{=}CH_2^+$ $C_4H_8S^+$ m/z 88.0347
60 (39) – [M-198] $C_2H_4S^+$ m/z 60.0034

Cf. similar spectrum at http://www.restek.com/compound/view/298-03-3/Demeton-O

Demeton-O sulphone **$C_8H_{19}O_5PS_2$** **M:290(1%)**

Theoretical molecular ion: m/z 290.0412 (100%), 291.0445 (8.7%), 292.0370 (9.0%)
Average MW: 290.33



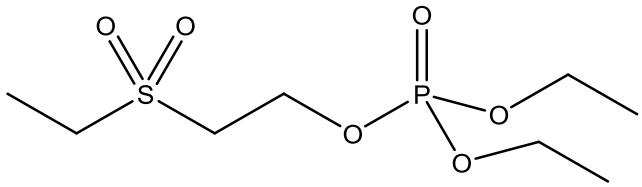
m/z	197	153	29	45	141	125	97	121
%	100	89	84	77	71	51	44	42

290 (1) – M^+
197 (100) – [M-93] loss of $CH_3CH_2SO_2$ to $C_6H_{14}O_3PS^+$ m/z 197.0401
153 (89) – [M-137] $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (51) – [M-165] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826

No NIST spectrum available.

Demeton-O oxon sulphone **$C_8H_{19}O_3PS$** **M:274(2%)**

Theoretical molecular ion: m/z 274.0640 (100%), 275.0674 (8.7%), 276.05979 (4.5%)
Average MW: 274.27



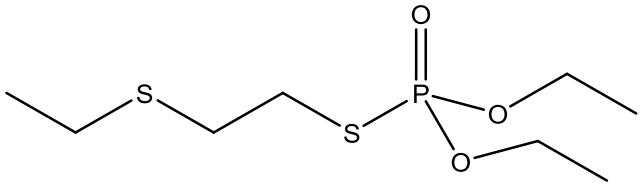
m/z	125	99	181	121	127	153	155	29
%	100	85	73	45	45	44	43	34

274 (2) – M^+
181 (73) – [M-93] loss of $CH_3CH_2SO_2$ to $C_6H_{14}O_4P^+$ m/z 181.0630
155 (43) – [M-119] $(CH_3CH_2O)_2(HO)_2P^+$ $C_4H_{12}O_4P^+$ m/z 155.0473
153 (44) – [M-121] loss of $CH_3CH_2SO_2CH_2CH_2$ to $C_4H_{10}O_4P^+$ m/z 153.0317
127 (45) – [M-147] $(CH_3CH_2O)(HO)_3P^+$ $C_2H_8O_4P^+$ m/z 127.0160
125 (51) – [M-149] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121 (100) – [M-153] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
99 (85) – [M-175] $(HO)_4P^+$ $H_4O_4P^+$ m/z 98.9845

No NIST spectrum available.

Demeton-S $C_8H_{19}O_3PS_2$ **M:258(0.8%)**

Theoretical molecular ion: m/z 258.0513 (100%), 259.0547 (8.7%), 260.0471 (9.0%)
Average MW: 258.33



Equivalent to **disulfoton oxon**.

Rapidly metabolised to sulphoxide and sulphone.

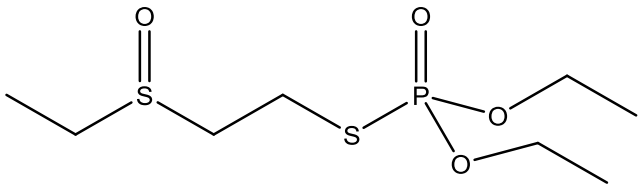
m/z	88	60	29	89	61	114	115	93
%	100	42	14	13	13	10	9	9

258 (1) – M^+
170 (5) - [M-88] $(CH_3CH_2O)_2(HO)P{=}S^+$ $C_4H_{11}O_3PS^+$ m/z 170.0167
142 (5) – [M-116] $(CH_3CH_2O)(HO)_2P{=}S^+$ $C_2H_7O_3PS^+$ m/z 141.9854
114 (10) – [M-144] $(HO)_3P{=}S^+$ $H_3O_3PS^+$ m/z 113.9541
88 (100) – [M-170] $CH_3CH_2SCH{=}CH_2^+$ $C_4H_8S^+$ m/z 88.0347
60 (42) – [M-198] $C_2H_4S^+$ m/z 60.0034

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C126750&Mask=200

Demeton-S sulphoxide $C_8H_{19}O_4PS_2$ **M:274(0%)**

Theoretical molecular ion: m/z 274.0462 (100%), 275.0496 (8.7%), 276.0420 (9.0%)
Average MW: 274.33



Rapidly metabolised to sulphone. Not amenable to GC.

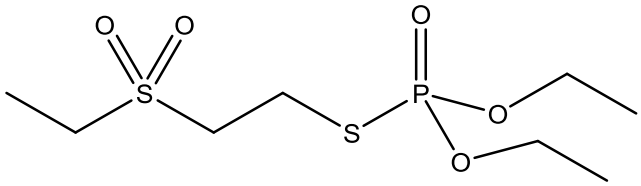
m/z	109	197	141	29	81	137	45	61
%	100	89	77	28	27	26	24	23

274 (0) – M^+ absent
197 (89) - [M-77] loss of CH_3CH_2SO to $C_6H_{14}O_3PS^+$ m/z 197.0401
169 (10) - [M-105] $(CH_3CH_2O)_2P{=}O.S^+$ $C_4H_{10}O_3PS^+$ m/z 169.0088
141 (77) - [M-133] $(CH_3CH_2O)(HO)P{=}O.S^+$ $C_2H_6O_3PS^+$ m/z 140.9775
137 (26) - [M-137] $(CH_3CH_2O)_2P{=}O^+$ $C_4H_{10}O_3P^+$ m/z 137.0368
109 (100) - [M-165] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
81 (27) - [M-193] $(HO)_2P{=}O^+$ $H_2O_3P^+$ m/z 80.9742
61 (23) - [M-213] $CH_3CH_2S^+$ $C_2H_5S^+$ m/z 61.0112 (reduction/rearrangement?)
45 (24) - [M-229] $CH_3CH_2O^+$ $C_2H_5O^+$ m/z 45.0340

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2496926&Mask=200#Mass-Spec

Demeton-S sulphone **$C_8H_{19}O_5PS_2$** **M:290(0%)**

Theoretical molecular ion: m/z 290.0412 (100%), 291.0445 (8.7%), 292.0370 (9.0%)
Average MW: 290.33



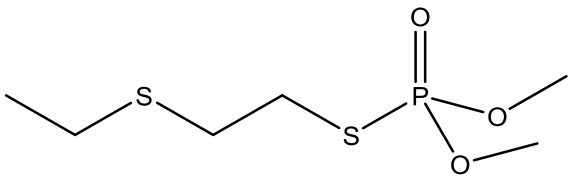
m/z	109	197	141	29	81	61	169	45
%	100	95	73	40	32	28	28	27

290 (0) – M^+ absent
197 (95) – [M-93] loss of $CH_3CH_2SO_2$ to $C_6H_{14}O_3PS^+$ m/z 197.0401
169 (28) – [M-121] $(CH_3CH_2O)_2P{=}O.S^+$ $C_4H_{10}O_3PS^+$ m/z 169.0088
141 (73) – [M-149] $(CH_3CH_2O)(HO)P{=}O.S^+$ $C_2H_6O_3PS^+$ m/z 140.9775
109 (100) – [M-181] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
81 (32) – [M-209] $(HO)_2P{=}O^+$ $H_2O_3P^+$ m/z 80.9742
61 (28) – [M-229] $CH_3CH_2S^+$ $C_2H_5S^+$ m/z 61.0112 (reduction/rearrangement?)

Cf. similar spectrum for m/z 50-200 ions at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2496915&Mask=200#Mass-Spec
But dominated by m/z 29 (100%) and 27. The weak high mass ion is not the molecular ion (m/z 290) but m/z 291 (perhaps from auto-CI to give $(M+H)^+$ at m/z 291, due to high sample concentration in ion source.)

Demeton-S-methyl **$C_6H_{15}O_3PS_2$** **M:230(1%)**

Theoretical molecular ion: m/z 230.0200 (100%), 231.0234 (6.5%) ,232.0158 (9.0%)
Average MW: 230.28



Rapidly metabolised to sulphoxide and sulphone.

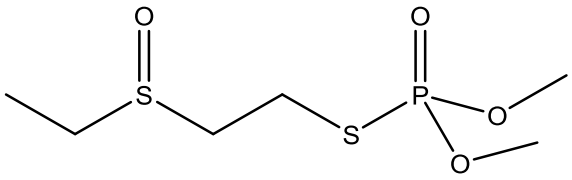
m/z	88	60	142	109	89	61	79	112
%	100	54	12	12	10	9	8	8

230 (1) – M^+
142 (12,5) – [M-88] $(CH_3O)_2(HO)P{=}S^+$ $C_2H_7O_3PS^+$ m/z 141.9854
112 (8) – [M-118] $(CH_3O)(HO)(HS)P^+$ $CH_5O_2PS^+$ m/z 111.9748
109 (100) – [M-121] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
88 (100) – [M-142] $CH_3CH_2SCH{=}CH_2^+$ $C_4H_8S^+$ m/z 88.0347
79 (8) – [M-151] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
60 (54) – [M-170] $C_2H_4S^+$ m/z 60.0034

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C919868&Mask=200 though it exhibits a much stronger molecular ion at m/z 230 (5-10%).

Demeton-S-methyl sulphoxide $C_6H_{15}O_4PS_2$ **M:246(0%)**

Theoretical molecular ion: m/z 246.0149 (100%), 247.0183 (6.5%), 248.0107 (9.0%)
Average MW: 246.28



A metabolite of demeton-S-methyl and a pesticide in its own right ("Oxydemeton-methyl" or "Metasystox R")
Very poor GC transmission (spectrum obtained by direct insertion MS).
It may be determined by LC-electrospray MS (Beike 2002).

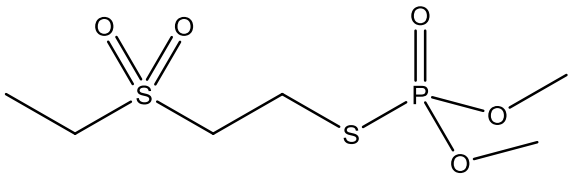
m/z	169	109	125	110	168	105	60	142
%	100	90	50	15	10	10	10	5

246 (0) – M^+
169 (100) – [M-77] loss of CH_3CH_2SO to $(CH_3O)_2P{=}O.SCH_2CH_2^+$ $C_4H_{10}O_3PS^+$ m/z 169.0088
142 (5) – [M-104] $(CH_3O)_2(HO)P{=}S^+$ $C_2H_7O_3PS^+$ m/z 141.9854
125 (50) – [M-121] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (90) – [M-137] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
105 (10) – [M-241] $CH_3CH_2SOCH_2CH_2^+$ $C_4H_9OS^+$ m/z 105.0374

No NIST spectrum available

Demeton-S-methyl sulphone $C_6H_{15}O_5PS_2$ **M:262(0%)**

Theoretical molecular ion: m/z 262.0099 (100%), 263.0132 (6.5%), 264.0057 (9.0%)
Average MW: 262.27



Sometimes poor GC transmission.

m/z	169	109	125	110	168	142	29	170
%	100	51	33	15	15	9	8	7

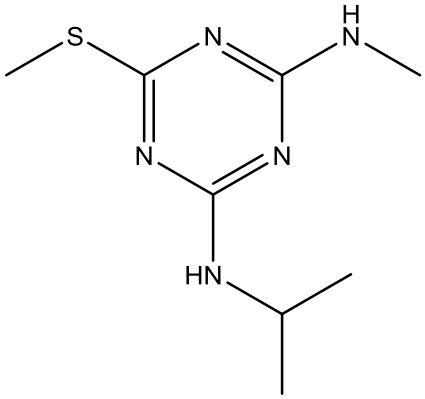
262 (0) – M^+ absent
169 (100) – [M-93] loss of $CH_3CH_2SO_2$ to $(CH_3O)_2P{=}O.SCH_2CH_2^+$ $C_4H_{10}O_3PS^+$ m/z 169.0088
142 (9) – [M-120] $(CH_3O)_2(HO)PS^+$ $C_2H_7O_3PS^+$ m/z 141.9854
125 (50) – [M-121] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
110 (15) – [M-152] $(CH_3O)_2(HO)P^+$ $C_2H_7O_3P^+$ m/z 110.0133
109 (51) – [M-153] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055

Cf. similar but poor spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C17040196&Mask=200

Also – compare slightly noisy spectrum for **Demeton-O-methyl** at http://webbook.nist.gov/cgi/cbook.cgi?ID=C867276&Mask=200 which exhibits ions at m/z 88, 91, 106, 60 109 and 142.

Desmetryn **$C_8H_{15}N_5S$** **M:213(100%)**

Theoretical molecular ion: m/z 213.1048 (100.0%), 214.1082 (8.7%), 215.1006 (4.5%)
Average MW: 213.30



Methylthiotriazine herbicide. Used to control annual broad-leaved weeds and some grasses. Not approved for use in EU.

Acute oral LD50 for rat approx. 1,000 mg/kg (moderate toxicity).

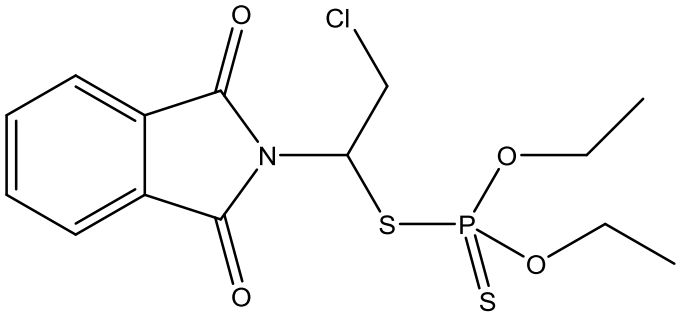
m/z	213	198	171	57	82	124	99	156
%	100	65	35	35	25	20	15	15

213 (100) – M^+
198 (65) – [M-15] loss of CH_3 to $C_7H_{12}N_5S^+$ m/z 198.0813
171 (35) – [M-42] loss of C_3H_6 to $C_5H_9N_5S_+$ m/z 171.05787

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1014693&Mask=200

Dialifos / Dialifor **$C_{14}H_{17}ClNO_4PS_2$** **M:393(1%)**

Theoretical molecular ion: m/z 393.0025 (100%), 394.9996 (32%)
Average MW: 393.84



Organophosphorus insecticide and acaricide, used on a variety of crops including potatoes, vegetables, fruit and cotton. No longer approved for use in EU.

Acute oral LD50 for rat approx. 70 mg/kg (high toxicity).

May be oxidised to dialifos oxon. Long GC RT.

m/z	208	210	76	97	357	65	129	130

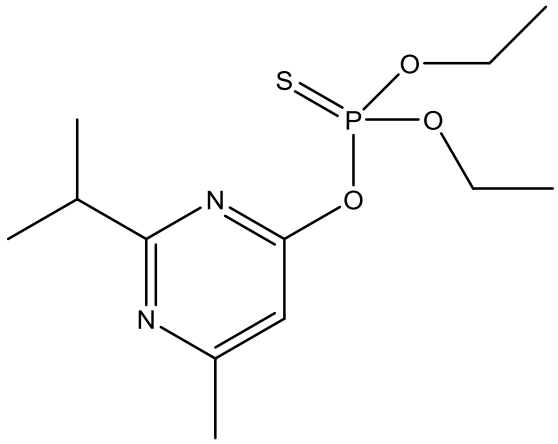
%	100	35	10	10	10	10	10	10

393 (1) – M^+ weak
357 (10) – [M-36] loss of HCl to $C_{14}H_{16}NO_4PS_2^+$ m/z 357.0258
208,210 (100,35) – [M-185] $C_6H_4.C_2NO_2.CHCH_2Cl^+$ $C_{10}H_7ClNO_2^+$ m/z 208.0165 etc.
130 (10) – [M-263] $(HO)_2(HS)PS^+$ $H_3O_2PS_2^+$ m/z 129.9312
129 (10) – [M-264] $(HO)_2PS_2^+$ $H_2O_2PS_2^+$ m/z 128.9234
97 (10) – [M-296] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
65 (10) – [M-328] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. Similar spectrum at http://www.restek.com/compound/view/10311-84-9/Dialifos

Diazinon **$C_{12}H_{21}N_2O_3PS$** **M:304(65%)**

Theoretical molecular ion: m/z 304.1011
Average MW: 304.35



Organophosphorus insecticide. Used to control sucking and chewing insects on a wide range of crops including top fruit. It also has livestock applications. No longer approved for use in EU.

Acute oral LD50 for rat approx. 1,000 mg/kg (moderate toxicity).

m/z	179	137	152	304	199	93	153	97
%	100	95	85	65	50	45	40	35

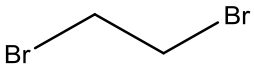
Assignments confirmed by accurate mass (Cardiff GCT)
304 (65) – M^+ m/z 304.1011
289 (11) – [M-15] loss of CH_3 to $C_{11}H_{18}N_2O_3PS^+$ m/z 289.0776
276 (20) – [M-28] loss of C_2H_4 from OP ester to $C_{10}H_{17}N_2O_3PS^+$ m/z 276.0698
260 (15) – [M-44] loss of C_2H_4O to $C_{10}H_{17}N_2O_2PS^+$ m/z 260.0748
248 (20) – [M-56] loss of $2C_2H_4$ from OP ester to $C_8H_{13}N_2O_3PS^+$ m/z 248.0385
227 (30) – [M-77] loss of C_2H_5OS to $C_{10}H_{16}N_2O_2P^+$ m/z 227.0949
216 (25) – [M-88] loss of $C_4H_8O_2$ to $C_8H_{13}N_2O_2PS^+$ m/z 216.0486
215 (20) – [M-89] loss of C_4H_9S to $C_8H_{12}N_2OPS^+$ m/z 215.0586
199 (50) – [M-105] loss of C_4H_9OS to $C_8H_{12}N_2O_2P^+$ m/z 199.0636
179 (100) – [M-125] $(C_3H_7)(CH_3)C_4N_2H.\underline{OCH_2CH_3}^+$ $C_{10}H_{15}N_2O^+$ m/z 179.1184
(interesting rearrangement - transfer of ethoxy group from OP ester to diazine)
163 (15) – [M-141] $(C_3H_7)(CH_3)C_4N_2H.\underline{CH_2CH_3}^+$ $C_{10}H_{15}N_2^+$ m/z 163.1235
(interesting rearrangement - transfer of ethyl group from OP ester to diazine)
152 (85) – [M-152] $(C_3H_7)(CH_3)C_4N_2H.OH^+$ $C_8H_{12}N_2O^+$ m/z 152.0950
137 (95) – [M-167] $(C_3H_7)C_4N_2H.OH^+$ $C_7H_9N_2O^+$ m/z 137.0715

135 (20) – [M-169] $C_8H_{11}N_2^+$ m/z 135.0922
125 (10) – [M-179] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
124 (20) – [M-180] $(C_2H_6)C_4N_2H.OH^+$ $C_6H_8N_2O^+$ m/z 124.0637
97 (35) – [M-207] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
93 (45) – [M-211] $C_5H_5N_2^+$ m/z 93.0453 (NOT usual $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105)
84 (15) – [M-220] $C_4H_6NO^+$ m/z 84.0449
66 (20) – [M-238] $C_4H_4N^+$ m/z 66.0344
65 (15) – [M-239] $H_2O_2P^+$ m/z 64.9792
54 (10) – [M-250] $C_3H_4N^+$ m/z 54.0344

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C333415&Mask=200

N.B. See also rather weak spectrum of **diazinon oxon** (MW 288) at http://webbook.nist.gov/cgi/cbook.cgi?ID=C962583&Mask=200 which exhibits ions at m/z 288, 273, 152, 137 and 84.

1,2-Dibromoethane **$C_2H_4Br_2$** **M:186,188,190(1,2,1%)**
Theoretical molecular ion: m/z 187.8659 (100%), 185.8680 (51.4%), 189.8639 (48.6%)
Average MW: 187.87



Fumigant, has been used in soil and on citrus, vegetable, and cereal crops to control termites, beetles and moths. Now largely obsolete.

Acute oral LD50 for rat approx. 100 mg//kg (moderate toxicity). Carcinogen.

m/z	27	107	109	26	28	79	81	93
%	100	80	80	15	10	5	5	5

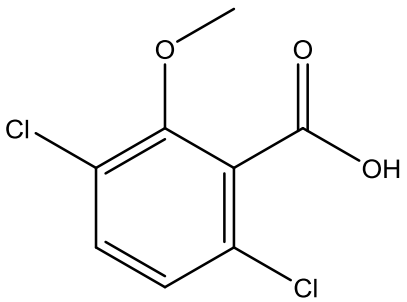
186,188,190 (1,2,1) – M^+
107,109 (80,80) – [M-79] loss of Br to C2H4Br+ m/z 106.9494 etc.
27 (100) – [M-159] $C_2H_3^+$ m/z 27.0235

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C106934&Mask=200#Mass-Spec

Dicamba acid **$C_8H_6Cl_2O_3$** **M:220,222,224(100,65,10%)**
Theoretical molecular ion: m/z 219.9694 (100%), 221.9665 (64%), 223.9635 (10.2%)
Average MW: 221.03

Selective, systemic herbicide, approved for use in the EU for general weed control.

Acute oral LD50 for rat approx. 1500 mg/kg (moderate toxicity).



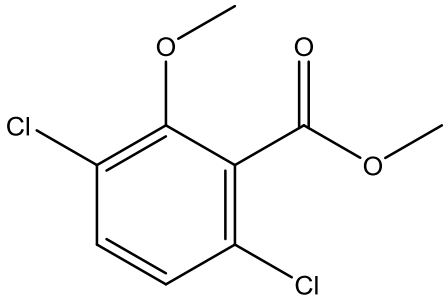
Poor GC transmission.

m/z	173	220	175	222	203	174	191	97
%	100	100	85	65	50	50	45	40

220,222 (100,65) – M^+
203,205 (50,30) – [M-17] loss of OH to $C_8H_5Cl_2O_2^+$ m/z 202.9667 etc.
173,175 (100,85) – [M-47] loss of CH_3O_2 to $C_7H_3Cl_2O^+$ m/z 172.9561 etc.

Cf. similar spectra at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1918009&Mask=200#Mass-Spec

Dicamba, methyl ester **$C_9H_8Cl_2O_3$** **M:234,236(25,15%)**
Theoretical molecular ion: m/z 233.9851 (100%), 235.9821 (64%), 237.9792 (10.2%)
Average MW: 223.06

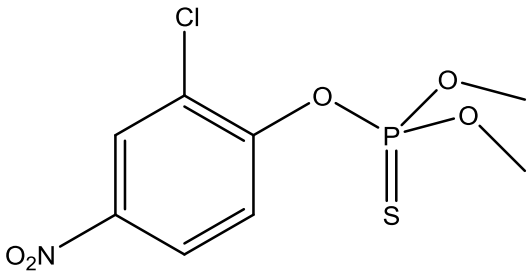


m/z	203	205	234	188	236	201	190	175
%	100	65	25	20	15	15	10	10

234,236 (25,15) – M+
203,205 (100,65) – [M-31] loss of CH_3O to $C_8H_5Cl_2O_2^+$ m/z 202.9667 etc.
188,190 (20,10) – [M-46] loss of C_2H_6O to $C_7H_2Cl_2O_2^+$ m/z 187.9432 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C6597780&Mask=200#Mass-Spec

Dicapthon **$C_8H_9ClNO_5PS$** **M:297,299(0,0%)**
Theoretical molecular ion: m/z 296.9628 (100%), 298.9598 (32%), 298.9586 (4.5%)
Average MW: 297.65



Organophosphorus thiophosphate insecticide. No longer approved for use.

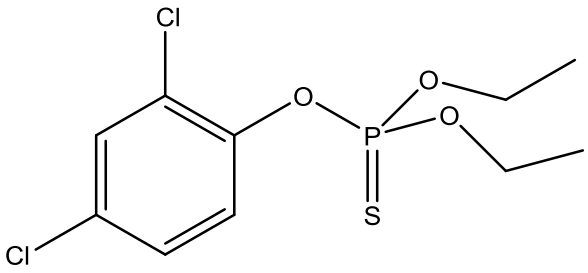
Acute oral LD50 for rat >500 mg/kg.

m/z	262	125	79	47	63	109	93	216
%	100	65	25	20	20	20	15	15

297 (0) – M^+ absent, due to powerful *ortho*-effect of chlorine.
262 (100) – [M-35] loss of Cl to $C_8H_9NO_5PS^+$ m/z 261.9939
216 (15) – [M-81] loss of Cl & SCH_2 to $C_7H_7NO_5P^+$ m/z 216.0062 [interesting rearrangement to cyclic ion?]
125 (65) – [M-172] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (20) – [M-188] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (25) – [M-218] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (20) – [M-234] PS^+ m/z 62.9458

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C2463845&Mask=200

Dichlofenthion **$C_{10}H_{13}Cl_2O_3PS$** **M:314,316,318(2,1.4,0.3%)**
Theoretical molecular ion: m/z 313.9700 (100%), 315.9671 (64%), 317.9641 (10%)
Average MW: 313.14



Organophosphorus insecticide and nematicide. Used to control soil dwelling insects and nematodes, and screwworms in cattle.

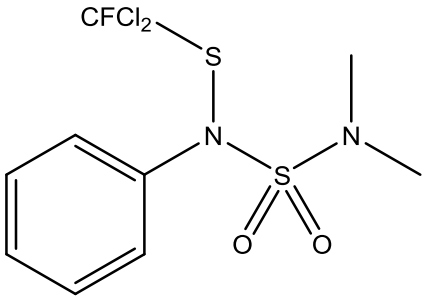
Acute oral LD50 for rat approx 100 mg/kg (moderate toxicity).

m/z	279	97	223	162	109	251	164	125
%	100	80	75	50	45	35	35	30

314,316,318(2,1,0.3) – M^+
279,281 (100,35) – [M-35] loss of Cl to $C_{10}H_{13}ClO_3PS^+$ m/z 279.0012 etc.
251,253 (100,35) – [M-63] loss of Cl & C_2H_4 to $C_8H_9ClO_3PS^+$ m/z 250.9699 etc.
223,225 (75,25) – [M-91] loss of Cl & $2C_2H_4$ to $C_6H_5ClO_3PS^+$ m/z 222.939
162,164 (50,35) – [M-152] dichlorophenol $Cl_2C_6H_3OH$ $C_6H_4Cl_2O^+$ m/z 161.9639 etc.
125 (30) – [M-189] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (45) – [M-205] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (80) – [M-217] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
63 (15) – [M-251] PS^+ m/z 62.9458

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C97176&Mask=200

Dichlofluanid **$C_9H_{11}Cl_2FN_2O_2S_2$** **M:332,334(7,5%)**
Theoretical molecular ion: m/z 331.9623 (100%), 333.9594(64%), 335.95640 (10.2%)
Average MW: 333.22



Fungicide used control a wide range of diseases including scab, brown spot, *Botrytis spp.*, *Alternaria sp*p. and storage diseases. Not approved for use in EU.
Cf. **tolylfluanid** (homologue).

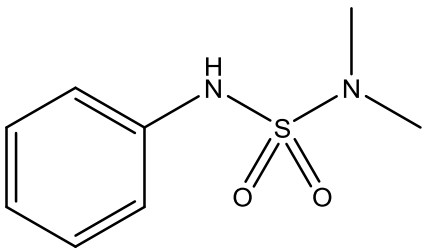
Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

m/z	123	167	224	226	92	124	77	108
%	100	50	40	30	20	15	15	10

332,334 (7,5) – M^+
224,226 (40,30) – [M-108] loss of $SO_2N(CH_3)_2$ to $C_7H_5Cl_2FNS^+$ m/z 223.9504 etc.
167 (50) – [M-165] loss of CCl_2F & SO_2 to $C_8H_{11}N_2S^+$ m/z 169.0643 [rearrangement]
123 (100) – [M-209] $C_6H_5NS^+$ m/z 123.0143

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1085989&Mask=200

Dichlofluanid related **$C_8H_{12}N_2O_2S$** **M:200(45%)**
N-(dimethylsulphamoyl)aniline
Theoretical molecular ion: m/z
Average MW:



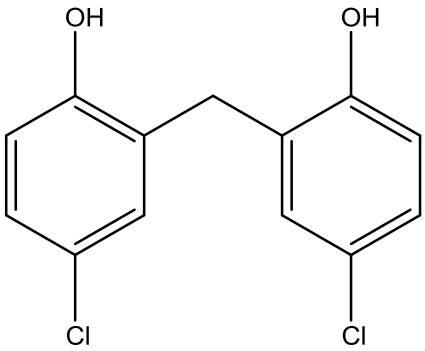
N-(dimethylsulphamoyl)aniline

Dichlofluanid may decompose during GC analysis to this compound:

m/z	92	65	200	39	93	108	64	121
%	100	65	45	30	25	15	10	5

200 (45) – M+
92 (100) – [M-108] loss of C_6H_6N to $SO_2N(CH_3)_2^+$ $C_2H_6NO_2S^+$ m/z 108.0119

Dichlorophen **$C_{13}H_{10}Cl_2O_2$** **M:268,270(40,25%)**
Theoretical molecular ion: m/z 268.0058 (100%), 270.0028 (64%), 271.9999 (10%),
Average MW: 269.12



Fungicide, bactericide and algicide. Not approved for use in the EU.

Acute oral LD50 for rat >2,000 mg/kg (low toxicity).

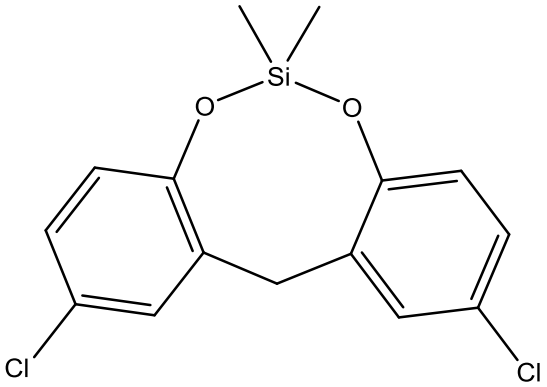
Very poor GC transmission.

m/z	128	141	268	130	270	143	233	77
%	100	60	40	35	25	20	15	15

268,270 (40,25) – M^+
128,130 (100,35) – [M-140] "chlorophenol" $C_6H_5ClO^+$ m/z 128.0029 etc.
141,143 (40,20) – [M-127] "chlorocresol" $C_7H_7ClO^+$ m/z 142.0185

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C97234&Mask=200#Mass-Spec

Dichlorophen related **$C_{15}H_{14}Cl_2O_2Si$** **M:324,326,328(100,70,15%)**
Theoretical molecular ion: m/z 324.0140 (100%), 326.0111 (64%), 328.0081 (10%)
Average MW: 325.26



Dichlorophen may produce GC artefact peaks, by reaction with GC dimethylsilicone stationary phases, if injected in large (µg) quantities. These unexpected products are cyclic silicones, of which the dimethyl form is usually dominant:

m/z	324	326	309	311	289	325	215	291
%	100	70	55	35	35	25	20	15

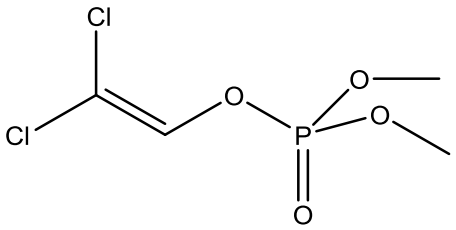
324,326 (100,70) – M^+
309,311 (55,35) – [M-15] loss of CH_3 to $C_{14}H_{11}Cl_2O_2Si^+$ m/z 308.9905 etc.
289,291 (35,15) – [M-35] loss of Cl to $C_{15}H_{14}ClO_2Si^+$ m/z 289.02516 etc.

215 (20) – [M-109] loss of ClC_6H_2 $C_9H_{12}ClO_2Si^+$ m/z 215.0295

No NIST spectrum available.

Dichlorvos **$C_4H_7Cl_2O_4P$** **M:220,222(5,3%)**

Theoretical molecular ion: m/z 219.9459 (100%), 221.9430 (64%), 223.9400 (10%)
Average MW: 220.97



Very volatile, so may be lost during concentration of sample extracts.

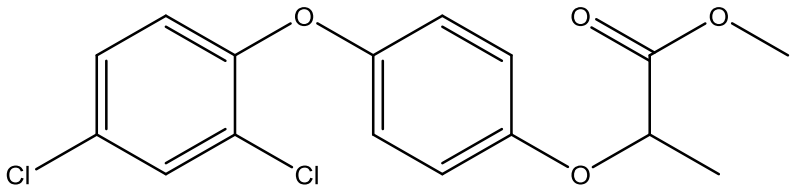
m/z	109	79	185	47	145	220	187	222
%	100	15	15	10	10	5	5	3

Assignments confirmed by accurate mass (Cardiff GCT):
220,222 (5,3) – M^+ $C_4H_7Cl_2O_4P^+$ m/z 219.9459
185,187 (15,5) – [M-35] loss of Cl to $C_4H_7ClO_4P^+$ m/z 184.9771 etc.
145,147 (10,3) – [M-75] $(CH_3O)_2(HO)PCl^+$ $C_2H_7ClO_3P^+$ m/z 144.9821 etc. [rearrangement]
109 (100) – [M-111] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
83,85 (20,15) – [M-137] $CHCl_2^+$ m/z 82.9455 etc.
79 (15) – [M-141] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
60,62 (10,5) – [M-160] C_2HCl^+ m/z 59.9767 etc.
47 (10) – [M-173] almost isobaric PO^+ m/z 46.9687
(Not CCl^+ m/z 46.9689)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C62737&Mask=200#Mass-Spec

Diclofop-methyl **$C_{16}H_{14}Cl_2O_4$** **M:340,342,344(100,65,10%)**

Theoretical molecular ion: m/z 340.0269 (100%), 342.0240 (65%), 344.0210 (10%)
Average MW: 325.18



Herbicide. Used for post-emergence control of annual grasses including wild oats. Approved for use in EU.

Acute oral LD50 for rat >500 mg/kg (moderate toxicity).

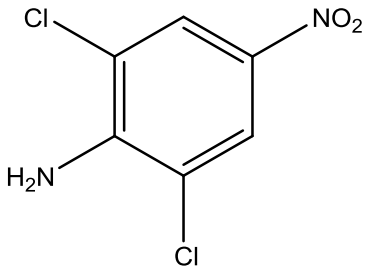
m/z	340	253	342	255	254	256	281	283
%	100	90	65	65	50	30	30	25

340,342,344 (100,65,10) – M^+

281,283 (30,25) – [M-59] loss of $COOCH_3$ to $C_{14}H_{11}Cl_2O_2^+$ m/z 281
253,255 (90,65) – [M-87] loss of $CH_3CHCOOCH_3$ to $C_{12}H_7O_2Cl_2^+$ m/z 253

Cf. similar (noisy) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C51338273&Mask=200#Mass-Spec

Dicloran **$C_6H_4Cl_2N_2O_2$** **M:206,208,210(100,65,10%)**
Theoretical molecular ion: m/z 205.9650 (100%), 207.9620 (64%), 209.9591 (10.2%)
Average MW: 207.01



Fungicide. Used for various pre- and post-harvest diseases on fruit and vegetables. Not approved for use in EU.

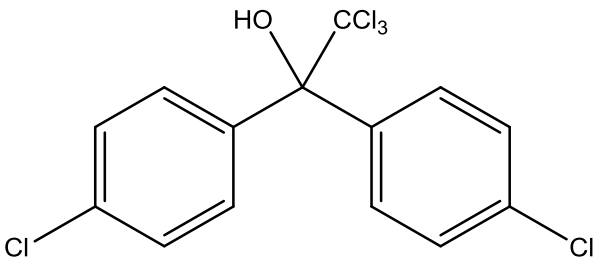
Acute oral LD50 for rat >2,000 mg/kg (moderate toxicity).

m/z	206	124	176	208	160	178	126	133
%	100	95	70	65	55	45	30	25

206,208,210 (100,65,10) – M^+
176,178 (70,45) – [M-30] loss of NO from nitro group, to $C_6H_4Cl_2NO^+$ m/z 175.9670 etc.
160,162 (55,25) – [M-46] loss of NO_2 to $C_6H_4Cl_2N^+$ m/z 159.9721
124,126 (95,30) – [M-82] loss of NO_2 & HCl to $C_6H_3ClN^+$ m/z 123.9954

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C99309&Mask=200#Mass-Spec

Dicofol **$C_{14}H_9Cl_5O$** **M:368(0%)**
Theoretical molecular ion: m/z 367.9096 (63%), 369.9067 (100%), 371.9037 (64%)
Average MW: 370.48



Obsolete organochlorine acaricide. “Hydroxy-DDT”

Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity). Irritant. Neurotoxin.

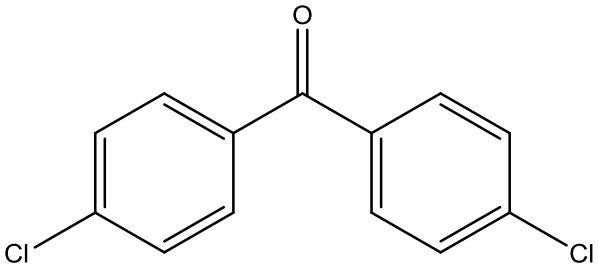
Very susceptible to GC degradation to dichlorobenzophenone (see below).

m/z	139	251	253	111	141	75	252	140
%	100	60	45	35	30	15	10	10

368,370,372 (0) – M^+ absent
316,318,320 (1,2,1) – [M-52] loss of Cl & OH to "DDE" $C_{14}H_8Cl_4^+$ m/z 315.9380 etc.
251,253 (65,43) – [M-117] loss of CCl_3 to $C_{13}H_9Cl_2O^+$ m/z 251.00305 etc.
111,113 (35,10) – [M-257] $ClC_6H_4^+$ m/z 111.0002 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C115322&Mask=200#Mass-Spec

Dicofol related **$C_{13}H_8Cl_2O$** **M:250,252(30,20%)**
dichlorobenzophenone
Theoretical molecular ion: m/z 249.9952 (100%), 251.9923 (64%), 253.9893 (10.2%)
Average MW: 251.11



4,4'-dichlorobenzophenone

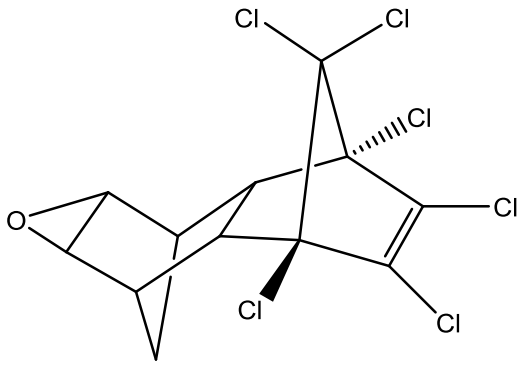
Dicofol may undergo degradation during GC analysis to p,p'- dichlorobenzophenone ("DCBP"), *cf.* chlorobenzilate:

m/z	139	141	111	250	252	75	113	215
%	100	35	30	30	20	15	10	10

250,252 (30,20) – M^+
215,217 (10,3) – [M-35] loss of Cl to $C_{13}H_8ClO^+$ m/z 215.0264
139,141 (100,35) – [M-111] $ClC_6H_4CO^+$ m/z 138.9951
111,113 (30,10) – [M-139] $ClC_6H_4^+$ m/z 111.0002
75 (15) – [M-175] $C_6H_3^+$ m/z 75.0235

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C90982&Units=CAL&Mask=200#Mass-Spec

Dieldrin **$C_{12}H_8Cl_6O$** **M:378,380,382,384(3,6,5,2%)**
Theoretical molecular ion: m/z 377.8706 (51%), 379.8677 (100%), 381.8647 (81%), 383.8618 (35%)
Average MW: 380.91



Obsolete organochlorine insecticide. Also a metabolite of aldrin.

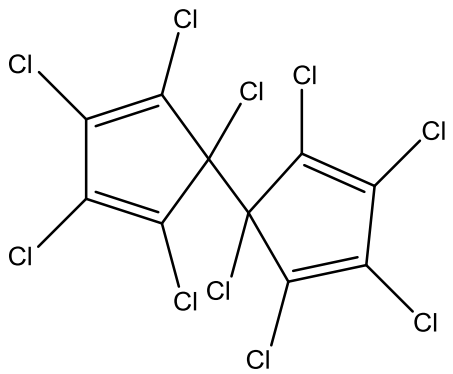
KI (SE-30) = 21.0

m/z	79	82	81	108	263	277	279	77
%	100	30	25	15	15	10	10	10

378,380,382,384 (3,6,5,2) – M^+
343,345,347 (5,7,5) – [M-35] loss of Cl
275,277,279,281 (7,15,13,6) – [M-103] loss of 3Cl
261,263,265 (11,15,11) – [M-117]
79 (100) – [M-299] $C_5H_3O^+$

Cf. similar (weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C60571&Mask=200#Mass-Spec
Plus several other isomers of $C_{12}H_8Cl_6O$ – endrin, endrin ketone & photodieldrin etc.

Dienochlor **$C_{10}Cl_{10}$** **M:470,472,474,476,478(2,5,10,7,3%)**
Theoretical molecular ion: m/z 469.6885 (21%), 471.6856 (69%), 473.6826 (100%), 475.6797 (86%)
Average MW: 474.61



Obsolete organochlorine insecticide.

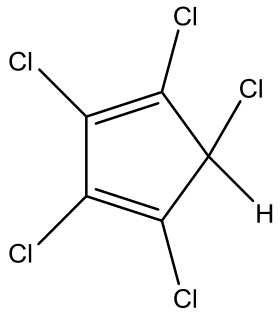
Acute oral LD50 for rat approx. 3,000 mg/kg (low toxicity).

m/z	237	239	235	404	402	406	332	334
%	100	65	65	50	45	30	30	25

470,472,474,476,478 (2,5,10,7,3) – M^+
435,437,439,441 (1,2,3,2,1) – [M-35] loss of Cl to $C_{10}Cl_9^+$
400,402,404,406,408 (15,45,50,30,15) – [M-70] loss of 2Cl to $C_{10}Cl8^+$
235,237,239 (65,100,65) – [M-235] $C_5Cl_5^+$ m/z 234.8443, 236.8413, 238.8384 etc.

Cf. generally similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2227170&Mask=200 but which lacks the cluster of ions due to $C_{10}Cl_9^+$ at m/z 435-445 (effect of different source temperature on fragmentation?)

Dienochlor related **C_5HCl_5** **M:236,238,240(15,25,15%)**
Pentachlorocyclopentadiene
Theoretical molecular ion: m/z 235.8521 (63%), 237.8491 (100%), 239.8462 (64%), 241.8432 (20%)
Average MW: 238.31



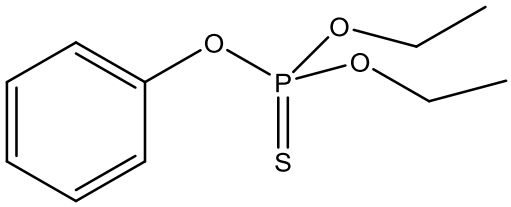
1,2,3,4,5-pentachlorocyclopentadiene may be observed as a minor, shorter GC RT contaminant:

m/z	203	201	205	96	61	238	240	236
%	100	75	50	30	25	25	15	15

236,238,240 (15,25,15) – M^+
201,203,205 (75,100,50) – [M-35] loss of Cl to $C_5HCl_4^+$ m/z 200.8832 etc.

No NIST spectrum available.

O,O-Diethyl-O-phenyl phosphorothioate $C_{10}H_{15}O_3PS$ M:246(78%)
Theoretical molecular ion: m/z 246.0480 (100%), 247.0513 (10.8%), 248.0438 (4.5%)
Average MW: 246.26

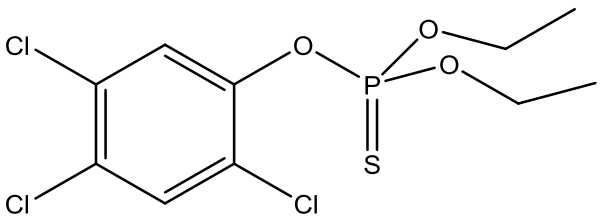


Organophosphorus pesticide formulation contaminant.

m/z	94	246	110	109	97	105	141	190
%	100	78	63	43	26	20	17	17

No NIST spectrum available.

O,O-Diethyl-O-(2,4,5-trichlorophenyl) phosphorothioate $C_{10}H_{12}Cl_3O_3PS$ M:348(0%)
Theoretical molecular ion: m/z 347.9310 (100%), 349.9281 (96%), 351.9251 (31%)
Average MW: 349.59



Organophosphorus pesticide formulation contaminant and ethyl analogue of **fenchlorphos**.

m/z	97	313	257	315	259	125	285	109

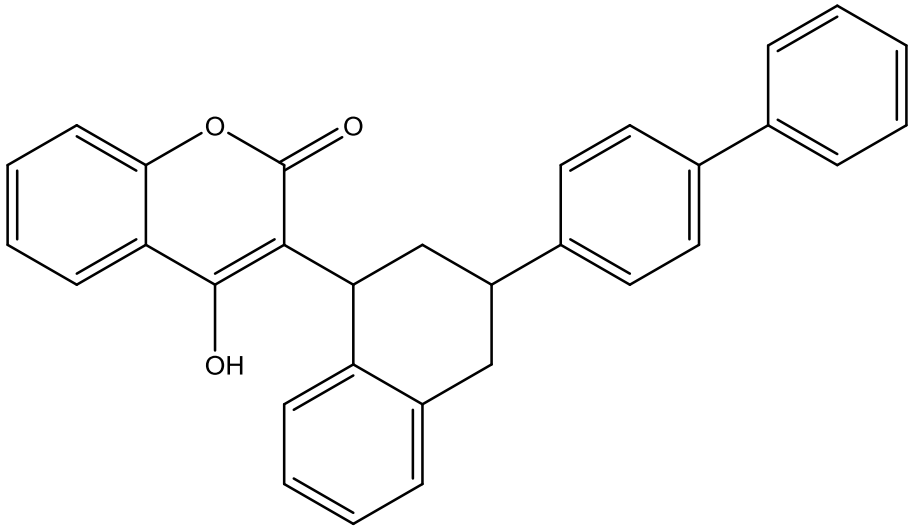
%	100	64	59	47	40	35	33	33

348 (0) – M^+ absent
313,315 (64,47) – [M-35] loss of Cl to $C_{10}H_{12}Cl_2O_3PS^+$ m/z 312.9622 etc
285,287 (33,15) – [M-63] loss of Cl & C_2H_4 to $C_8H_8Cl_2O_3PS^+$ m/z 284.9309
257,259 (59,40) – [M-91] loss of Cl & $2C_2H_4$ to $C_6H_4Cl_2O_3PS^+$ m/z 256.8996

No NIST spectrum available.

Difenacoum **$C_{31}H_{24}O_3$** **M:444(75%)**

Theoretical molecular ion: m/z 444.1725 (100%), 445.1759 (34%)
Average MW: 444.53



Anticoagulant rodenticide. Approve for use in EU.

Acute oral LD50 for rat approx.1 mg/kg (high toxicity).

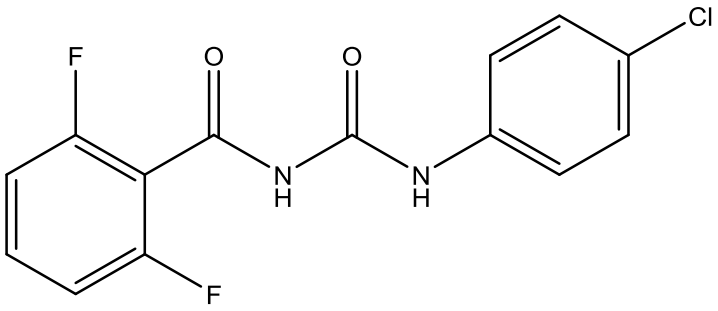
Poor GC transmission.

m/z	167	444	282	290	121	163	277	129
%	100	75	50	50	50	35	25	20

444 (75) – M^+
282 (50) – [M-162] $C_{22}H_{18}^+$ m/z 282.1409
167 (100) – [M-277] $C_{13}H_{11}^+$ m/z 167.0861 – interesting
163 (35) – [M-281] 4-hydroxycoumarin moiety, $C_9H_7O_3^+$ m/z 163.0395

No NIST spectrum available.

Diflubenzuron $C_{14}H_{19}ClF_2N_2O_2$ **M:310,312(10,3%)**
Theoretical molecular ion: m/z 310.0321 (100%), 312.0291 (32%)
Average MW: 310.68



Benzoylurea insecticide & chemosterilant. Approved for use in EU.

Acute oral LD50 for rat >4,600 mg/kg (low toxicity).

Diflubenzuron is not amenable to GC analysis.

m/z	153	141	155	157	113	63	125	127
%	100	80	30	25	25	25	25	25

310,312 (10,3) – M^+
153,155 (100,30) – [M-157] $ClC_6H_4NCO^+$ $C_7H_4ClNO^+$ m/z 152.9981
141 (80) [M-169] $C_7H_3F_2O^+$ m/z 141.0152

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C35367385&Mask=200#Mass-Spec

Diflubenzuron related, i) 4-chloroaniline C_6H_6ClN **M:127,129(100,35%)**
Theoretical molecular ion: m/z 127.0189 (100%), 129.0159 (32%)
Average MW: 127.57

$Cl\text{-}C_6H_4\text{-}NH_2$

4-chloroaniline is one of several GC degradation products / contaminants of diflubenzuron.
KI (OV-17) = 13

m/z	127	129	65	92	-	-	-	-
%	100	35	25	15	-	-	-	-

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C106478&Units=SI&Mask=200#Mass-Spec

Diflubenzuron related, ii) C_7H_4ClNO **M:153,155(100,35%)**
Theoretical molecular ion: m/z 152.9981 (100%), 154.9952 (32%)
Average MW: 153.57

$Cl\text{-}C_6H_4\text{-}N{=}C{=}O$

4-chlorophenyl isocyanate is one of several GC degradation products / contaminants of diflubenzuron.
KI (OV-17) = 12

m/z	153	125	155	90	63	127	-	-
%	100	40	35	30	20	15	-	-

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C104121&Units=SI&Mask=200#Mass-Spec

Diflubenzuron related, iii) **$C_7H_5F_2NO$** **M:157(50%)**

Theoretical molecular ion: m/z 157.0339 (100%), 158.0373 (8%)
Average MW: 157.12

$C_6H_3F_2$-$CONH_2$

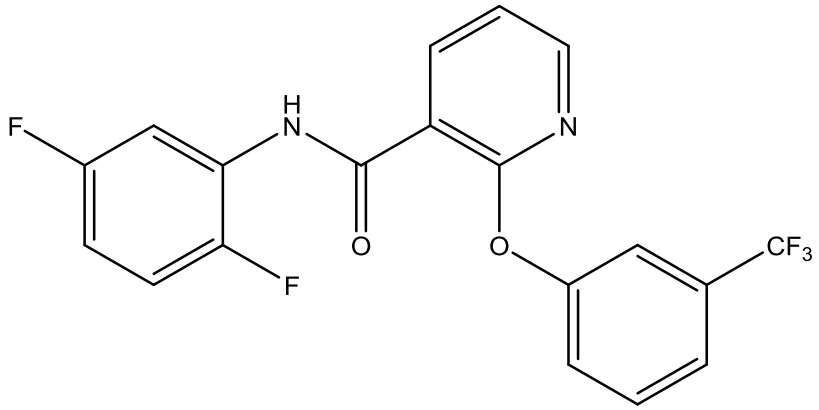
2,6-difluorobenzamide is one of several GC degradation products / contaminants of diflubenzuron.
KI (OV-17) = 15

m/z	141	157	113	63	-	-	-	-
%	100	50	35	20	-	-	-	-

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C18063031&Units=SI&Mask=200#Mass-Spec

Diflufenican **$C_{19}H_{11}F_5N_2O_2$** **M:394(25%)**

Theoretical molecular ion: m/z 394.0741 (100%), 395.0774 (21%)
Average MW: 394.29



Herbicide. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

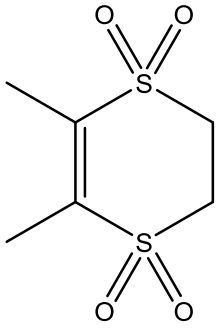
m/z	266	394	101	267	169	145	218	246
%	100	25	25	20	15	15	15	15

394 (25) – M^+
266 (100) – [M-128] $C_{13}H_7F_3NO_2^+$ m/z 266.0429

No NIST spectrum available.

Dimethipin $C_6H_{10}O_4S_2$ **M:210(5%)**

Theoretical molecular ion: m/z 210.0021 (100%), 211.9979 (9.0%), 211.0054 (6.5%)
Average MW: 210.62



Plant growth regulator and defoliant. No longer approved for use in EU.

Acute oral LD50 for rat approx. 400 mg/kg (moderate toxicity).

KI (OV-17) = 22.0

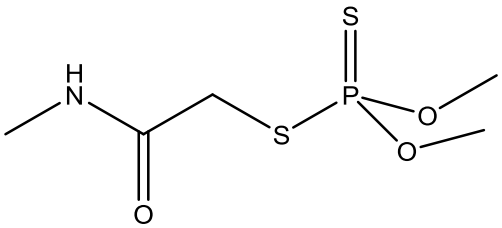
m/z	54	43	39	53	27	118	76	59
%	100	70	50	35	35	25	20	15

210 (5) – M^+
124 (10) – [M-86] $SO_2CH_2CH_2S^+$ $C_2H_8O_2S_2^+$ m/z 123.9653
118 (25) – [M-92] $CH_3C{=}C(CH_3)SO_2^+$ $C_4H_6O_2S^+$ m/z 118.0089
54 (100) – [M-156] $C_4H_6^+$ m/z 54.0920

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C55290647&Units=SI&Mask=200#Mass-Spec listed under "1,4-Dithiin, 2,3-dihydro-5,6-dimethyl-, 1,1,4,4-tetraoxide"

Dimethoate $C_5H_{12}NO_3PS_2$ **M:229(5%)**

Theoretical molecular ion: m/z 228.9996 (100%), 230.0030 (5%), 230.9954 (9%)
Average MW: 229.26



Organophosphorus insecticide and acaricide. Approved for use in EU.

Acute oral LD50 for rat approx. 250 mg/kg (moderate toxicity).

The oxidative metabolite, dimethoate oxon, is **omethoate**.

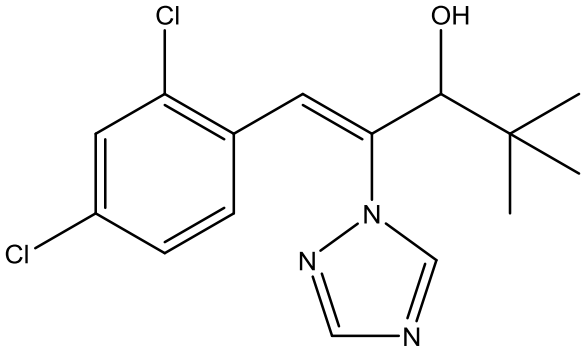
m/z	87	93	125	229	143	47	79	104
%	100	35	30	5	5	5	5	5

Assignments confirmed by accurate mass data (Cardiff GCT)
229 (5) – M^+ $C_5H_{12}NO_3PS_2$ m/z 228.9996
157 (5) – [M-72] $(CH_3O)_2PS.S^+$ $C_2H_6O_2PS_2^+$ m/z 156.9547
143 (5) – [M-86] rearrangement ion $(CH_3O)_2(HO)P(SH)^+$ $C_2H_8O_3PS^+$ m/z 142.9932

(NOT similar predicted OP ion $(CH_3O)(HO)PS.S^+$ $CH_4O_2PS_2^+$ m/z 142.9390, which differs by CH_4/O)
125 (30) – [M-104] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
104 (5) – [M-125] $SCH_2CONHCH_3^+$ $C_3H_6NOS^+$ m/z 104.0170
93 (35) – [M-136] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
87 (100) – [M-142] $C_3H_5NS^+$ m/z 87.0143
79 (100) – [M-150] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (100) – [M-166] PS^+ m/z 62.9458
58 (100) – [M-171] CH_3NHCO^+ $C_2H_4NO^+$ m/z 58.0293

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C60515&Mask=200#Mass-Spec

Diniconazole **$C_{15}H_{17}Cl_2N_3O$** **M:325(0%)**
Theoretical molecular ion: m/z 325.0749 (100%), 327.0719 (64%), 329.0690 (10%)
Average MW: 326.22



Conazole fungicide. Used to control a range of diseases including mildew, bunts and smuts. Not approved for use in EU.

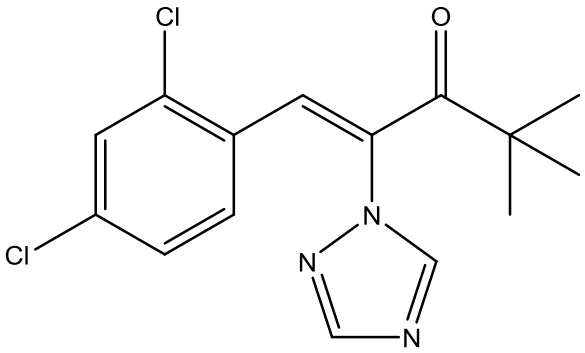
Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity).

m/z	268	70	57	270	41	29	165	269
%	100	80	70	65	35	25	20	20

325,327 (0,0) – M^+
268,270,272 (100,65,15) – [M-57] $C_{11}H_8Cl_2N_3O^+$ m/z 268.0044 etc.
70 (80) – [M-255] $(C_2H_2N_3)H_2^+$ $C_2H_4N_3^+$ m/z 74.0405

No NIST spectrum available.

Diniconazole ketone **$C_{15}H_{15}Cl_2N_3O$** **M:323(0%)**
Theoretical molecular ion: m/z 323.0592 (100%), 325.0563 (64%), 327.0533 (10%)
Average MW: 324.21



An oxidation product of **diniconazole**.

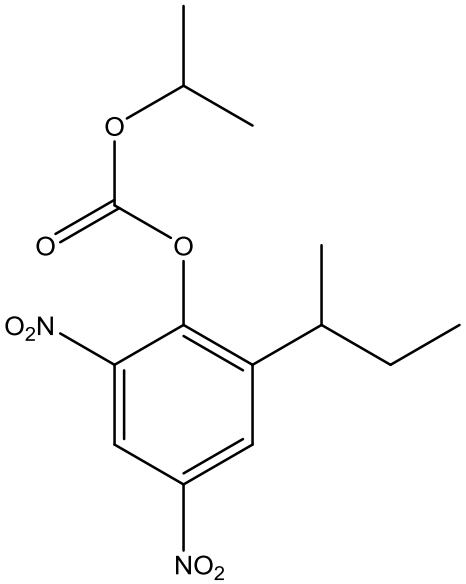
m/z	57	288	204	41	29	184	232	290
%	100	50	30	30	25	20	15	15

323,325 (0,0) – M^+
288,290 (50,15) – [M-35] loss of Cl to $C_{15}H_{15}ClN_3O^+$ m/z 288.0904 etc.
204,206 (30,10) – [M-121] loss of Cl & C4H9 & HCN to $C_{10}H_5ClN_2O^+$ m/z 204.0090

No NIST spectrum available.

Dinobuton **$C_{14}H_{18}N_2O_7$** **M:326(0%)**

Theoretical molecular ion: m/z 326.1114 (100%), 327.1148 (15%)
Average MW: 326.31



Dinitrophenol acaricide and fungicide. Used against red spider mites and powdery mildew. No longer approved for use in EU.

Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

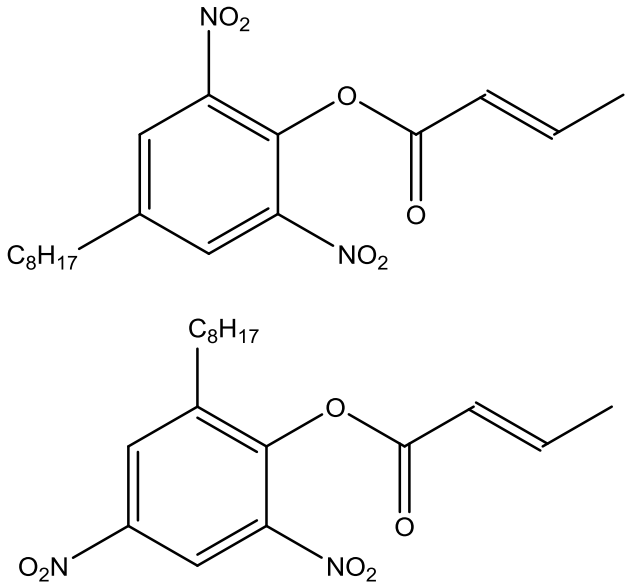
m/z	43	211	41	163	240	205	147	212
%	100	45	15	10	10	10	10	5

326 (0) – M+
267 (2) – [M-59] loss of OC_3H_7 to $C_{11}H_{11}N_2O_6^+$ m/z 267.0617
211 (45) – [M-115] loss of $C_3H_7O.C{=}O.OC$ to $C_9H_{11}N_2O_4^+$ m/z 211.0355
43 (100) – [M-283] $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C973217&Mask=200

Dinocap **$C_{18}H_{24}N_2O_6$** **M:364(0%)**

Theoretical molecular ion: m/z
Average MW: 364.39



Dinocap isomers (2,6- and 2,4-dinitro forms)
(C_8H_{17} is a mixture of 1-methylheptyl, 1-ethylhexyl and 1-propylpentyl)

Acaricide and fungicide, used for control of powdery mildew. Approved for use in EU.

Acute oral LD50 for rat >1,000 mg/kg (moderate toxicity).

Dinocap is an isomeric reaction mixture of six major components, which may be resolved on capillary GC (to give a characteristic peak profile), with very similar (very uninformative) mass spectra.

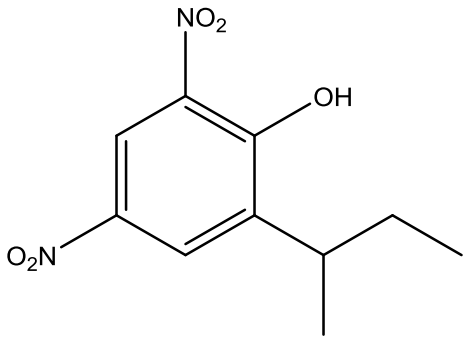
m/z	69	41	70	-	-	-	-	-
%	100	5	5	-	-	-	-	-

364 (0) – M^+
69 (100) – [M-295] $CH_3CH{=}CHCO^+$ $C_4H_5O^+$ m/z 69.0340

No NIST spectrum available.

Dinoseb $C_{10}H_{12}N_2O_5$ **M:240(15%)**

Theoretical molecular ion: m/z 240.0746 (100%), 241.0780 (10.8%)
Average MW: 240.21



Dinitrophenol herbicide. No longer approved for use in EU.

Acute oral LD50 for rat 25 mg/kg (high toxicity). Suspect carcinogen.

Metabolite of binapacryl. Isomer of dinoterb, with very different spectrum due to different alkyl chain fragmentation. Poor GC transmission.

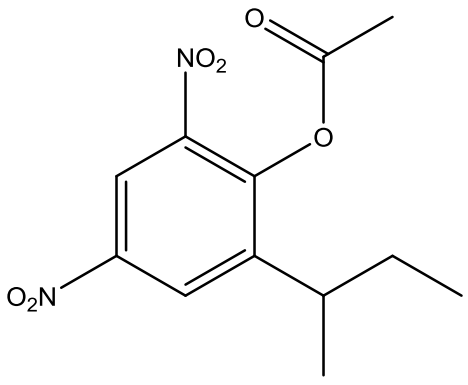
m/z	211	163	147	117	240	29	41	57
%	100	45	25	20	15	15	15	15

240 (15) – M^+
211 (100) – [M-29] loss of CH_3CH_2 to $C_8H_7N_2O_5^+$ m/z 211.0355
163 (45) – [M-77] loss of NO_2 & NOH to $C_{10}H_{11}O_2^+$ m/z 163.0759
147 (25) – [M-93] loss of $2NO_2$ & H to $C_{10}H_{11}O^+$ m/z 147.0810

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C88857&Mask=200#Mass-Spec

Dinoseb acetate $C_{12}H_{14}N_2O_6$ **M:282(1%)**

Theoretical molecular ion: m/z 282.0852 (100%), 283.0885 (13.0%)
Average MW: 282.25



Remarkably unhelpful spectrum! Abundant acetyl ion m/z 43 and little else.

m/z	43	211	240	44	163	147	117	205
%	100	10	10	10	5	5	5	5

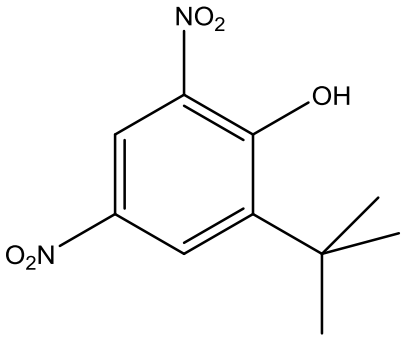
282(1) – M^+

240 (10) – [M-42] loss of CH_2CO to dinoseb M^+ $C_{10}H_{12}N_2O_5^+$ m/z 240.0746
43 (100) – [M-197] CH_3CO^+ $C_2H_3O^+$ m/z 43.0184

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2813958&Mask=200

Dinoterb **$C_{10}H_{12}N_2O_5$** **M:240(15%)**

Theoretical molecular ion: m/z 240.0746 (100.0%), 241.0780 (10.8%)
Average MW: 240.21



Dinitrophenol herbicide. No longer approved for use in EU.

Acute oral LD50 for rat 25 mg/kg (high toxicity).

Isomer of dinoseb, with very different spectrum due to different alkyl chain fragmentation. Poor GC transmission.

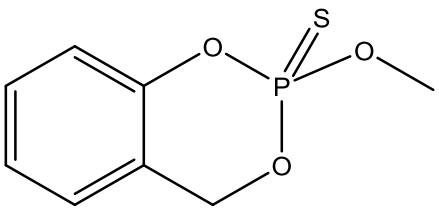
m/z	225	177	131	240	161	41	103	226
%	100	45	25	15	15	10	10	10

240 (15) – M^+
225 (100) – [M-15] loss of CH_3 to $C_9H_9N_2O_5^+$ m/z 225.0512
177 (45) – [M-63] loss of NO_2 & OH to $C_{10}H_{11}NO_2^+$ m/z 177.0790
131 (25) – [M-109] loss of $2NO_2$ & OH to $C_{10}H_{11}^+$ m/z 131.0861

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1420071&Mask=200

Dioxabenzofos / Salithion **$C_8H_9O_3PS$** **M:216(100%)**

Theoretical molecular ion: m/z 216.0010 (100%), 217.0044 (8.7%), 217.9968 (4.5%)
Average MW: 216.19



m/z	216	183	78	153	201	138	137	121
%	100	55	45	30	25	20	20	15

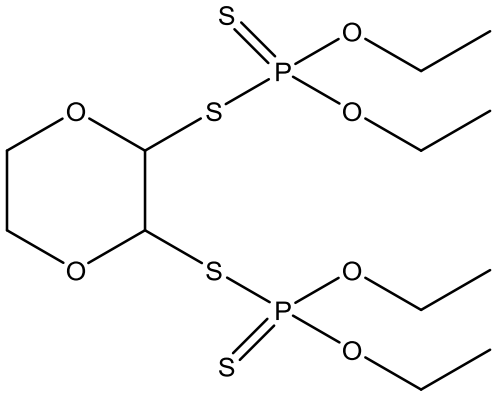
216 (100) – M^+
201 (25) – [M-15] loss of CH_3 to $C_7H_6O_3PS^+$ m/z 201.9775
183 (55) – [M-33] loss of SH to $C_8H_8O_3P^+$ m/z 183.0211
153 (30) – [M-63] loss of CH_3OS to $C_7H_6O_2P^+$ m/z 153.0105
138 (20) – [M-78] loss of C_6H_6 to $C_2H_3O_3PS^+$ m/z 137.9541 (interesting rearrangement)

78 (45) – [M-138] $C_6H_6^+$ m/z 78.0470
63 (10) – [M-153] PS^+ m/z 68.9458
47 (10) – [169] PO^+ m/z 46.9687

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3811492&Units=SI&Mask=200#Mass-Spec

Dioxathion **$C_{12}H_{26}O_6P_2S_4$** **M:456(0%)**

Theoretical molecular ion: m/z 456.0087(100%), 458.0045 (18%)
Average MW: 456.54



Organophosphorus insecticide and acaricide. Used on livestock to control ticks, fleas and mites and as an acaricide on citrus fruits and nuts. No longer approved for use in EU.

Acute oral LD50 for rat approx. 25 mg/kg (high toxicity).

Poor GC transmission and long RT.

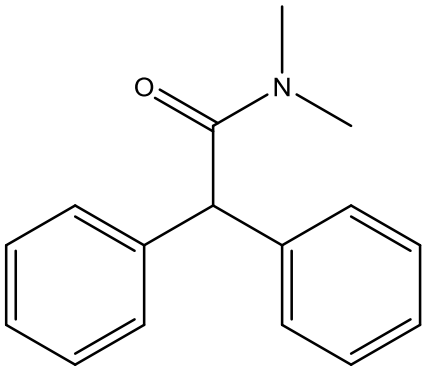
m/z	97	125	153	271	65	185	270	86
%	100	60	70	65	35	30	25	15

456 (0) – M^+
271 (65) – [M-185] $C_8H_{16}O_4PS_2^+$ m/z 271.0228
185 (30) – [M-271] $(CH_3CH_2O)_2PS_2^+$ $C_4H_{10}O_2PS_2^+$ m/z 184.9860
153 (70) – [M-303] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (60) – [M-331] $(CH_3CH_2O)(HO)PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (100) – [M-357] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
86 (15) – [M-370] $C_4H_6O_2^+$ dioxane moiety, m/z 86.0368

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C78342&Mask=200#Mass-Spec

Diphenamid **$C_{16}H_{17}NO$** **M:239(5%)**

Theoretical molecular ion: m/z 239.1310 (100%), 240.1344 (17%)
Average MW: 239.31



Alkanamide herbicide. Used for pre-emergence control of annual grasses and broad-leaved weeds. Not approved for use in EU.

Acute oral LD50 for rat approx. 900 mg/kg (moderate toxicity).

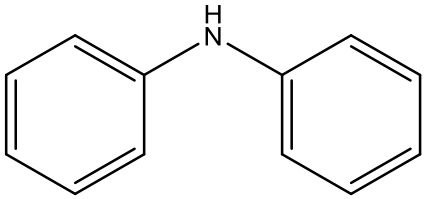
m/z	72	167	165	239	152	166	168	239
%	100	60	25	20	20	15	5	5

239 (5) – M^+
167 (60) – [M-73] loss of $(CH_3)_2NCOH$ to $C_{13}H_{11}^+$ m/z 167.0861
165 (25) – [M-75] $C_{13}H_9^+$ m/z 165.0704
72 (100) – [M-168] $(CH_3)_2NCO^+$ $C_3H_6NO^+$ m/z 72.0449

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C957517&Mask=200#Mass-Spec

Diphenylamine **$C_{12}H_{11}N$** **M:169(100%)**

Theoretical molecular ion: m/z 169.0892 (100%), 170.0925 (13%)
Average MW: 169.23



Fungicide. Used mainly to control superficial scald in apples and pears via both pre- and post-harvest treatment. No longer approved for use in EU.

Acute oral LD50 for rat >15,000 mg/kg (low toxicity).

m/z	169	168	167	51	***84.5***	77	170	66
%	100	50	30	20	15	15	15	10

169 (100) – M^+
168 (5) – [M-1] loss of H to $C_{12}H_{10}N^+$ m/z 168.0813
84.5 (15%) – doubly charged molecular ion 169/2 = m/z 84.5 (note lack of ^{13}C isotope peak in NIST spectrum)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C122394&Mask=200#Mass-Spec

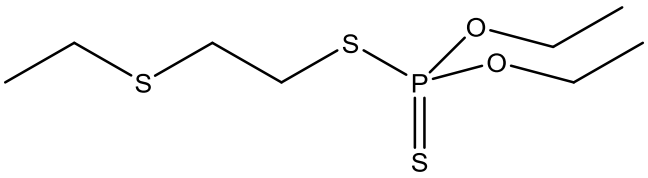
Disulfoton $C_8H_{19}O_2PS_3$ **M:274(10%)**

Theoretical molecular ion: m/z 274.0285 (100%), 275.0318 (8.7%), 276.0243 (13.6%)
Average MW: 274.39

Organophosphorus insecticide and acaricide. Systemic action. Used to control aphids, thrips, mealybugs, spider mites and other sucking insects. No longer approved for use in EU.

Acute oral LD50 for rat approx. 2 mg/kg (high toxicity).

Disulfoton is the diethyl homologue of thiometon (a dimethyl ester).
The sulphoxide and sulphone oxidative metabolites are also important. The oxon analogues are much less commonly observed (though included in MRLs).



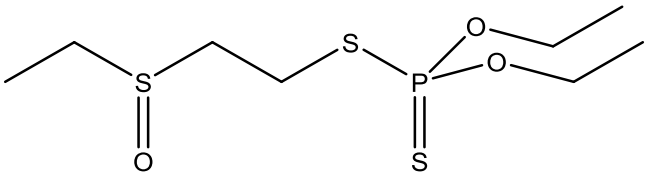
m/z	88	89	60	61	153	186	142	274
%	100	35	20	15	10	10	10	10

Assignments confirmed by accurate mass (Cardiff GCT)
274 (10) – M^+ $C_8H_{19}O_2PS_2^+$ m/z 274.0285
245 (5) – [M-29] loss of C_2H_5 to $C_6H_{14}O_2PS_2^+$ m/z 244.9884
219(10) – [M-55] loss of C_4H_7 to $C_4H_{12}O_2PS_2^+$ m/z 218.9800
186 (10) – [M-88] $(CH_3CH_2O)_2(HS)P{=}S^+$ $C_4H_{11}O_2PS_2^+$ m/z 185.9938
153 (10) – [M-121] $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
142 (10) – [M-132] $(C_2H_5O)(HS)PSH^+$ $C_2H_7OPS_2^+$ m/z 141.9676 (O/S swap)
NOT expected ion $(HO)_2PS.SCH^+$ $CH_4O_2PS_2^+$ m/z 141.9312
129 (5) – [M-145] $(HO)_2PS_2^+$ $H_2O_2PS_2^+$ m/z 128.9234
125 (5) – [M-149] $(C_2H_5O)(HO)PS^+$ $C_2H_6O_2PS^+$ m/z 124.9789
97 (5) – [M-177] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9481
88 (100) – [M-186] $CH_3CH_2SCH{=}CH_2^+$ $C_4H_8S^+$ m/z 88.0347
60 (20) – [M-214] $CH_2CH_2S^+$ $C_2H_4S^+$ m/z 60.0034
59 (30) – [M-215] CH_2CHS^+ $C_2H_3S^+$ m/z 58.9955

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C298044&Mask=200#Mass-Spec but m/z 97 stronger.

Disulfoton sulphoxide $C_8H_{19}O_3PS_3$ **M:290(0.5%)**

Theoretical molecular ion: m/z 290.0234 (100%), 291.02675 (8.7%), 292.0192 (14%)
Average MW: 290.49



Very poor GC transmission.

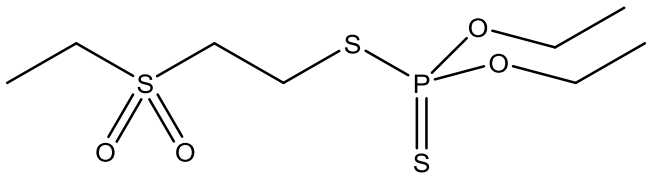
m/z	125	213	153	97	185	61	157	29
%	100	85	80	80	60	40	35	25

290 (0) – M^+ absent
213 (85) – [M-77] loss of CH_3CH_2SO to $C_6H_{14}O_2PS_2^+$ m/z 213.0173
185 (60) – [M-105] loss of $CH_3CH_2SOCH_2CH_2$ to $C_4H_{10}O_2PS_2^+$ m/z 184.9860
157 (35) – [M-133] loss of CH_3CH_2SO & $2C_2H_4$ to $C_2H_6O_2PS_2^+$ m/z 156.9547
153 (80) – [M-137] $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
129 (20) – [M-161] $(HO)_2PS_2^+$ $H_2O_2PS_2^+$ m/z 128.9234
125 (100) – [M-165] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (80) – [M-193] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
61 (40) – [M-229] $CH_3CH_2S^+$ $C_2H_5S^+$ m/z 61.0112 (reduction/rearrangement?)

Cf. "Oxydisulfoton" spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2497076&Units=SI&Mask=200#Mass-Spec which exhibits similar ions, but exaggerated intensities at low mass.

Disulfoton sulphone **$C_8H_{19}O_4PS_3$** **M:306(1%)**

Theoretical molecular ion: m/z 306.0183 (100%), 307.0217 (8.7%), 308.0141 (13.6%)
Average MW: 306.39



m/z	213	153	61	125	97	157	185	186
%	100	75	40	30	30	20	15	10

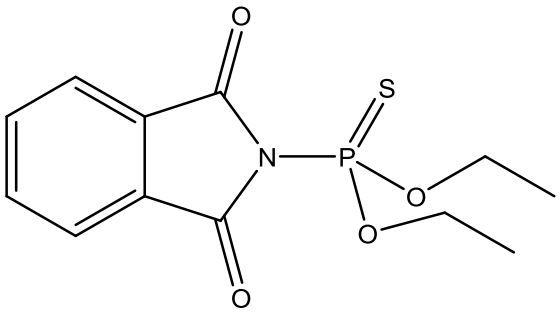
306 (1) – M^+ weak
213 (100) – [M-93] loss of $CH_3CH_2SO_2$ to $C_6H_{14}O_2PS_2^+$ m/z 213.0173
185 (15) – [M-121] loss of $CH_3CH_2SO_2$ & C_2H_4 to $C_4H_{10}O_2PS_2^+$ m/z 184.9860
157 (20) – [M-149] loss of $CH_3CH_2SO_2$ & $2C_2H_4$ to $C_2H_6O_2PS_2^+$ m/z 156.9547
153 (5) – [M-153] $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
129 (5) – [M-177] $(HO)_2PS_2^+$ $H_2O_2PS_2^+$ m/z 128.9234
125 (30) – [M-181]] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (30) – [M-209] $H_2O_2PS^+$ m/z 96.9513
65 (5) – [M-241] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792 (and/or SO_2H m/z 64.9697)
61 (40) – [M-245] $CH_3CH_2S^+$ $C_2H_5S^+$ m/z 61.0112 (reduction/rearrangement?)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2497065&Units=SI&Mask=200#Mass-Spec

Disulfoton oxon, see Demeton-S **$C_8H_{19}O_2PS_3$** **M:274(10%)**

Ditalimfos $C_{12}H_{14}NO_4PS$ **M:299(85%)**

Theoretical molecular ion: m/z 299.0381 (100%), 300.0415 (13%), 301.0339 (4.5%)
Average MW: 299.28



Organophosphorus fungicide. Used to control powdery mildew on fruit and vegetables. No longer approved in EU.

Acute oral LD50 for rat approx. 5,000 mg/kg (low toxicity)

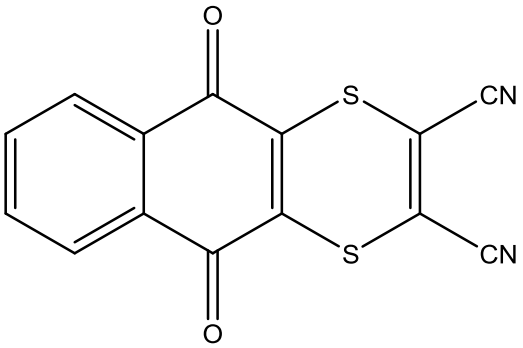
m/z	130	299	148	209	243	194	271	102
%	100	85	75	60	55	50	35	25

299 (85) – M^+
271 (35) – [M-28] loss of C_2H_4 to $C_{10}H_{10}NO_4PS^+$ m/z 271.0068
243 (55) – [M-56] loss of $2C_2H_4$ to $C_8H_6NO_4PS^+$ m/z 242.9789
209 (60) – [M-90] loss of $2(CH_3CH_2O)$ to $C_8H_4NO_2PS^+$ m/z 208.9700
194 (50) – [M-105] loss of C_6H_4CO+H to $C_5H_9NO_3PS^+$ m/z 194.0041
148 (75) – [M-151] $C_6H_4(COH)_2N^+$ C8H6NO2+ m/z 148.0399
130 (100) – [M-169] $C_6H_4NC_2O^+$ $C_8H_4NO^+$ m/z 130.0293
102 (25) – [M-197] $C_6H_4NC^+$ $C_7H_4N^+$ m/z 102.0343
76 (20) – [M-223] $C_6H_4^+$ m/z 76.0313

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C5131248&Mask=200#Mass-Spec

Dithianon $C_{14}H_4N_2O_2S_2$ **M:296(100%)**

Theoretical molecular ion: m/z 295.9714 (100%), 296.9748 (15%), 297.9672 (9.0%)
Average MW: 296.32



Quinone fungicide. Used for control of scab and foliar diseases. Approved for use in EU.

Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

Very poor GC transmission.

m/z	296	76	240	104	50	295	268	297
%	100	90	50	50	40	30	30	20

296 (100) – M^+
268 (30) – [M-28] loss of CO to $C_{13}H_4N_2OS_2^+$ m/z 267.9765
240 (50) – [M-56] loss of 2CO to $C_{12}H_4N_2S_2^+$ m/z 239.9816
104 (50) – [M-192] $C_6H_4CO^+$ $C_7H_4O_2^+$ m/z 104.0262
76 (90) – [M-220] NC-C=C-CN^+ $C_4N_2^+$ m/z 76.0062 and/or $C_6H_4^+$ m/z 76.0313
50 (40) – [M-246] NC-C=C^+ $C_4N_2^+$ m/z 50.0031

Cf. similar (though weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3347226&Mask=200#Mass-Spec

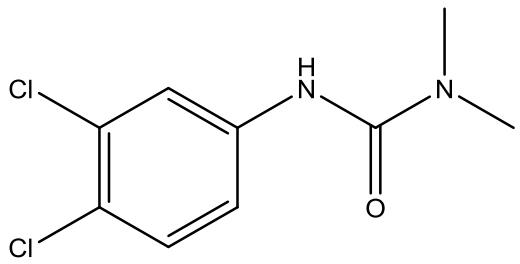
Dithiocarbamates

Residues of dithiocarbamates (whether metal complexes, e.g. maneb, mancozeb, nabam and zineb, or not, e.g. thiram) may be determined by measuring the carbon disulphide generated from them under acidic, reducing conditions (Hill 1982).

Ethylenethiourea (ETU, see separate entry) is an analytically troublesome (poor GC transmission) toxic metabolite that may be produced from ethylenebisdithiocarbamate (EBDC) fungicides. It may be determined by GC-MS following derivatisation (e.g. S-butylation), but is directly amenable to LC-MS determination (Tran 2013).

Cf. Propineb, which can produce iso-propylene thiourea.

Diuron **$C_9H_{10}Cl_2N_2O$** **M:232,234(15,10%)**
Theoretical molecular ion: m/z 232.0170 (100%), 234.0141 (64%)
Average MW: 223.09



Herbicide. Used for pre-emergence control of weeds and mosses in non-crop areas and woody crops. Approved for use in EU.

Acute oral LD50 for rat approx. 400 mg/kg (moderate toxicity).

Very poor GC transmission.

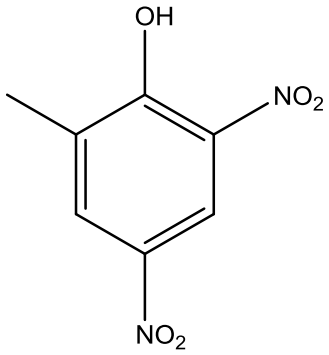
m/z	72	232	234	44	73	187	189	45
%	100	15	10	5	5	5	5	5

232,234 (15,10) – M^+
187,189 (5,5) – [M-45] loss of $(CH_3)_2NH$ to $Cl_2.C_6H_4.NCO^+$ $C_7H_3Cl_2NO^+$ m/z 186.9592 etc.
72 (100) – [M-160] $(CH_3)_2NCO^+$ $C_3H_6NO^+$ m/z 72.0449
44 (5) – [M-188] $(CH_3)_2N^+$ $C_2H_6N^+$ m/z 44.0500

Cf. similar (weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C330541&Mask=200#Mass-Spec

DNOC **$C_7H_6N_2O_5$** **M:198(100%)**

Theoretical molecular ion: m/z 198.0277 (100%), 199.0310 (7.6%)
Average MW: 198.13



Dinitro-*ortho*-cresol (DNOC)

Dinitrophenol acaricide, fungicide, herbicide and insecticide (and dangerous, human, accelerated weight loss aid of the 1930s).

Poor GC transmission.

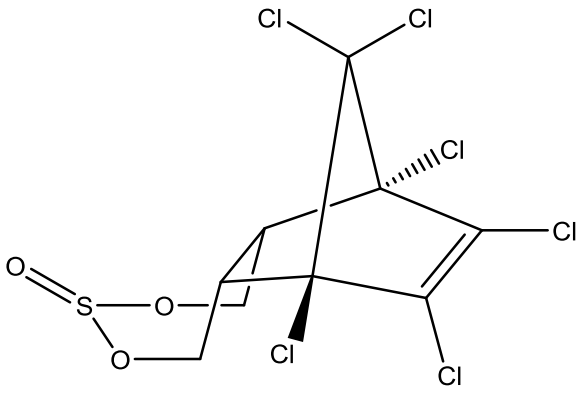
m/z	198	105	121	51	53	168	106	30
%	100	35	30	20	20	20	15	15

198 (100) – M^+
168 (20) – [M-30] loss of NO from nitro group, to $C_7H_6NO_4^+$ m/z 168.0297
121 (30) – [M-77] loss of NO & NO_2 & H to $C_7H_5O_2^+$ m/z 121.0290
106 (15) – [M-92] loss of $2NO_2$ to $C_7H_6O^+$ m/z 106.0419
105 (35) – [M-93] loss of $2NO_2$ & H to $C_7H_5O^+$ m/z 105.0340
51 (20) – [M-147] $C_4H_3^+$ m/z 51.0235

Cf. similar (weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C534521&Mask=200#Mass-Spec

Endosulfan **$C_9H_6Cl_6SO_3$** **M:404,406,408(1,1,1%)**

Theoretical molecular ion: m/z 403.8169 (52%), 405.8141 (100%), 407.8110 (53%), 409.8080 (34%)
Average MW: 406.90



alpha-endosulfan

Organochlorine insecticide and acaricide. Not approved for use in the EU. It is highly toxic to mammals, a neurotoxin and possibly a mutagen. It is moderately toxic to birds, honeybees and earthworms but slightly more toxic to aquatic organisms.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

Technical endosulfan (ca. 95% pure) is a mixture of alpha (65%) and beta (30%) isomers. These isomers, plus endosulfan sulphate, are included in MRLs.

Endosulfan, alpha - major isomer, shorter GC RT. KI(SE-30) = 20.8

m/z	195	197	241	239	207	237	160	69
%	100	75	75	65	65	60	60	60

404,406,408(1,1,1) – M^+
337,339,341(19,30,21) – [M-67] loss of Cl+S/O_2
321,323,325(10,15,10) – [M-83]
305,307,309(13,25,15) – [M-99]
293,295,297(7,15,8) – [M-111]
275,277,279(32,50,37) – [M-129]
237,239,241 (60,75,75) – [M-167]
193,195,197 (45,100,90) – [M-211]

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C959988&Mask=200 though slightly different relative intensities.

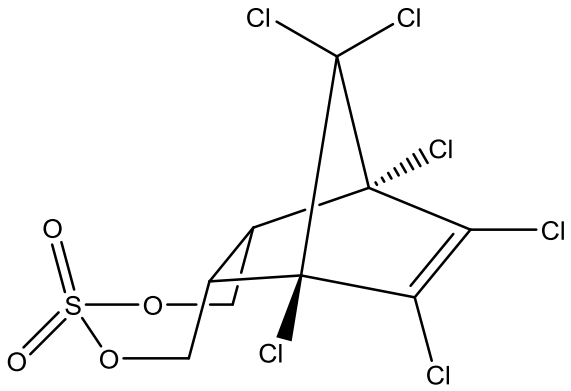
Endosulfan, beta - minor isomer, longer GC RT. KI(SE-30) = 21.8

m/z	195	197	159	160	241	237	207	89
%	100	75	70	65	60	60	60	50

404,406,408(1,1,1)
337,339,341(15,25,17)
321,323,325(10,15,10)
305,307,309(15,25,15)
293,295,297(6,12,6)
275,277,279(20,40,30)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C33213659&Mask=200

Endosulfan sulphate **$C_9H_6Cl_6SO_4$** **M:420,422,424,426(8,17,15,5%)**
Theoretical molecular ion: m/z 419.8118 (52%), 421.8089 (100%), 423.8059 (53%), 425.8030 (34%)
Average MW: 422.90



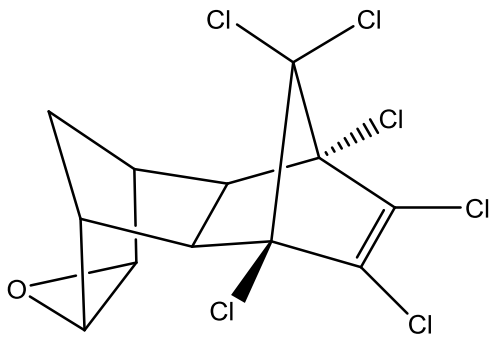
Alpha- and beta-endosulfan produce endosulfan sulphate by oxidation. It is included in MRLs for endosulfan.

m/z	272	274	229	387	227	270	239	237
%	100	80	75	60	55	50	45	45

420,422,424,426(8,17,15,5) – M^+
385,387,389,391(35,60,38,13) – [M-35] loss of Cl
355,357,359(3,7,4) – [M-65] loss of SO_2H
287,289,291(7,10,8) – [M-133] loss of $C_4H_5O_3S$ to $C_5Cl_6OH^+$
270,272,274 (50,100,80) – [M-150] loss of $C_4H_6O_4S$ to hexachlorocyclopentadiene $C_5Cl_6^+$

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1031078&Mask=200#Mass-Spec though slightly different relative intensities.

Endrin **$C_{12}H_8Cl_6O$** **M:378,380,382(1,2,1%)**
Theoretical molecular ion: m/z 377.8706 (70%), 379.8677 (89%), 381.8647 (100%), 383.8618 (37%)
Average MW: 380.90



Obsolete, organochlorine insecticide. Not approved for use in the EU. Endrin tends to be persistent in soil systems. It is highly toxic to mammals and is a neurotoxin. It is also highly toxic to birds, honeybees and most aquatic organisms.

Acute oral LD50 for rat >7.5 mg/kg (high toxicity)

May degrade on GC. The spectrum of endrin contains many ions of similar intensity, thus all are relatively weak. This makes trace detection difficult by EI+ MS.

Endrin may undergo acid-catalysed conversion to "endrin aldehyde" and "endrin ketone" (Chau 1969), which have spectra rather similar to that of endrin, but with longer GC RTs.

KI (SE-30) = 21.5

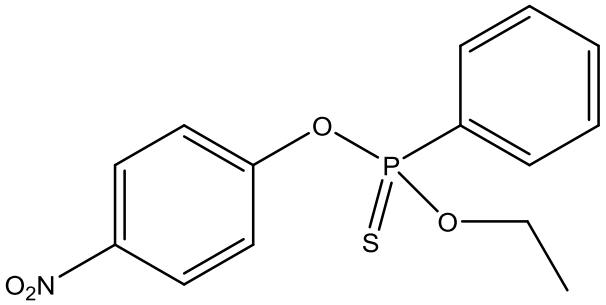
m/z	67	317	315	319	345	281	79	147
%	100	55	35	35	30	30	25	25

378,380,382(2,4,3) – M+
343,345,347(16,28,17) – [M-35] loss of Cl
315,317,319(33,53,32) – [M-63] loss of Cl+CO
279,281,283(21,25,12) – [M-99] loss of 2Cl+CO+H
261,263,265(12,18,11) – [M-117] loss of CCl3
67 (100) – [M-311] C5H7+

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C72208&Units=CAL&Mask=1A8F#Mass-Spec which also displays many polychlorinated isotope clusters, but which has base peak at m/z 81 rather than 67, and the most dominant poly-Cl cluster at m/z 261,263,265 rather than at m/z 315,317,319.

EPN **$C_{14}H_{14}NO_4PS$** **M:323(10%)**

Theoretical molecular ion: m/z 323.0381 (100%), 324.0415 (15%), 325.0339 (4.5%)
Average MW: 323.30



Organophosphorus phenylphosphonothioate insecticide. Used to control Lepidoptera larva, especially bollworms in a range of crops including cotton, rice, fruit and vegetables.

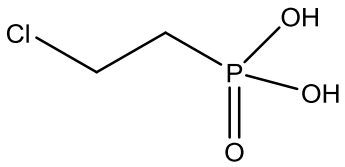
Acute oral LD50 for rat approx 14 mg/kg (high toxicity).

m/z	157	169	185	141	63	77	110	323
%	100	60	40	40	25	20	15	10

323 (10) – M^+
278 (5) – [M-45] loss of CH_3CH_2O to $C_{12}H_9NO_3PS^+$ m/z 278.0041
248 (5) – [M-75] loss of CH_3CH_2O+NO to $C_{12}H_9O_2PS^+$ m/z 248.0061
185 (40) – [M-138] $C_6H_5.PS.OCH_2CH_3^+$ $C_8H_{10}OPS^+$ m/z 185.0190
169 (60) – [M-127] $C_6H_5.PO.OCH_2CH_3^+$ $C_8H_{10}O_2P^+$ m/z 169.0418
157 (100) – [M-166] $C_6H_5.PS.OH^+$ $C_6H_6OPS^+$ m/z 156.9877
141 (40) – [M-182] $C_6H_5.PO.OH^+$ $C_6H_6O_2P^+$ m/z 141.0105
77 (20) – [M-246] $C_6H_5^+$ m/z 77.0391
63 (25) – [M-260] PS^+ m/z 62.9458

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2104645&Mask=200
filed as "Phosphonothioic acid, phenyl-, O-ethyl O-(4-nitrophenyl) ester"

Ethephon **$C_2H_6ClO_3P$** **M:144,146(0,0%)**
Theoretical molecular ion: m/z 143.9743 (100%), 144.9777 (2.2%), 145.9714 (32%)
Average MW: 144.49



Organophosphorus plant growth regulator with a range of uses, including the prevention of lodging (collapse of the cereal stem) in cereals and promotion of pre-harvest ripening of fruit. Approved for use in EU.

Acute oral LD50 for rat approx. 1,500 mg/kg (moderate toxicity).

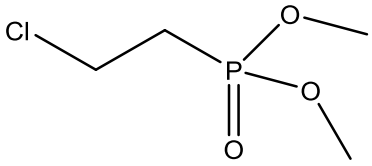
Not amenable to GC.

m/z	82	81	109	65	27	44	47	91
%	100	30	25	25	20	15	10	10

144,146 (0) – M^+ absent
109 (25) – [M-35] loss of Cl to $(CH_2CH_2)(HO)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
91 (10) [M-53] loss of Cl & H_2O to $(CH_2CH_2)PO_2^+$ $C_2H_4O_2P^+$ m/z 90.9949
82 (100) – [M-62] $(HO)_3P^+$ $H_3O_3P^+$ m/z 81.9820
81 (100) – [M-62] $(HO)_2PO^+$ $H_2O_3P^+$ m/z 80.9742
65 (25) – [M-79] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
47 (10) – [M-97] PO^+ m/z 46.9687

Cf. generally similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C16672870&Mask=200#Mass-Spec, listed under "Phosphonic acid, (2-chloroethyl)-", but with additional, atypical $(M+H)^+$ at m/z 145, 146 (6,2%), due to auto-CI, indicative of excessive MS source concentration.

Ethephon, dimethyl **$C_4H_{10}ClO_3P$** **M:172,174(0,0%)**
Theoretical molecular ion: m/z 172.0056 (100%), 174.0027 (32%)
Average MW: 172.54



Ethephon derivative.

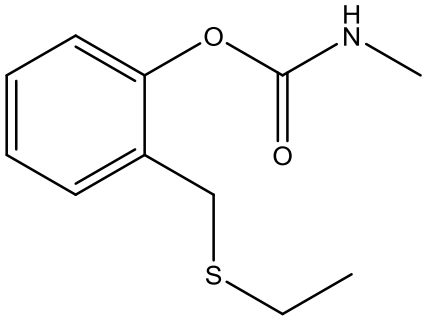
m/z	110	109	79	80	113	47	145	137
%	100	30	30	15	10	10	10	5

172,174 (0,0) – M^+ absent
137 (5) – [M-35] loss of Cl to $C_4H_{10}O_3P^+$ m/z 137.0368
110 (100) – [M-62] loss of $ClCHCH_2$ to $(CH_3O)_2(HO)P^+$ $C_2H_7O_3P^+$ m/z 110.0488

No NIST spectrum available.

Ethiofencarb **$C_{11}H_{15}NO_2S$** **M:225(2%)**

Theoretical molecular ion: m/z 225.08235 (100%), 226.0857 (11.9%), 227.07815 (4.5%)
Average MW: 225.31



Carbamate insecticide. Used to control aphids. No longer approved in EU.

Acute oral LD50 for rat approx. 200 mg/kg (moderate toxicity)

Poor GC transmission.

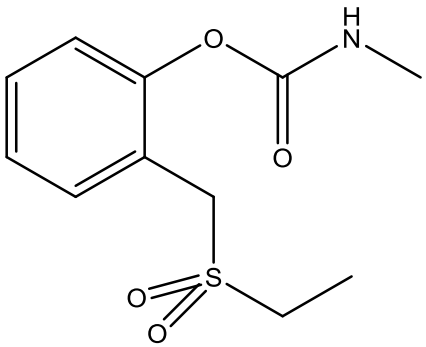
m/z	107	168	78	57	77	106	108	62
%	100	30	20	20	15	10	10	10

225 (2) – M^+
168 (30) – [M-57] loss of CH_3NCO methyl isocyanate to $C_9H_{12}OS+$ m/z 168.2540
107 (100) – [M-118] loss of CH_3NCO & SCH_2CH_3 to $C_7H_7O^+$ m/z 107.0497
62 (10) – [M-163] $HSCH_2CH_3^+$ $C_2H_6S^+$ m/z 62.0190

No NIST spectrum available.

Ethiofencarb sulphone **$C_{11}H_{15}NO_4S$** **M:257(0%)**

Theoretical molecular ion: m/z 257.0722 (100%), 258.0755 (11.9%), 259.0680 (4.5%)
Average MW: 257.30



Poor GC transmission.

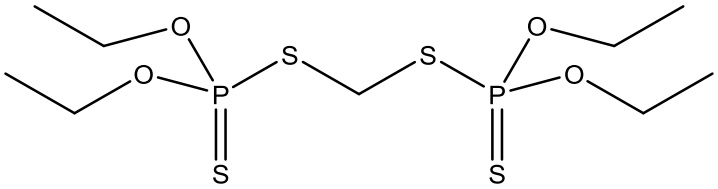
m/z	107	200	77	78	79	108	52	-
%	100	10	10	5	5	5	5	-

257 (0) – M^+ absent
200 (10) – [M-57] loss of CH_3NCO methyl isocyanate to $C_9H_{12}O_3S^+$ m/z 200.0507
107 (100) – [M-140] loss of CH_3NCO & $SO_2CH_2CH_3$ to $C_7H_7O^+$ m/z 107.0497

No NIST spectrum available.

Ethion $C_9H_{22}O_4P_2S_4$ **M:384,385,386(20,3,5%)**

Theoretical molecular ion: m/z 383.9876 (100%), 384.9910 (9.7%), 385.98341 (18.1%)
Average MW: 384.46



Organophosphorus insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 200 mg/kg (moderate toxicity).

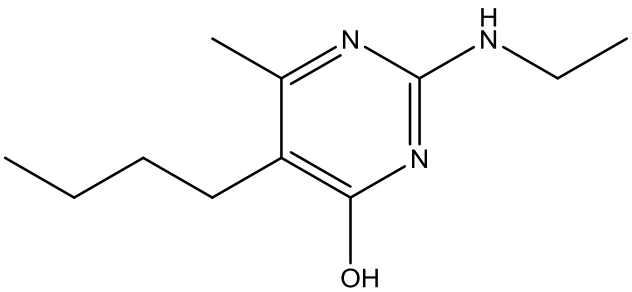
m/z	231	153	97	121	125	93	65	384
%	100	65	50	45	45	25	20	20

384,385,386 (20,3,5) – M^+
261 (3) – [M-123] loss of 2(CH_3CH_2O) & SH to $C_5H_{11}O_2P_2S_3^+$ m/z 260.9396
231 (100) – [M-153] $SCH_2S.PS(OCH_2CH_3)_2^+$ $C_5H_{12}O_2PS_3^+$ m/z 231.9737
153 (65) – [M-231] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.1039
125 (45) – [M-259] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121 (45) – [M-263] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
97 (50) – [M-287] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C563122&Mask=200#Mass-Spec

Ethirimol $C_{11}H_{19}N_3O$ **M:209(20%)**

Theoretical molecular ion: m/z 209.1528 (100%), 210.1562 (11.9%)
Average MW: 209.29



Pyrimidine fungicide. Often used as a seed treatment. May also be a pesticide transformation product (from hydrolysis of **bupirimate)**. No longer approved for use in EU.

Acute oral LD50 for rat >4,000 mg/kg (low toxicity).

Poor GC transmission.

m/z	166	96	209	42	55	167	71	194

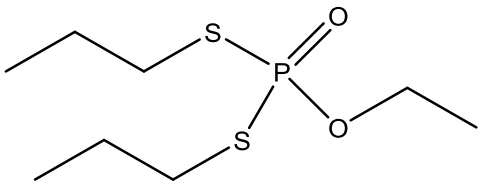
%	100	25	20	15	15	10	10	5

209 (20) – M+
194 (5) – [M-15] loss of CH_3 to $C_{10}H_{16}N_3O^+$ m/z 194.1293
166 (100) – [M-43] loss of C_3H_7 to $C_8H_{12}N_3O^+$ m/z 166.0980
96 (25) – [M-113] $C_6H_8O^+$ m/z 96.0575 and/or $C_5H_8N_2^+$ m/z 96.06875

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C23947606&Mask=200#Mass-Spec

Ethoprophos **$C_8H_{19}O_2PS_2$** **M:242(25%)**

Theoretical molecular ion: m/z 242.0564 (100%), 243.0598 (8.7%), 244.0522 (9.0%)
Average MW: 242.33



Organophosphorus insecticide and nematicide. Used to control plant parasitic nematodes and soil insects. Approved for use in EU.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

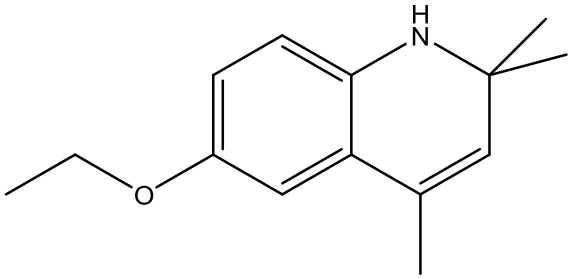
m/z	43	158	97	41	139	126	74	93
%	100	90	70	60	50	50	40	40

Assignments confirmed by accurate mass (Cardiff GCT)
242 (25) – M^+ m/z 242.0564
200 (25) – [M-42] loss of C_3H_6 to $C_5H_{13}O_2PS_2^+$ m/z 200.0095
168 (15) – [M-74] loss of C_3H_6S to $C_5H_{13}O_2PS^+$ m/z 168.0374
167 (5) – [M-75] loss of C_3H_7S to $C_5H_{12}O_2PS^+$ m/z 167.0296
158 (100) – [M-84] loss of $2C_3H_6$ to $(HS)_2PO.OCH_2CH_3^+$ $C_2H_7O_2PS_2^+$ m/z 157.9625
139 (50) – [M-103] $C_3H_8OPS^+$ m/z 138.9983
126 (50) – [M-116] loss of C_3H_6 & C_3H_6S to $C_2H_7O_2PS^+$ m/z 125.9904
125 (50) – [M-117] $C_2H_6O_2PS^+$ m/z 124.9826
97 (70) – [M-145] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
93 (40) – [M-149] $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105
74 (40) – [M-168] $C_3H_6S^+$ m/z 74.0190
43 (100) – [M-201] $C_3H_7^+$ m/z 43.0548

Cf. similar (but weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C13194484&Mask=200#Mass-Spec

Ethoxyquin **$C_{14}H_{19}NO$** **M:217(20%)**

Theoretical molecular ion: m/z 217.1467 (100%), 218.1500 (15.1%)
Average MW: 217.31



Quinoline fungicide. Used to control scald and other diseases, and post-harvest in top fruit. Approved for use in EU.

Acute oral LD50 for rat >1,500 mg/kg (moderate toxicity).

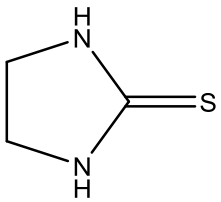
m/z	202	174	173	203	217	145	144	188
%	100	50	20	20	20	15	10	5

217 (20) – M^+
202 (100) – [M-15] loss of CH_3 to $C_{13}H_{16}NO^+$ m/z 202.1232
174 (50) – [M-43] loss of CH_3 & C_2H_5 to $C_{11}H_{11}NO^+$ m/z 173.0841

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C91532&Mask=200

Ethylenethiourea (ETU) **$C_3H_6N_2S$** **M:102(100%)**

Theoretical molecular ion: m/z 102.0252 (100%), 103.0285 (3.2%), 104.0210 (4.5%)
Average MW: 102.16



ethylenethiourea (ETU), or 2-imidazolidinethione

ETU is a genotoxic metabolite of ethylenebisdithiocarbamate (EBDC) fungicides, e.g. mancozeb, maneb, zineb.

Poor GC transmission, but may be derivatised (e.g. S-butyl), or analysed by LC-MS (Tran 2013).

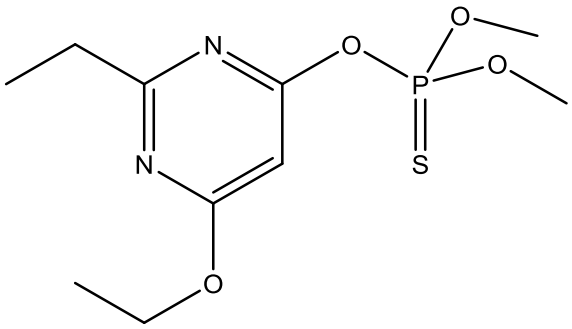
m/z	102	30	73	45	42	72	103	104
%	100	30	15	10	10	10	5	5

102 (100) – M^+
30 (30) – [M-72] loss of CH_2NH_2 to CH_3NCS^+ $C_2H_2NS^+$ m/z 71.9908

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C96457&Mask=200#Mass-Spec

Etrimfos $C_{10}H_{17}N_2O_4PS$ **M:292(100%)**

Theoretical molecular ion: m/z 292.0647 (100%), 293.0680 (10.8%), 294.0605 (4.5%)
Average MW: 292.29



Organophosphorus insecticide. Used to control various pests of stored grain.
No longer approved for use in EU.

Acute oral LD50 for rat > 1,500 mg/kg (moderate toxicity).

m/z	292	181	56	125	153	168	79	277
%	100	75	65	55	50	45	35	30

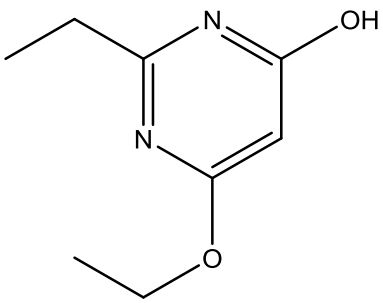
292 (100) – M^+
277 (30) – [M-15] loss of CH_3 to $C_9H_{14}N_2O_4PS^+$ m/z 277.0412
181 (75) – [M-111] loss of C_6H_9NO to $C_4H_8NO_3PS^+$ m/z 180.9963
168 (45) – [M-124] loss of $C_2H_5O_2PS$ to $C_8H_{12}N_2O_2^+$ m/z 168.0899
153 (50) – [M-139] $C_2H_4NO_3PS^+$ m/z 152.9650 (??)
125 (55) – [M-167] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
93 (20) – [M-199] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (20) – [213] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
56 (65) – [M-236] $CH_3CH_2C{=}NH^+$ $C_3H_6N^+$ m/z 56.0500

Cf. generally similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C38260547&Mask=200#Mass-Spec
Listed under "Phosphorothioic acid, O-(6-ethoxy-2-ethyl-4-pyrimidinyl) O,O-dimethyl ester" with similar major ions, but different relative abundances.

Etrimfos related $C_8H_{12}N_2O_2$ **M:168(35%)**

6-ethoxy-2-ethyl-4-hydroxypyrimidine

Theoretical molecular ion: m/z 168.0899 (100%), 169.0932 (8.7%)
Average MW: 168.20



An hydrolysis product of etrimfos (6-ethoxy-2-ethyl-4-hydroxypyrimidine):

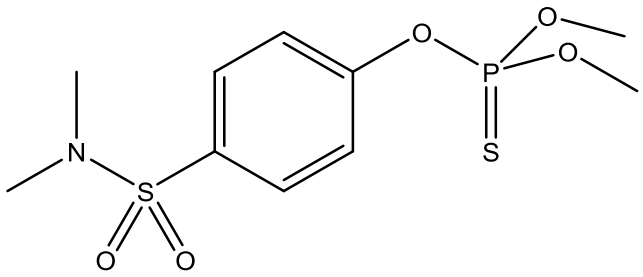
m/z	153	56	69	140	112	168	124	99
%	100	75	50	50	45	35	25	25

168 (35) – M^+
153 (100) – [M-15] loss of CH_3 to $C_7H_9N_2O_2^+$ m/z 153.0664
140 (50) – [M-28] loss of C_2H_4 to $C_6H_8N_2O_2^+$ m/z 140.0586
112 (45) – [M-56] loss of $CH_3CH_2C{=}NH$ to $C_5H_6NO_2^+$ m/z 112.0399

No NIST spectrum available.

Famphur **$C_{10}H_{16}NO_5PS_2$** **M:325(1%)**

Theoretical molecular ion: m/z 325.0208 (100%), 326.0241 (10.8%), 327.0165 (9.0%)
Average MW: 325.33



Organophosphorus insecticide. Used as veterinary systemic parasiticide for cattle. Also used illegally to poison birds of prey etc. (magpies being particularly sensitive). No longer approved for use in EU.

Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

Long GC RT.

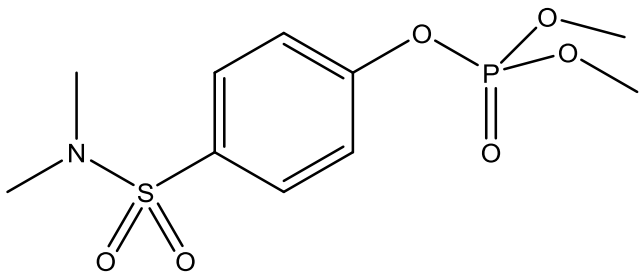
m/z	218	93	125	217	44	109	219	79
%	100	30	25	25	15	15	10	5

Assignments confirmed by accurate mass (Cardiff GCT)
325 (1) – M^+ m/z 325.0208 (not detected on GCT)
282 (5) – [M-43] loss of C_2H_5N to $C_8H_{11}O_5PS_2^+$ m/z 281.9786
218 (100) – [M-107] loss of $C_2H_5NSO_2$ to $C_8H_{11}O_3PS^+$ m/z 218.0167
136 (20) – [M-189] $(CH_3)_2NC_6H_4^+$ by expulsion of SO_2, to $C_8H_{10}NO^+$ m/z 136.0762
125 (25) – [M-200] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (15) – [M-216] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 190.0055
93 (30) – [M-232] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (10) – [M-246] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C52857&Mask=200#Mass-Spec

Famphur oxon **$C_{10}H_{16}NO_6PS$** **M:309(9%)**

Theoretical molecular ion: m/z 309.0436 (100%), 310.0470 (10.8%), 311.0394 (4.5%)
Average MW: 309.27



Oxidative metabolite of **famphur**. Long GC RT.

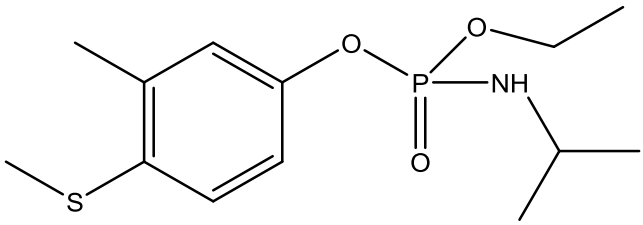
m/z	202	201	44	265	109	186	93	309
%	100	69	39	21	18	18	12	9

309 (9) – M+
265 (21) – [M-44] loss of $(CH_3)_2N$ to $C_8H_{10}O_6PS^+$ m/z 264.9936
202 (100) – [M-107] loss of $C_2H_5NSO_2$ to $C_8H_{11}O_4P^+$ m/z 202.0395
109 (15) – [M-200] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 190.0055

No NIST spectrum available.

Fenamiphos **$C_{13}H_{22}NO_3PS$** **M:303(100%)**

Theoretical molecular ion: m/z 303.1058 (100%), 304.1092 (14.1%), 305.1016 (4.5%)
Average MW: 303.3568



Organophosphorus insecticide and nematicide. Used to control ectoparasitic, endoparasitic, free-living and cyst-forming nematodes. Approved for use in EU.

Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

Chiral molecule. Several oxidative metabolites. The sulphone is included in MRLs.

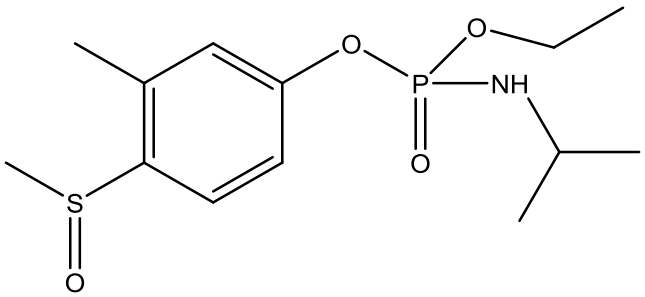
m/z	303	288	260	154	195	44	217	304
%	100	40	30	30	25	20	15	15

Assignments confirmed by accurate mass (Cardiff GCT)
303 (100) – M^+ $C_{13}H_{22}NO_3PS^+$ m/z 303.1058
288 (40) – [M-15] loss of CH_3 to $C_{12}H_{19}NO_3PS^+$ m/z 288.0823
260 (30) – [M-43] loss of C_3H_7 to $C_{10}H_{15}NO_3PS^+$ m/z 260.05103
243 (15) – [M-60] loss of $C_3H_{10}N$ to $C_{10}H_{12}O_3PS^+$ m/z 243.0245
217 (15) – [M-86] loss of $C_5H_{12}N$ to $C_8H_{10}O_3PS^+$ m/z 217.0088
195 (25) – [M-108] rearrangement and loss of $C_3H_8O_3P$ to $C_{11}N_{17}NS^+$ m/z 195.1082

180 (5) – [M-123] $C_{10}H_{14}NS^+$ m/z 180.0847
154 (30) – [M-149] phenol $(CH_3S)(CH_3)C_6H_3.OH^+$ $C_8H_{10}OS^+$ m/z 154.0452
139 (20) – [M-164] phenol fragment $(S)(CH_3)C_6H_3.OH^+$ $C_7H_7OS^+$ m/z 139.0218
122 (25) – [M-181] $(C_3H_7NH)P(OH)O^+$ $C_3H_9NO_2P^+$ m/z 122.0371
110 (15) – [M-193] $C_6H_6S^+$ m/z 110.0190
109 (10) – [M-195] $C_6H_5S^+$ m/z 109.0112
91 (10) – [M-212] $C_7H_7^+$ m/z 91.0548
80 (15) – [M-223] $(HO)_2(NH)P^+$ $H_3NO_2P^+$ m/z 79.9901
77 (10) – [M-226] $C_6H_5^+$ m/z 77.0391
44 (20) – [M-259] $C_2H_6N^+$ m/z 44.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C22224926&Mask=200#Mass-Spec with similar major ions, but different relative abundances.

Fenamiphos sulphoxide **$C_{13}H_{22}NO_4PS$** **M:319(30%)**
Theoretical molecular ion: m/z 319.1007 (100%), 320.10411 (14.1%), 321.0965 (4.5%)
Average MW: 319.34



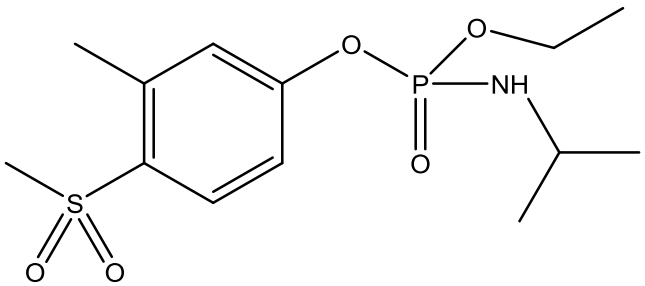
Oxidative metabolite of fenamiphos.

m/z	304	122	303	319	154	196	80	44
%	100	85	35	30	30	25	25	20

319 (30) – M^+
304 (100) – [M-15] loss of CH_3 to $C_{12}H_{19}NO_4PS^+$ m/z 304.0772
196 (25) – [M-123]
122 (85) – [M-197] $(HO)(C_3H_8N)P{=}O^+$ $C_3H_9NO_2P^+$ m/z 122.0371
80 (25) – [M-239] $(H_2N)(HO)_2P^+$ $H_3NO_2P^+$ m/z 79.9901
44 (20) – [M-275] $C_2H_6N^+$ m/z 44.0500

No NIST spectrum available.

Fenamiphos sulphone **$C_{13}H_{22}NO_5PS$** **M:335(10%)**
Theoretical molecular ion: m/z
Average MW:



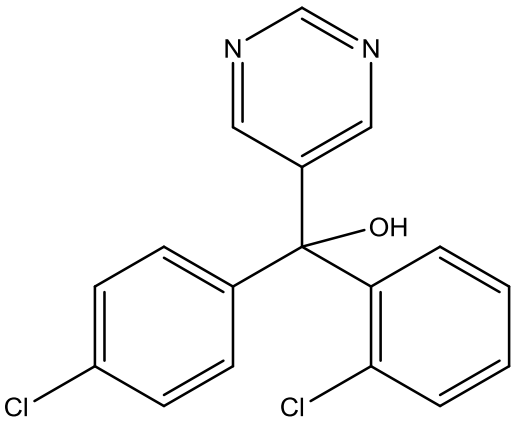
Oxidative metabolite of fenamiphos.

m/z	320	292	58	44	321	122	293	335
%	100	65	20	15	15	10	10	10

335 (10) – M^+
320 (100) – [M-15] loss of CH_3 to $C_{12}H_{19}NO_5PS^+$ m/z 320.0722
292 (65) – [M-43] loss of C_3H_7 to $C_{10}H_{15}NO_5PS^+$ m/z 292.0409
122 (85) – [M-213] $(HO)(C_3H_8N)P{=}O^+$ $C_3H_9NO_2P^+$ m/z 122.0371
80 (25) – [M-239] $(H_2N)(HO)_2P^+$ $H_3NO_2P^+$ m/z 79.9901
58 (20) – [M-277] $(CH_3)_2CHNH^+$ $C_3H_8N^+$ m/z 58.0657
44 (20) – [M-291] $C_2H_6N^+$ m/z 44.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C31972448&Units=SI&Mask=200#Mass-Spec, though some low mass ions, e.g. m/z 80, rather stronger.

Fenarimol **$C_{17}H_{12}Cl_2N_2O$** **M:330,332(30,20%)**
Theoretical molecular ion: m/z 330.0327 (100%), 332.0297 (63.9%), 334.0268 (10.2%)
Average MW: 331.20



Pyrimidine fungicide. No longer approved for use in EU.

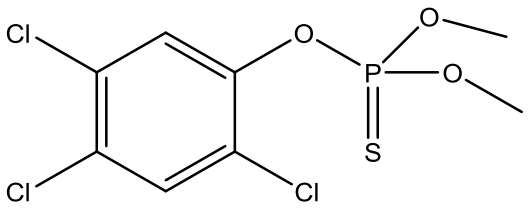
Acute oral LD50 for rat approx. 2,500 mg/kg (low toxicity).

m/z	139	107	219	251	330	141	253	111
%	100	80	65	50	30	30	30	25

330,332 (30,20) – M^+
251,253 (50,30) – [M-79] loss of $C_4H_3N_2$ to $C_{13}H_9Cl_2O^+$ m/z 251.0031 etc.
139 (100) – [M-191] $ClC_6H_4CO^+$ $C_7H_4ClO^+$ m/z138.9951 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C60168889&Mask=200#Mass-Spec

Fenchlorphos / Ronnel **$C_8H_8Cl_3O_3PS$** **M:320,322,324(2,2,1%)**
Theoretical molecular ion: m/z 319.8997 (100%), 321.8968 (96%), 323.8938 (31%)
Average MW: 321.53



Organophosphorus insecticide. Used to control warble fly larvae. No longer approved in EU.

Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity).

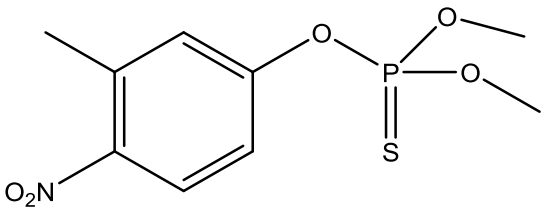
m/z	285	287	125	79	109	93	47	289
%	100	80	60	25	25	25	20	15

Assignments confirmed by accurate mass (Cardiff GCT)
320,322,324 (2,2,1) – M^+ $C_8H_8Cl_3O_3PS^+$ m/z 319.8997 etc
285,287,289 (100,80,15) – [M-35] loss of Cl to $C_8H_8Cl_2O_3PS^+$ m/z 284.9309 etc.
270,272,274 (10,7,3) – [M-50] loss of Cl & CH_3 to $C_7H_5Cl_2O_3PS^+$ m/z 269.9074 etc.
196,198,200 (10,10,3) – [M-124] $C_6H_3Cl_3O_3^+$ m/z 195.9249 etc.
195,197,199 (10,10,3) – [M-125] $C_6H_2Cl_3O_3^+$ m/z 194.9171 etc.
167,169,171 (30,30,10) – [M-153] $C_5H_2Cl_3^+$ m/z 166.9171 etc.
125 (60) – [M-195] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (25) – [M-211] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055 [O/S swap]
97,99 (25,5) – [M-223] $C_5H_2Cl^+$ m/z 96.9845 etc.
97 (10) – [M-223] $H_2O_2PS^+$ m/z 96.9513 etc.
93 (25) – [M-227] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (25) – [M-241] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
62 (15) – [M-258] $C_5H_2^+$ m/z 62.0157
47 (20) – [M-273] PO^+ m/z 46.9687

Cf. similar, but very weak spectrum, at http://webbook.nist.gov/cgi/cbook.cgi?ID=C299843&Units=SI&Mask=200#Mass-Spec which lacks the less abundant but informative $^{13}C/^{34}S$ isotope peaks.

Fenchlorphos oxon spectrum also available at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3983457&Mask=200
Exhibits main ions at m/z 109 (100%), $[M-35]^+$ at 269,271,273 (50,35,5%), 79 (30%) and weak M^+ at m/z 304,306 (5,5%).

Fenitrothion **$C_9H_{12}NO_5PS$** **M:277(50%)**
Theoretical molecular ion: m/z 277.0174 (100%), 278.0207 (9.7%), 279.0132 (4.5%)
Average MW: 277.23



Organophosphorus (phenyl organothiophosphate) insecticide, used to control chewing, sucking and boring pests on a range of crops.

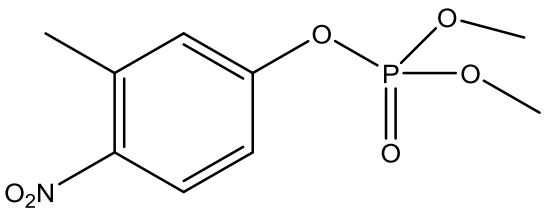
Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

m/z	125	109	277	260	79	47	93	63
%	100	90	50	30	30	35	35	15

277 (50) – M^+.
260 (30) – [M-17] loss of OH to $C_9H_{11}NO_4PS^+$ m/z 260.0146 (surprising fragmentation)
125 (100) – [M-152] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (90) – [M-168] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (35) – [M-184] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (30) – [M-198] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (15) – [M-214] PS^+ m/z 62.9458
47 (35) - [M-230] PO^+ m/z 46.9687

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C122145&Mask=200#Mass-Spec

Fenitrothion oxon **$C_9H_{12}NO_6P$** **M:261(15%)**
Theoretical molecular ion: m/z 261.0402 (100%), 262.0436 (9.7%), 263.0445 (1.2%)
Average MW: 261.17



Oxidative metabolite of fenitrothion.

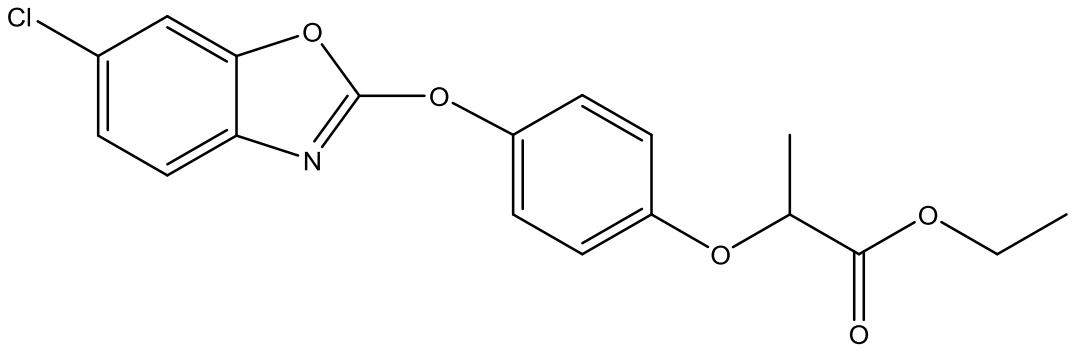
m/z	109	244	79	127	63	261	90	77
%	100	55	20	15	15	15	15	15

261 (15) – M^+
244 (55) – [M-17] loss of OH to $C_9H_{11}NO_5P^+$ m/z 244.0375 (surprising fragment – cyclic product?)
127 (15) – [M-152] $(CH_3O)_2(HO)_2P^+$ $C_2H_8O_4P^+$ m/z 127.0160
109 (100) – [M-152] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
90 (15) – [M-171] $C_7H_6^+$ m/z 90.0470
79 (30) – [M-182] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2255176&Mask=200#Mass-Spec

Fenoxaprop-ethyl **$C_{18}H_{16}ClNO_5$** **M:361,363(70,25%)**

Theoretical molecular ion: m/z 361.0717 (100%), 363.0688 (32%)
Average MW: 361.78



Herbicide. No longer approved in EU.
Acute oral LD50 for rat approx. 2,500 mg/kg (low toxicity).
Chiral molecule.

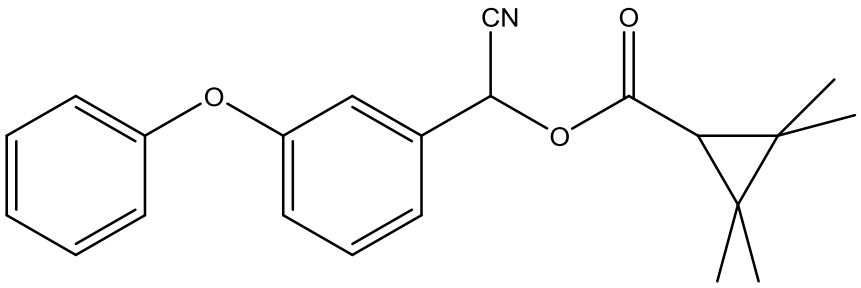
m/z	288	361	290	261	119	363	289	182
%	100	70	35	30	25	25	20	15

361,363 (70,25) – M^+
288,290 (100,35) – [M-73] loss of CH_3CH_2OOC to $C_{15}H_{11}ClNO_3^+$ m/z 288.0428
261 (30) – [M-100] loss of $C_5H_8O_2$ to phenol $C_{13}H_8ClNO_3^+$ m/z 261.0193

No NIST spectrum available.

Fenpropathrin **$C_{22}H_{23}NO_3$** **M:349(5%)**

Theoretical molecular ion: m/z 349.1678 (100%), 350.1712 (24%), 351.1745 (2.7%)
Average MW: 349.43



Synthetic pyrethroid insecticide.
Acute oral LD50 for rat approx. 800 mg/kg (moderate toxicity).

One peak on capillary GC (unlike many other pyrethroids).

m/z	97	55	125	181	208	83	209	141
%	100	55	45	40	30	30	20	20

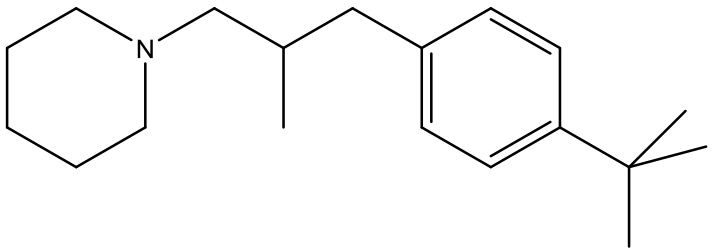
349 (5) – M^+
265 (15) – [M-84] loss of $(CH_3)_4C_2$, tetramethylethene, to $C_{16}H_{11}NO_3^+$ m/z 265.0739
208 (30) – [M-141] $C_6H_5O.C_6H_4.CHCN^+$ $C_{14}H_{10}NO^+$ m/z 208.0762
125 (45) – [M-224] $(CH_3)_4.C_3H.CO^+$ $C_8H_{13}O^+$ m/z 125.0966
97 (100) – [M-252] $(CH_3)_4C_3H^+$ tetramethylcyclopropane $C_7H_{13}^+$ m/z 97.1017

55 (55) – [M-294]] $(CH_3)_2.CCH^+$ $C_4H_7^+$ m/z 55.0548

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C39515418&Mask=200#Mass-Spec

Fenpropidin **$C_{19}H_{31}N$** **M:273(2%)**

Theoretical molecular ion: m/z 273.24565 (100%), 274.2490 (20.5%), 275.2524 (2.0%)
Average MW: 273.46



Piperidine fungicide used to control powdery mildew, rusts and leaf spots in cereals. Approved for use in the EU.

Acute oral LD50 for rat approx. 1,400 mg/kg (moderate toxicity).

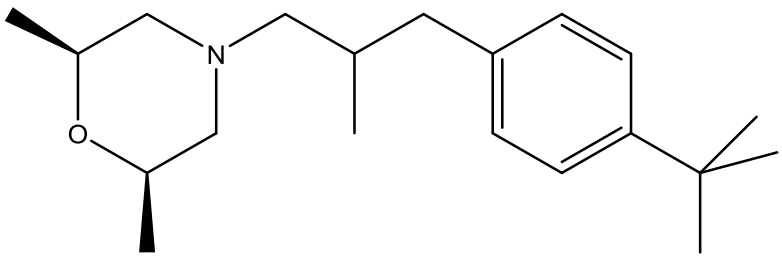
m/z	98	99	41	55	273	42	-	-
%	100	5	5	5	2	2	-	-

273 (2) – M^+
98 (100) – [M-175] $C_5H_{10}N\text{-}CH_2^+$ $C_6H_{12}N^+$ m/z 98.0970

Cf. weak and noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C67306007&Mask=200#Mass-Spec that has m/z 98 base peak, plus several additional ions e.g. m/z 70, 117, 145, 173 not observed here. Evidence of contaminant?

Fenpropimorph **$C_{20}H_{33}NO$** **M:303(5%)**

Theoretical molecular ion: m/z 303.2562 (100%), 304.2596 (21.6%), 305.2629 (2.2%)
Average MW: 303.49



Fungicide. Used to control powdery mildew, scald, rusts and other fungal pathogens.

Acute oral LD50 for rat approx. 1,500 mg/kg (moderate toxicity).

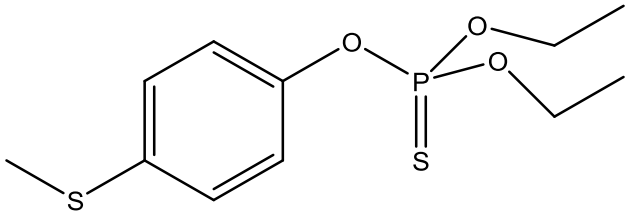
m/z	128	43	129	42	303	-	-	-
%	100	10	10	5	5	-	-	-

303 (5) – M^+
128 (100) – [M-175] $(CH_3)_2[C_4H_6NO]CH_2^+$ $C_7H_{14}NO^+$ m/z 128.1075

No NIST spectrum, but similar to that at http://www.restek.com/compound/view/67306-03-0/Fenpropimorph

Fensulfothion sulphide $C_{11}H_{17}O_3PS_2$ **M:292(100%)**

Theoretical molecular ion: m/z 292.0357 (100%), 293.0390 (11.9%), 294.0315 (9.0%)
Average MW: 292.35



Fensulfothion reduction product.

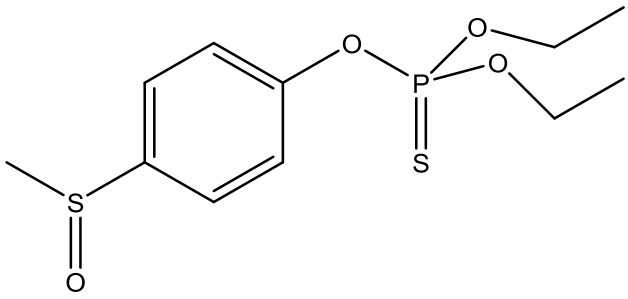
m/z	292	156	140	97	264	125	109	236
%	100	60	45	35	25	20	20	20

292 (100) – M^+
264 (25) – [M-28] loss of C_2H_4 to $C_9H_{13}O_3PS_2^+$ m/z 264.2938
236 (20) – [M-56] loss of $2C_2H_4$ to $C_7H_9O_3PS_2^+$ m/z 236.2398
156 (60) – [M-136] $CH_3S.C_6H_4.\underline{S}H^+$ $C_7H_8S_2^+$ m/z 156.0067 [O/S swap]
140 (45) – [M-152] $CH_3S.C_6H_4.\underline{O}H^+$ $C_7H_8OS^+$ m/z 140.0296 [O/S swap]
125 (20) – [M-167] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (20) – [M-183] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (35) – [M-195] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513

No NIST spectrum, but very similar to that reported by Wood (1977).

Fensulfothion $C_{11}H_{17}O_4PS_2$ **M:308(50%)**

Theoretical molecular ion: m/z 308.0306 (100%), 309.0339 (11.9%), 310.0264 (9.0%)
Average MW: 308.35



Organophosphorus insecticide. Used against soil nematodes and soil insects in field crops. No longer approved for use in EU.

Acute oral LD50 for rat approx. 2 mg/kg (high toxicity).

NOTE: The EI mass spectrum appears to be concentration dependent: At high source concentrations, the "true" (sulphoxide) spectrum is obtained, but at lower concentrations, the "sulphide" spectrum takes over (presumably because of reduction in the ion source of the parent compound, which contains a sulphoxide moiety (CH_3SO-), to the sulphide).

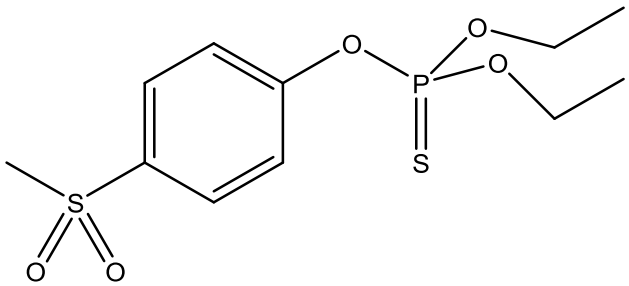
See Sugitate (2012).

m/z	293	97	125	141	308	109	153	265
%	100	95	85	85	50	50	50	25

308 (50) – M^+
293 (100) – [M-15] loss of CH_3 to $C_{10}H_{14}O_4PS_2^+$ m/z 293.0071
265 (25) – [M-43] loss of CH_3 & C_2H_4 to $C_8H_{10}O_4PS_2^+$ m/z 264.9758
153 (50) – [M-155] $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2P^+$ m/z 153.0139
141 (85) – [M-167] $OS.C_6H_4.OH^+$ $C_6H_5O_2S^+$ m/z 141.0010
125 (85) – [M-183] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (50) – [M-199] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (95) – [M-211] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C115902&Mask=200#Mass-Spec

Fensulfothion sulphone **$C_{11}H_{17}O_5PS_2$** **M:324(100%)**
Theoretical molecular ion: m/z 324.0255 (100%), 325.0289 (11.9%), 326.0213 (9.0%)
Average MW: 324.35



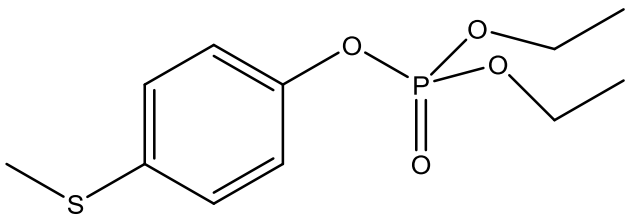
Fensulfothion oxidation product. Included in MRL of fensulfothion.

m/z	324	188	109	97	125	172	157	219
%	100	60	60	60	50	35	30	30

324 (100) – M^+
296 (100) – [M-28] loss of C_2H_4 to $C_9H_{13}O_5PS_2^+$ m/z 295.9948
188 (60) – [M-136] $CH_3SO_2.C_6H_4.SH^+$ $C_7H_8S_2^+$ m/z 187.9966 [O/S swap]
172 (35) – [M-152] $CH_3SO_2.C_6H_4.OH^+$ $C_7H_8O_3S^+$ m/z 172.0194
157 (30) – [M-167] $SO_2.C_6H_4.OH^+$ $C_6H_5O_3S^+$ m/z 156.9959
125 (85) – [M-199] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (50) – [M-215] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (95) – [M-227] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C14255722&Mask=200#Mass-Spec

Fensulfothion oxon sulphide **$C_{11}H_{17}O_4PS$** **M:276(100%)**
Theoretical molecular ion: m/z 276.0585 (100%), 277.0619 (11.9%), 278.0543 (4.5%)
Average MW: 276.29



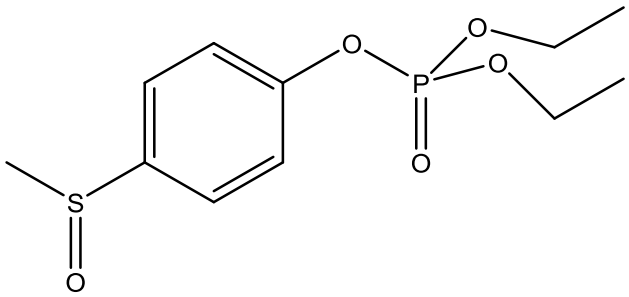
Fensulfothion related compound.

m/z	276	140	220	248	125	202	139	109
%	100	75	60	40	25	20	15	15

276 (100) – M^+
248 (40) – [M-28] loss of C_2H_4 to $C_9H_{13}O_4PS^+$ m/z 248.2328
220 (60) – [M-56] loss of $2C_2H_4$ to $C_7H_9O_4PS^+$ m/z 219.9959
202 (20) – [M-74] loss of C_2H_4+CH_2S to $C_8H_{11}O_4P^+$ m/z 202.0395
140 (45) – [M-136] $CH_3S.C_6H_4.OH^+$ $C_7H_8OS^+$ m/z 140.0296
125 (20) – [M-151] ? cannot be the "usual" m/z 125 ion $(CH_3CH_2O)(HO)P{=}S^+$ because no sulphur!
Perhaps loss of CH_3 from $CH_3S.C_6H_4.OH^+$ m/z 140.
109 (20) – [M-167] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055

No NIST spectrum available

Fensulfothion oxon **$C_{11}H_{17}O_5PS$** **M:292(20%)**
Theoretical molecular ion: m/z 292.0534 (100%), 293.0568 (11.9%), 294.0492 (4.5%)
Average MW: 292.29



Fensulfothion oxidation product. See note about parent compound.

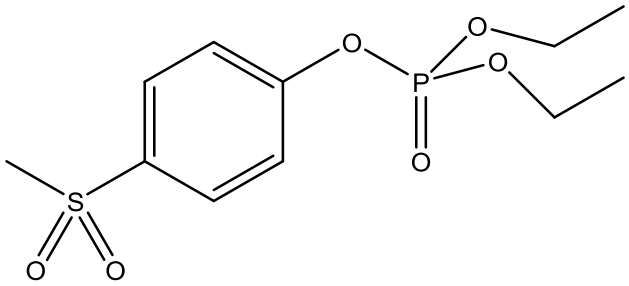
m/z	277	141	249	109	221	292	278	81
%	100	40	25	25	20	20	15	15

292 (20) – M^+
277 (100) – [M-15] loss of CH_3 to $C_{10}H_{14}O_5PS^+$ m/z 277.0300
249 (25) – [M-43] loss of CH_3 & C_2H_4 to $C_6H_6O_5PS^+$ m/z 248.9987
221 (20) – [M-71] loss of CH_3 & $2C_2H_4$ to $C_8H_{10}O_5PS^+$ m/z 220.9674
141 (40) – [M-151] $OS.C_6H_4.OH^+$ $C_6H_5O_2S^+$ m/z 141.0010
109 (25) – [M-199] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
81 (15) – [M-211] $(HO)_2PO^+$ $H_2O_3P^+$ m/z 80.9742

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=U290099&Mask=200

Fensulfothion oxon sulphone **$C_{11}H_{17}O_6PS$** **M:308(60%)**

Theoretical molecular ion: m/z 308.04835 (100%), 309.0517 (11.9%), 310.0441 (4.5%)
Average MW: 308.29



Fensulfothion oxidation product. (Complicated MS fragmentation!)

m/z	182	127	99	119	109	308	201	280
%	100	85	75	65	65	60	55	50

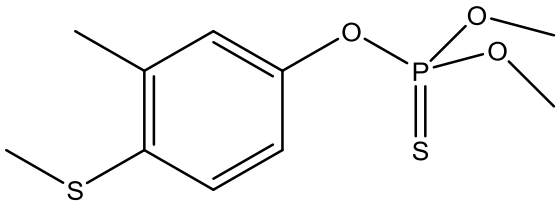
308 (100) – M^+
293 (20) – [M-15] loss of CH_3 from sulphone moiety to $C_{10}H_{14}O_6PS^+$ m/z 293.0249
280 (50) – [M-28] loss of C_2H_4 to $C_9H_{13}O_6PS^+$ m/z 280.0171
245 10) – [M-63] loss of CH_3SO to $C_{10}H_{14}O_5P^+$ m/z 245.0579
229 (20) – [M-79] loss of CH_3SO_2 to $C_{10}H_{14}O_4P^+$ m/z 229.0630
201 (55) – [M-107] loss of C_2H_4 & CH_3SO_2 to $C_8H_{10}O_4P^+$ m/z 201.0317
182 (100) – [M-126] $C_6H_4OPO(OC_2H_3)^+$ $C_8H_7O_3P_+$ m/z 182.01328 (??)
173 (30) – [M-135] loss of $2C_2H_4$ & CH_3SO_2 to $C_6H_6O_4P^+$ m/z 173.0004
127 (85) – [M-181] $(CH_3O)_2(HO)_2P^+$ $C_2H_6O_4P^+$ m/z 127.0160
119 (65) – [M-189] "m/z 182-63"?
109 (65) – [M-199] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
99 (75) – [M-209] $(HO)_4P^+$ $H_4O_4P^+$ m/z 98.9847

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C6132178&Mask=200#Mass-Spec
Listed under "Phosphoric acid, diethyl p-(methylsulfonyl)phenyl ester" which exhibits similar ions but with different relative intensities, e.g. m/z 109 is base peak, and elevated m/z 265 (M-43)
N.B. Compare NIST spectrum of C_6H_5-SO_2-CH_3 ***methyl phenyl sulfone*** $C_7H_8O_2S$, MW 156, which exhibits interesting fragmentation pathway from aromatic $-SO_2CH_3$ to aromatic –OH by loss of 62 dalton (CH_2OS)
Key ions in C_6H_5-SO_2-CH_3 spectrum:

m/z 156 (30) – M^+
m/z 141 (30) – [M-15]
m/z 94 (35) – [M-62] - rearrangement and loss of CH_2OS to phenol C_6H_5OH
m/z 77 (100) - [M-79] loss of CH_3SO_2 to C6H5+

Fenthion **$C_{10}H_{15}O_3PS_2$** **M:278(100%)**

Theoretical molecular ion: m/z 278.0200 (100%), 279.0234 (10.8%), 280.0158 (9.0%)
Average MW: 278.32



Organophosphorus insecticide used to control fruit flies, leafhoppers, leaf miners and other insect pests. No longer approved for use in EU.

Acute oral LD50 for rat approx. 250 mg/kg (moderate toxicity).

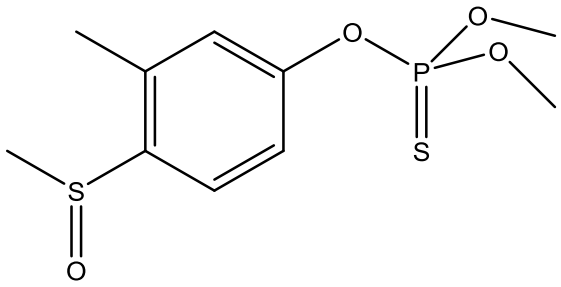
The oxidative metabolites are also important. Fenthion sulphoxide and sulphone are included in the MRL for fenthion.

m/z	278	109	279	169	280	125	245	137
%	100	20	15	15	10	10	10	10

278 (100) – M^+
245 (10) – [M-33] loss of SH to $C_{10}H_{14}O_3PS^+$ m/z 245.0401
169 (15) – [M-109] $CH_3S(CH_3)C_6H_3S^+$ $C_8H_9S_2^+$ m/z 169.0146 [O/S swap]
153 (5) – [M-125] $CH_3S(CH_3)C_6H_3O^+$ $C_8H_9OS^+$ m/z 153.0374
137 (10) – [M-141] $CH_3S(CH_3)C_6H_3^+$ $C_8H_9S^+$ m/z 137.0425
125 (10) – [M-153] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (10) – [M-169] $(CH_3O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (10) – [M-185] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (10) – [M-199] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C55389&Mask=200#Mass-Spec though some different relative intensities.

Fenthion sulphoxide **$C_{10}H_{15}O_4PS_2$** **M:294(60%)**
Theoretical molecular ion: m/z 294.0149 (100%), 295.0183 (10.8%), 296.0107 (9.0%)
Average MW: 294.32



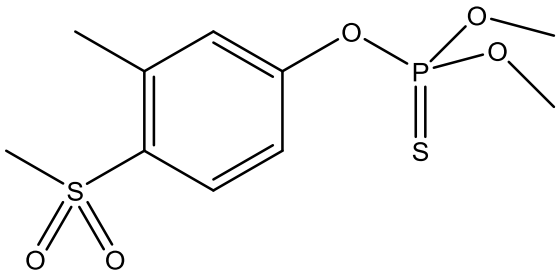
m/z	279	125	294	109	169	138	153	93
%	100	65	60	40	25	25	20	15

294 (100) – M^+
279 (10) – [M-15] loss of CH_3 to $C_9H_{12}O_4PS_2^+$ m/z 245.0401
125 (65) – [M-169] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
169 (25) – [M-109] $CH_3SO(CH_3)C_6H_3O^+$ $C_8H_9O_2S^+$ m/z 169.0323
109 (40) – [M-185] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
153 (20) – [M-141] $CH_3SO(CH_3)C_6H_3^+$ $C_8H_9OS^+$ m/z 153.0374
138 (10) – [M-141] $CH_3S(CH_3)C_6H_4^+$ $C_8H_{10}S^+$ m/z 138.0503

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3761419&Mask=200 [listed under "Mesulfenfos"]. Interestingly it exhibits elevated m/z 278 intensity (>20%), probably due to reduction of sulphoxide to sulphide in MS ion source (see Sugitate 2012).

Fenthion sulphone $C_{10}H_{15}O_5PS_2$ **M:310(95%)**

Theoretical molecular ion: m/z 310.0099 (100%), 311.0132 (10.8%), 312.00565 (9.0%)
Average MW: 310.32



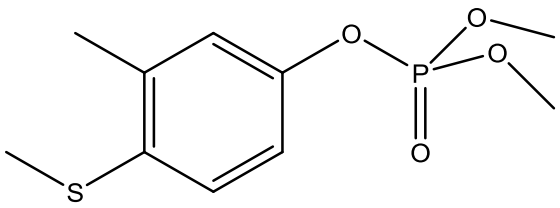
m/z	125	310	109	93	136	105	79	137
%	100	95	60	35	35	30	25	15

310 (95) – M^+
247 (5) – [M-63] rearrangement and loss of CH_3SO to $C_9H_{12}O_4PS^+$ m/z 247.0194
231 (10) – [M-79] loss of CH_3SO_2 to $C_9H_{12}O_3PS^+$ m/z 231.0245
137 (15) – [M-173] $CH_3(CH_3)C_6H_3S^+$ $C_8H_9S^+$ m/z 137.0425 - due to loss of SO2 and O/S swap
136 (10) – [M-174] $CH_3(CH_3)C_6H_2S^+$ $C_8H_8S^+$ m/z 136.0347 - due to loss of SO2 and O/S swap
125 (100) – [M-185] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (10) – [M-169] $(CH_3O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055 [O/S swap]
105 (30) – [M-205] $(CH_3)_2C_6H_3^+$ $C_8H_9^+$ m/z 105.0704 -- interesting, due to expulsion of SO_2
93 (35) – [M-217]] $(CH_3O)_2P{=}O^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (25) – [M-231] CH_3SO_2 and/or $(CH_3O)(HO)P^+$

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C3761420&Mask=200#Mass-Spec [listed under "Phosphorothioic acid, O,O-dimethyl O-[3-methyl-4-(methylsulfonyl)phenyl] ester"] which exhibits similar ions but some different relative intensities.

Fenthion oxon $C_{10}H_{15}O_4PS$ **M:262(100%)**

Theoretical molecular ion: m/z 262.0429 (100%), 263.0462 (10.8%), 264.0387 (4.5%)
Average MW: 262.26



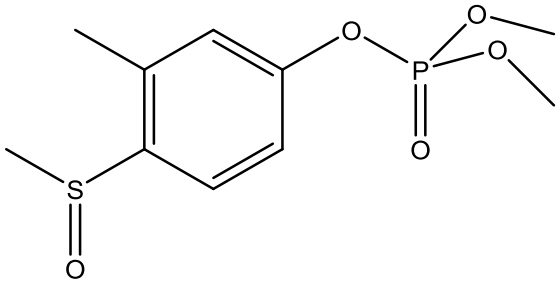
m/z	262	247	263	264	135	217	109	215
%	100	30	20	10	10	10	10	5

262 (100) – M^+
247 (30) – [M-15] loss of CH_3 to $C_9H_{12}O_4PS^+$ m/z 247.0194
217 (10) – [M-45] loss of CHS to $C_9H_{14}O_4P^+$ m/z 217.0630
215 (5) – [M-47] loss of CH_3S to $C_9H_{12}O_4P^+$ m/z 215.0473
135 (10) – [M-127] "$CH_3S(CH_3)C_6H_3$ minus H_2" $C_8H_7S^+$ m/z 135.02685
109 (10) – [M-153] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C6552121&Units=SI&Mask=200#Mass-Spec - rather uninformative, noisy spectrum with base peak at m/z 15, m/z 109 (65%) and m/z 262 (50%). [Listed rather unhelpfully under "Phosphoric acid, dimethyl 3-methyl-4-(methylthio)phenyl ester"]

Fenthion oxon sulphoxide **$C_{10}H_{15}O_5PS$** **M:278(25%)**

Theoretical molecular ion: m/z 278.0378 (100%), 279.0411 (10.8%), 280.0336 (4.5%)
Average MW: 278.26



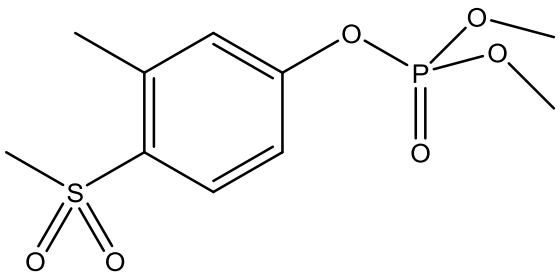
m/z	263	109	278	262	127	79	45	77
%	100	70	25	25	20	15	10	10

278 (25) – M^+
263 (10) – [M-15] loss of CH_3 to $C_9H_{12}O_5PS^+$ m/z 263.0143
262 (25) – [M-16] reduction to sulphide, $C_{10}H_{15}O_4PS^+$ m/z 262.0429
109 (70) – [M-169] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
127 (20) – [M-151] $(CH_3O)_2(HO)_2P^+$ $C_2H_8O_4P^+$ m/z 127.0160
79 (15) – [M-199] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
77 (10) – [M-201] ??
45 (20) – [M-233] ??

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C6552132&Mask=200#Mass-Spec [listed under "fenoxon sulfoxide"] Interestingly, it also exhibits elevated m/z 262 intensity (>20%), probably due to reduction of sulphoxide to sulphide in MS ion source (see Sugitate 2012).

Fenthion oxon sulphone **$C_{10}H_{15}O_6PS$** **M:294(100%)**

Theoretical molecular ion: m/z 294.0327 (100%), 295.03605 (10.8%), 296.0285 (4.5%)
Average MW: 294.26



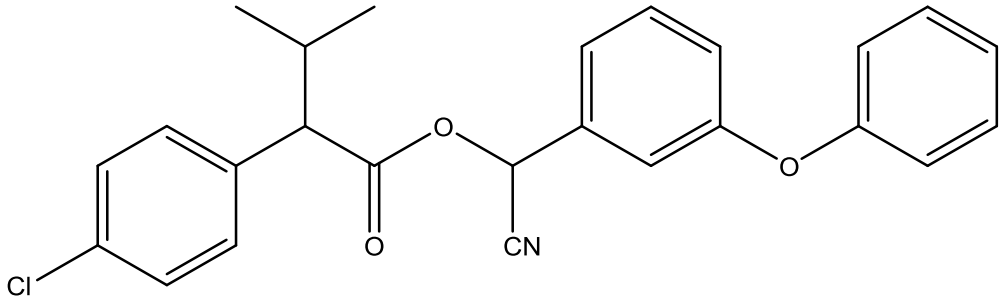
m/z	294	215	104	109	231	230	295	279
%	100	60	30	25	20	20	20	15

294 (100) – M^+
279 (15) – [M-15] loss of CH_3 to $C_9H_{12}O_6PS^+$ m/z 279.0092
231 (20) – [M-63] loss of SO2 but add H?
230 (20) – [M-64] loss of SO_2
215 (60) – [M-79] loss of CH_3SO_2 to $C_9H_{12}O_4P^+$ m/z 215.0473
109 (25) – [M-169] $(CH_3O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055 [O/S swap]
104 (30) – [M-189] $(CH_3)_2C_6H_2^+$ $C_8H_8^+$ m/z 104.0626 - interesting, due to expulsion of SO_2

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C14086352&Mask=200#Mass-Spec which exhibits elevated low mass ion intensities: base peak at m/z 109 (100%) and molecular ion m/z 278 only 20%.

Fenvalerate $C_{25}H_{22}ClNO_3$ **M:419,421(25,10%)**

Theoretical molecular ion: m/z 419.1288 (100%), 421.1259 (32%)
Average MW: 419.90



Synthetic pyrethroid insecticide.

May be resolved into two peaks on capillary GC (ca 3:1).

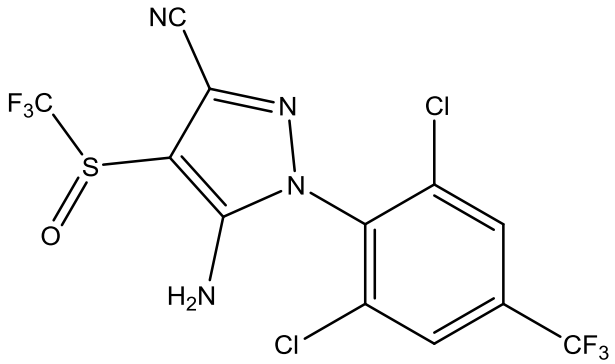
m/z	167	125	169	225	152	181	419	127
%	100	90	45	40	35	30	25	25

419,421 (25,10) – M^+
225 (40) – [M-194] $HOCH(CN)C_6H_4OC_6H_5^+$ $C_{14}H_{11}NO_2$+ m/z 225.0790
181 (30) – [M-238]
167,169 (100,45) – [M-252] $ClC_6H_4C_4H_7^+$ $C_{10}H_{12}Cl^+$ m/z 167.0628
152 (35) – [M-267]
125,127 (90) – [M-294] $ClC_6H_4CH_2^+$ $C_7H_6Cl^+$ m/z 125.0158 etc.

Cf. similar but very weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C51630581&Mask=200#Mass-Spec

Fipronil $C_{12}H_4Cl_2F_6N_4OS$ **M:436,438(0,0%)**

Theoretical molecular ion: 435.9387 (100%), 437.9358 (64%), 439.9328 (10%)
Average MW: 437.14



Phenylpyrazole insecticide which disrupts insect central nervous system by blocking GABA-gated chloride channels. Broad spectrum activity against e.g. thrips, rootworms, wireworms, weevils and termites. Approved for use in EU.

Acute oral LD50 for rat approx. 90 mg/kg (high toxicity).

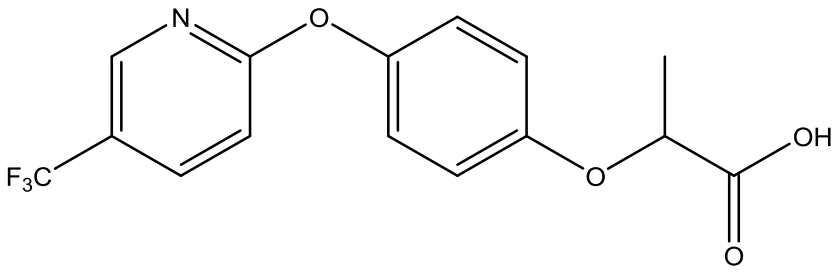
m/z	367	369	213	351	255	215	353	85

%	100	70	40	35	25	25	20	20

436,438 (0,0) – M^+
420,422 (5,3) – [M-16] loss of O, probably due to in-source reduction, $C_{12}H_4Cl_2F_6N_4S^+$ m/z 419.9438 etc.
417,419 (2,1) – [M-19] loss of F to $C_{12}H_4Cl_2F_5N_4OS^+$ m/z 416.9493 etc.
367,369 (100,70) – [M-69] loss of CF_3 to $C_{11}H_4Cl_2F_3N_4OS^+$ m/z 366.9435 etc
351,353 (35,20) – [M-85] loss of O/CF_3 to $C_{11}H_4Cl_2F_3N_4S^+$ m/z 350.9486
213,215 (40,25) – [M-223] $Cl_2C_6H_2.CF_3^+$ m/z 212.9486 etc.
85 (20) – [M-351] CF_3O^+ m/z 84.9901 (?)

No NIST spectrum available. Data from Ubukata (2009).
Cf. similar spectrum at http://www.nj.gov/dep/enforcement/pcp/bpo/pem/spectras/eispectra/Fipronil.pdf

Fluazifop acid **$C_{15}H_{12}F_3NO_4$** **M:327(85%)**
Theoretical molecular ion: m/z 327.0718 (100%), 328.0752 (16%), 329.07855 (1.2%)
Average MW: 327.26



Herbicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 3,000 mg/kg (low toxicity).

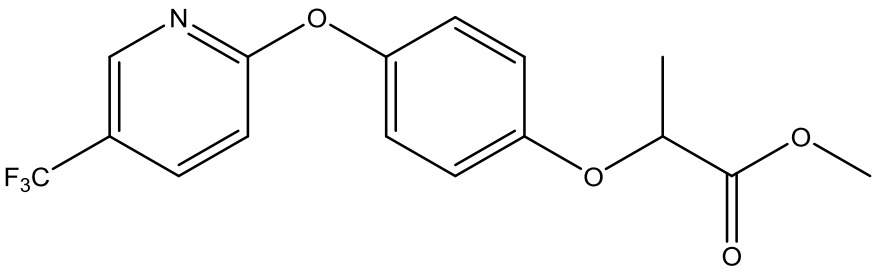
Chiral molecule. Poor GC transmission underivatised.

m/z	254	327	146	255	227	282	226	328
%	100	85	60	50	35	25	25	15

327 (85) – M^+
308 (7) – [M-19] loss of F (characteristic of trifluoromethyl aromatics) to $C_{15}H_{12}F_2NO_4^+$ m/z 308.0734
254 (100) – [M-73] loss of $C_3H_5O_2$ to $C_{12}H_7F_3NO_2^+$ m/z 254.1882
146 (60) – [M-181] $CF_3.C_6H_3N^+$ $C_6H_3F_3N^+$ m/z 146.0922

No NIST spectrum available.

Fluazifop methyl **$C_{16}H_{14}F_3NO_4$** **M:341(100%)**
Theoretical molecular ion: m/z 341.0875 (100%), 342.09085 (17%), 343.0942 (1.4%)
Average MW: 341.29



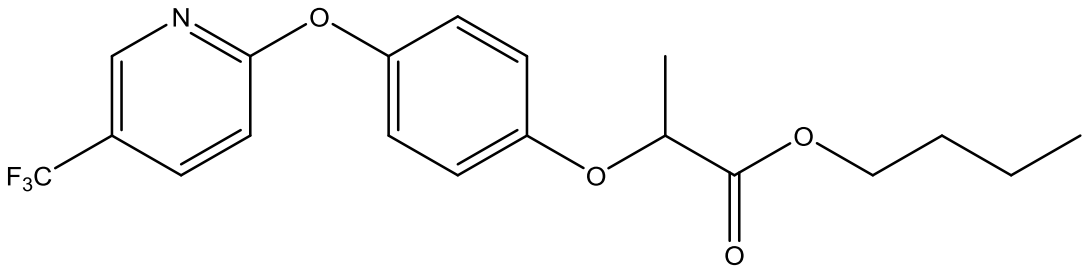
Herbicide.

m/z	341	282	254	146	255	227	342	238
%	100	90	75	35	30	25	20	15

341 (100) – M^+
322 (5) – [M-19] loss of F to $C_{16}H_{14}F_2NO_4^+$ m/z 322.0891
282 (90) – [M-59] loss of $COOCH_3$ to $C_{14}H_{11}F_3NO_2^+$ m/z 282.0741
254 (75) – [M-87] loss of $C_4H_7O_2$ to $C_{12}H_7F_3NO_2^+$ m/z 254.0429
146 (60) – [M-195] $CF_3.C_6H_3N^+$ $C_6H_3F_3N^+$ m/z 146.0922

No NIST spectrum available.

Fluazifop n-butyl **$C_{19}H_{20}F_3NO_4$** **M:383(50%)**
Theoretical molecular ion: m/z 383.1344 (100%), 384.1378 (21%), 385.14115 (2.0%)
Average MW: 383.37



Herbicide.

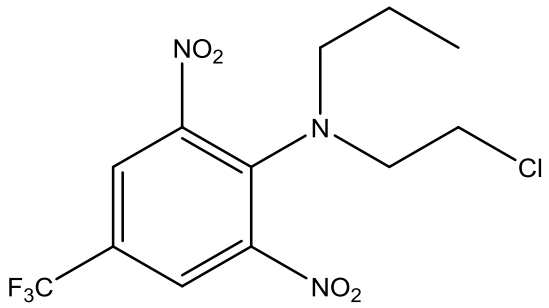
m/z	282	383	254	255	146	238	227	91
%	100	50	45	30	20	20	20	15

383 (50) – M^+
364 (5) – [M-19] loss of F to $C_{19}H_{20}F_2NO_4^+$ m/z 364.1360
282 (100) – [M-101] loss of $COOC_4H_7$ to $C_{14}H_{11}F_3NO_2^+$ m/z 282.0741
254 (75) – [M-129] loss of $C_7H_{13}O_2$ to $C_{12}H_7F_3NO_2^+$ m/z 254.0429
146 (60) – [M-237] $CF_3.C_6H_3N^+$ $C_6H_3F_3N^+$ m/z 146.0922

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C69806504&Units=SI&Mask=200#Mass-Spec

Fluchloralin **$C_{12}H_{13}ClN_3O_3F_3$** **M:355,357(5,2%)**

Theoretical molecular ion: m/z 355.0547 (100%), 357.0517 (32%)
Average MW: 355.70



Herbicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 1,500 mg/kg (moderate toxicity).

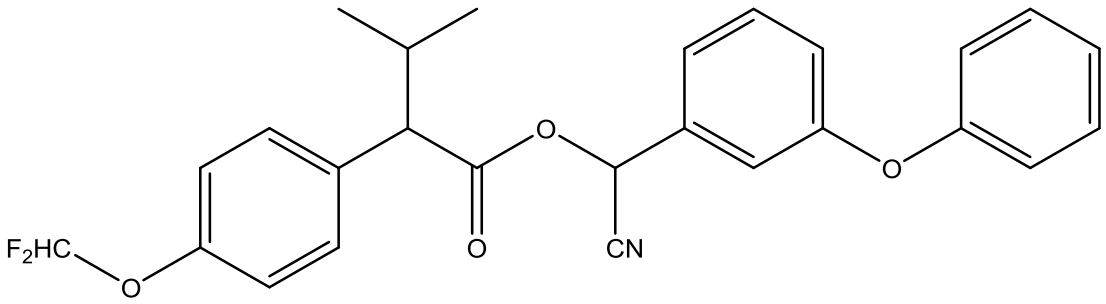
m/z	306	326	264	63	43	328	310	248
%	100	75	55	50	45	20	15	15

355,357 (5,2) – M^+
326,328 (75,20) – [M-29] loss of CH_3CH_2 to $C_{10}H_8ClF_3N_3O_4^+$ m/z 326.0155
306 (100) – [M-49] loss of CH_2Cl to C11H11F3N3O4+ m/z 306.0702
264 (55) – [M-91] $CF_3(NO_2)_2C_6H_2.N{=}CH_2^+$ $C_8H_5F_3N_3O_4^+$ m/z 264.0232
63 (50) – [M-292] $C_2H_4Cl^+$ m/z 63.0002 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C33245395&Mask=200#Mass-Spec

Flucythrinate **$C_{26}H_{23}F_2NO_4$** **M:451(20%)**

Theoretical molecular ion: m/z 451.1595 (100%), 452.1629 (28.1%)
Average MW: 451.47



Synthetic pyrethroid insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

May be resolved into two peaks on capillary GC (*ca* 4:3).

m/z	199	157	184	181	451	225	55	107
%	100	60	30	25	20	20	20	15

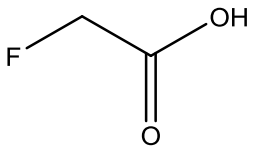
451 (20) – M^+
199 (100) – [M-252] $C_{15}H_{10}NO_3^+$ m/z 252.0661

157 (60) – [M-294] $CHF_2OC_6H_5.CH_2^+$ $C_8H_6F_2O^+$ m/z 156.0387

No NIST spectrum available.

Fluoroacetic acid **$C_2H_3FO_2$** **M:78(45%)**

Theoretical molecular ion: m/z 78.0117 (100%)
Average MW: 78.04



Rodenticide. No longer approved for use in EU.

Acute oral LD50 for rat 0.22 mg/kg (high toxicity).

Not directly amenable to GC analysis, but it may be determined following derivatisation, e.g. as:
- methyl ester (see spectrum of methyl fluoroacetate at http://webbook.nist.gov/cgi/cbook.cgi?ID=C453189&Mask=200#Mass-Spec
Methyl fluoroacetate, $C_3H_5FO_2$ MW 92, monitoring M^+ m/z 92.0690 (10%) and m/z 33.0141 (CH_2F^+ , 75% rel. abundance). Base peak due to m/z 59 $COOCH_3$).
- pentafluorobenzyl ester, $C_6F_5CH_2OCOCH_2F$, mw 258 (Miki 1998).

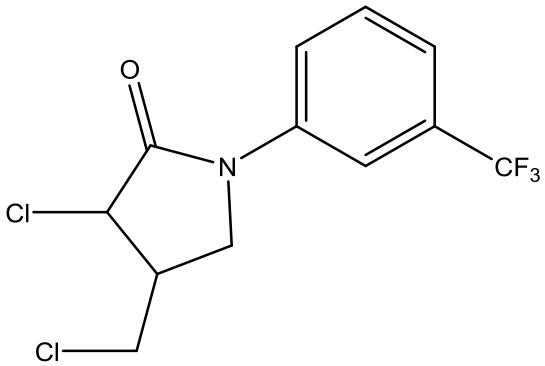
m/z	45	33	78	61	31	29	42	49
%	100	85	45	40	30	20	10	5

78 (45) – M^+
45 (100) – [M-33] $COOH^+$ CO_2H^+ m/z 44.9977
33 (85) – [M-45] CH_2F^+ m/z 33.0141

Data from NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C144490&Mask=200#Mass-Spec

Flurochloridone **$C_{12}H_{10}Cl_2F_3NO$** **M:311,313(100,70%)**

Theoretical molecular ion: m/z 311.0092 (100%), 313.0062 (64%), 315.00325 (10.2%)
Average MW: 312.11



Herbicide. Approved for use in EU.

Acute oral LD50 for rat >2,150 mg/kg (low toxicity).

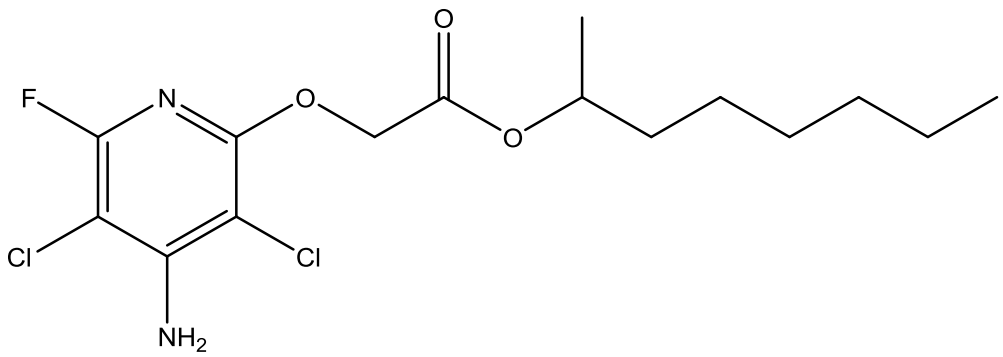
Technical flurochloridone is a 3:1 mixture of *trans*- and *cis*- isomers (the spectrum given was obtained from the *trans*-isomer).

m/z	311	187	174	313	103	145	75	172
%	100	95	70	70	55	50	45	35

311,313,315 (100,70,12) – M+
187 (95) – [M-124] loss of $C_4H_6Cl_2$ to isocyanate $CF_3C_6H_4NCO^+$ $C_8H_4F_3NO^+$ m/z 187.0245
174 (70) – [M-137] $CF_3C_6H_4NCH_3^+$ $C_8H_7F_3N^+$ m/z 174.0531
172 (35) – [M-139] $CF_3C_6H_4NCH^+$ $C_8H_5F_3N^+$ m/z 172.0374
145 (40) – [M-166] $CF_3C_6H_4^+$ m/z 145.0265

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C61213250&Mask=200#Mass-Spec though weaker molecular ion (75%).

Fluroxypyr-meptyl **$C_{15}H_{21}Cl_2FN_2O_3$** **M:366,368,370(10,7,2%)**
Theoretical molecular ion: m/z 366.0913 (100%), 368.0884 (64%), 369.0917 (10.4%)
Average MW: 367.24



Fluroxypyr-meptyl (1-methylheptyl)

Pre-emergence herbicide. Approved for use in EU.

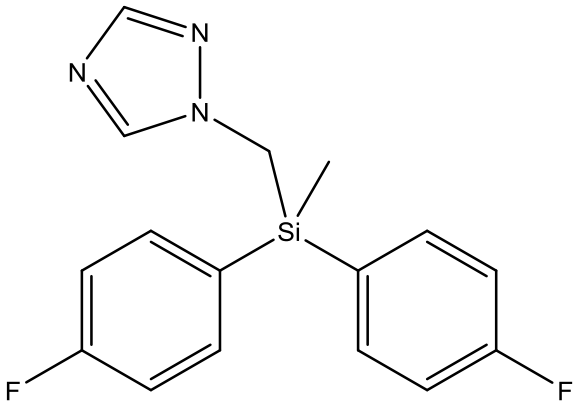
Acute oral LD50 for rat >2,000 mg/kg (moderate toxicity).

m/z	57	71	43	181	209	210	211	254
%	100	85	65	25	25	20	20	15

366,368,370(10,7,2) – M+
254,256, (15,10) – [M-112] loss of C_8H_{12} to $C_7H_5Cl_2FN_2O_3^+$ m/z 253.9661 etc.
209,211 (25,20) – [M-157] $C_6H_4Cl_2FN_2O^+$ m/z 208.9685
57 (100) – [M-309] $C_4H_7^+$ m/z 57.0704

No NIST spectrum available.

Flusilazole **$C_{16}H_{15}F_2N_3Si$** **M:315(10%)**
Theoretical molecular ion: m/z 315.1003 (100%), 316.1037 (17%), 317.0972 (3.3%)
Average MW: 315.39



Organosilicon conazole fungicide used to control a range of pathogens including *Ascomycetes, Basidiomycetes* and *Deuteromycete* on cereals, oilseed rape, sugar beet.

Approval for use withdrawn in EU in 2013.

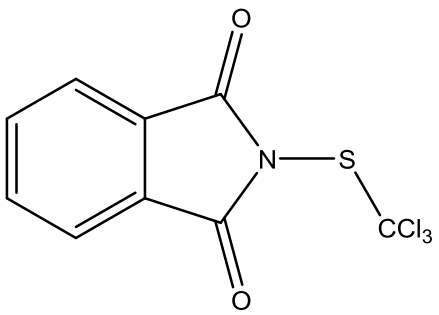
Acute oral LD50 for rat approx. 700 mg/kg (moderate toxicity).

m/z	233	206	47	234	315	123	220	300
%	100	35	25	25	10	10	10	5

315 (10) – M^+
300 (5) – [M-15] loss of CH_3 to $C_{15}H_{12}F_2N_3Si^+$ m/z 300.0769
233 (100) – [M-82] loss of $C_2H_2N_3$-CH_2 to $(FC_6H_4)_2(CH_3)Si^+$ $C_{13}H_{11}F_2Si^+$ m/z 233.0598
220 (10) – [M-95] loss of FC_6H_4 to $C_{10}H_{11}FN_3Si^+$ m/z 220.0706
206 (35) – [M-109] loss of FC_6H_4+CH_2 to $C_9H_9FN_3Si^+$ m/z 206.0550
123 (10) – [192] $FC_6H_4Si^+$ $C_6H_4FSi^+$ m/z 123.0066
47 (25) – [268] SiF^+ m/z 46.9753 – interesting rearrangement to energetically favoured ion

No NIST spectrum available. Cf. similar spectrum at Restek http://www.restek.com/compound/view/85509-19-9/Flusilazole

Folpet **$C_9H_4Cl_3NO_2S$** **M:295,297,299(10,10,3%)**
Theoretical molecular ion: m/z 294.9028 (100%), 296.8999 (96%), 298.8969 (31%)
Average MW: 296.55



Phthalimide fungicide (cf. captan, captafol, ditalimfos, folpet). Approved for use in EU.

Acute oral LD50 for rat > 2,000 mg/kg (moderate toxicity).

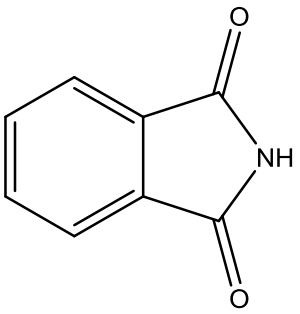
m/z	104	76	260	130	117	262	79	147
%	100	80	55	55	55	50	35	25

295,297 (10,10) – M^+
260,262 (55,35) – [M-35] loss of Cl to $C_9H_4Cl_2NO_2S^+$ m/z 259.9340 etc.
104 (100) – [M-191] $C_7H_4O^+$ m/z 104.0232
76 (80) – [M-279] $C_6H_4^+$ m/z 76.0313

Cf. generally similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C133073&Mask=200#Mass-Spec but noisy, and weaker lower mass ions.

Folpet related phthalimide **$C_8H_5NO_2$** **M:147(100%)**

Theoretical molecular ion: m/z 147.0320 (100%), 148.0354 (8.7%)
Average MW: 147.13



Folpet may degrade to phthalimide:

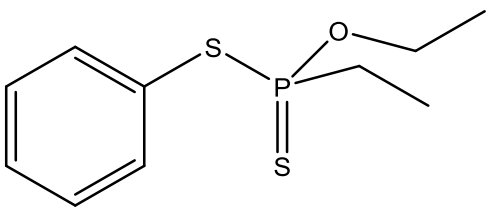
m/z	147	76	104	50	103	-	-	-
%	100	100	80	45	30	-	-	-

147 (100) – M^+
76 (100) – [M-71] $C_6H_4^+$ m/z 76.0313

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C85416&Mask=200#Mass-Spec

Fonofos **$C_{10}H_{15}OPS_2$** **M:246(35%)**

Theoretical molecular ion: m/z 246.0302 (100%), 247.0336 (10.8%), 248.0260 (9.0%)
Average MW: 246.32



Organophosphorus (phenyl ethylphosphonothionate) insecticide. Soil acting agent used predominately on corn to controls aphids, corn rootworm, corn wireworm, cutworms, white grubs and maggots. No longer approved for use in EU.

Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

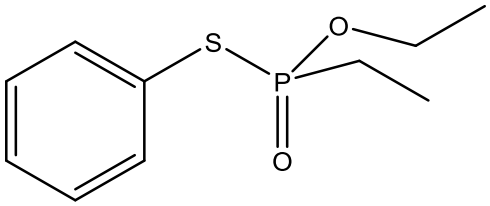
m/z	109	137	246	110	81	63	174	77
%	100	60	35	20	15	10	5	5

246 (35) – M^+
137 (60) – [M-109] loss of C_6H_5S to $(CH_3CH_2)(CH_3CH_2O)P{=}S^+$ $C_4H_{10}OPS^+$ m/z 137.0190
109 (100) – [M-137] loss of C_6H_5S & C_2H_4 to $(CH_3CH_2)(HO)P{=}S^+$ $C_2H_6OPS^+$ m/z 108.9877
N.B. m/z 109 may also be due to $C_6H_5S^+$ m/z 109.0112
81 (15) – [M-165] $(HO)(HS)P^+$ H_2OSP^+ m/z 80.9564
77 (5) – [M-169] $C_6H_5^+$ m/z 77.0391
63 (10) – [M-183] PS^+ m/z 62.9458

Cf. similar NIST MS at http://webbook.nist.gov/cgi/cbook.cgi?ID=C944229&Mask=200

Fonofos oxon **$C_{10}H_{15}O_2PS$** **M:230(25%)**

Theoretical molecular ion: m/z 230.0530 (100%), 231.0564 (11%), 232.0488 (4.5%)
Average MW: 230.26



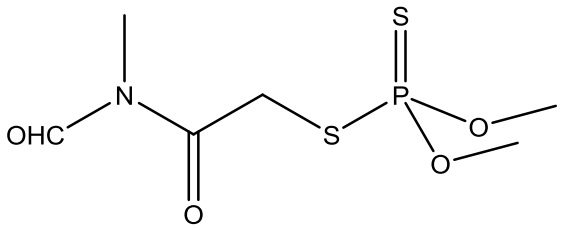
m/z	93	230	121	110	65	109	29	185
%	100	25	25	25	25	20	20	5

230 (25) – M^+
185 (5) – [M-45] loss of CH_3CH_2O to $C_8H_{10}OPS^+$ m/z 185.0190
121 (25) – [M-109] loss of C_6H_5S to $(CH_3CH_2)(CH_3CH_2O)P{=}O^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
109 (20) – [M-121] $C_6H_5S^+$ m/z 109.0112
93 (100) – [M-137] loss of C_6H_5S & C_2H_4 to $(CH_3CH_2)(HO)P{=}O^+$ $C_2H_6O_2PS^+$ m/z 93.0105
65 (25) – [M-165] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. similar NST MS at http://webbook.nist.gov/cgi/cbook.cgi?ID=C944218&Mask=200 though m/z 65 more abundant (60%).

Formothion **$C_6H_{12}NO_4PS_2$** **M:257(15%)**

Theoretical molecular ion: m/z 256.9945 (100%), 257.9979 (6.5%), 258.9903 (4.5%)
Average MW: 257.26



Organophosphorus insecticide and acaricide used to control spider mites, aphids, psyllids, mealy bugs, whiteflies and many other insect pests. No longer approved in EU.

Acute oral LD50 for rat approx 350 mg/kg (moderate toxicity)

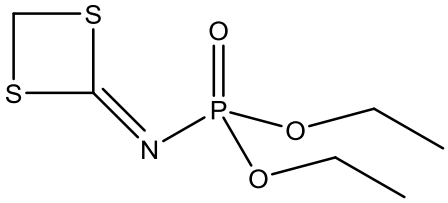
m/z	126	93	125	87	170	115	224	257
%	100	70	50	50	35	20	15	15

257 (15) – M^+
224 (15) – [M-33] loss of SH to $C_6H_{11}NO_4PS^+$ m/z 224.0146
198 (10) – [M-59] loss of $OHCNCH_3$/H to $C_4H_7O_3PS_2^+$ m/z 197.9574
170 (35) – [M-87] $CHS.P{=}S.(OCH_3)_2$ $C_3H_7O_2PS_2^+$ m/z 169.9625
126 (100) – [M-131] $(CH_3O)_2P(SH)^+$ $C_2H_7O_2PS^+$ m/z 125.9904
125 (50) – [M-132] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
93 (70) – [M-164] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
87 (50) – [M-170] $OHC.N(CH_3).COH^+$ $C_3H_5NO_2^+$ m/z 87.0320

Cf. Similar but weak and noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2540821&Mask=200

Fosthietan **$C_6H_{12}NO_3PS_2$** **M:241(0%)**

Theoretical molecular ion: m/z 240.999 (1.0%), 242.0030 (6.5%), 242.9954 (9.0%)
Average MW: 241.26



Organophosphorus (phosphoramidate) insecticide and nematicide. Previously used against a wide range of soil pests. No longer approved for use in EU.

Acute oral LD50 for rat approx. 20 mg/kg (high toxicity).

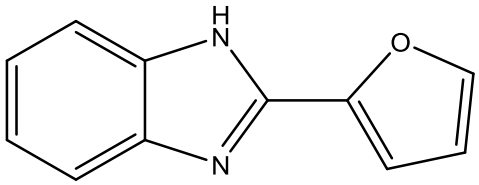
m/z	140	196	81	46	109	168	45	29
%	100	85	55	50	50	45	45	35

241 (0) – M^+ absent
196 (85) – [M-45] loss of CHS to $C_5H_{11}NO_3PS^+$ m/z 196.0197
168 (45) – [M-73] loss of CHS & C_2H_4 to $C_3H_7NO_3PS^+$ m/z 167.9884
140 (100) – [M-101] loss of CHS & $2C_2H_4$ to $(HO)_3P\text{-}NCS^+$ m/z $CH_3O_3PNS^+$ m/z 139.9571

109 (50) – [M-132] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
81 (55) – [M-160] $(HO)_2PO^+$ $H_2O_3P^+$ m/z 80.9742
46 (50) – [M-195] CH_2S^+ m/z 45.9877

No NIST spectrum available.

Fuberidazole **$C_{11}H_8N_2O$** **M:184(100%)**
Theoretical molecular ion: m/z 184.0637 (100%), 185.0670 (11.9%)
Average MW: 184.90



Fungicide. Used as a seed treatment to control *Fusarium spp*. in cereals.
Approved for use in EU.

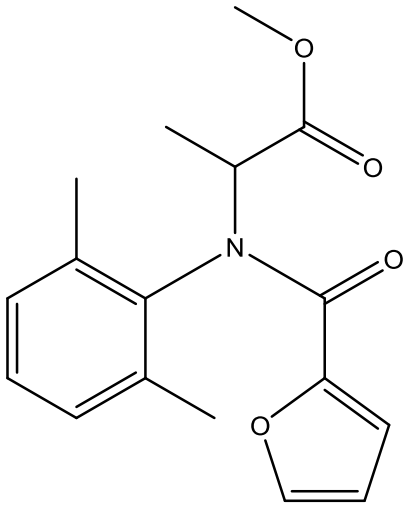
Acute oral LD50 for rat >300 mg/kg (moderate toxicity).

m/z	184	156	155	183	185	92	129	64
%	100	30	30	25	25	15	15	10

184 (100) – M+
156 (30) – [M-28] loss of CO to $C_{10}H_8N_2^+$ m/z 156.0688

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3878191&Mask=200#Mass-Spec

Furalaxyl **$C_{17}H_{19}NO_4$** **M:301(10%)**
Theoretical molecular ion: m/z 301.1314 (100%), 302.1348 (18.4%), 303.1381 (1.6%)
Average MW: 301.34



Fungicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 900 mg/kg (moderate toxicity).

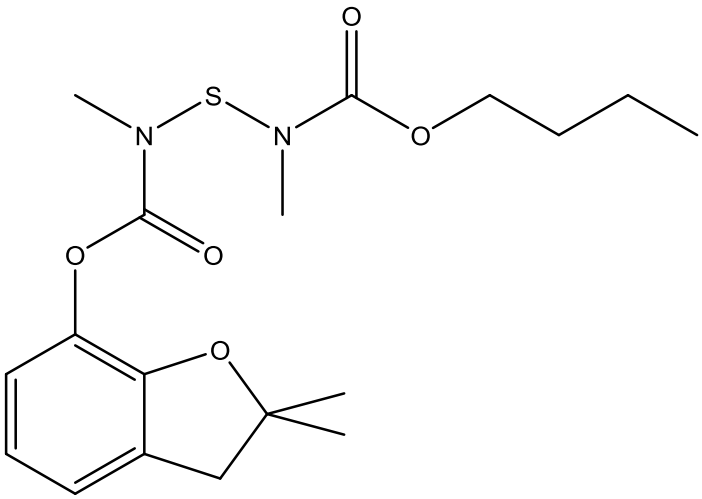
m/z	95	242	152	301	180	146	39	132
%	100	30	10	10	10	10	10	10

301 (10) – M^+
242 (30) – [M-59] loss of CH_3OCO to $C_{15}H_{16}NO_2^+$ m/z 242.1181
95 (100) – [M-206] $C_4H_2O.CO^+$ $C_5H_3O_2^+$ m/z 95.0133

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C57646307&Mask=200#Mass-Spec

Furathiocarb **$C_{18}H_{26}N_2O_5S$** **M:382(5%)**

Theoretical molecular ion: m/z 382.1562 (100%), 383.1596 (19.5%), 384.1520 (4.5%)
Average MW: 382.38



Benzofuranyl methylcarbamate insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

Sometimes poor GC transmission.

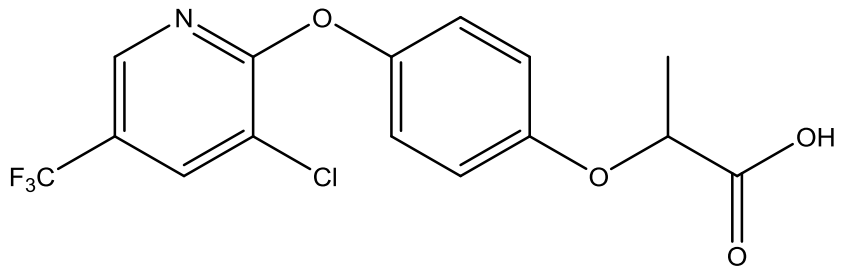
m/z	163	135	164	194	41	107	325	57
%	100	30	25	20	20	15	15	15

382 (5) – M^+
325 (15) – [M-57] $C_{14}H_{17}N_2O_5S^+$ m/z 325.0858
163 (100) – [M-219] $C_{10}H_{11}O_2^+$ m/z 163.0739
135 (30) – [M-247] $C_9H_{11}O^+$ m/z 135.0810

No NIST spectrum available, but most abundant ions similar to those reported by Suzuki (2006): m/z 163, 135, 194 & 325.

Haloxyfop acid **$C_{15}H_{11}ClF_3NO_4$** **M:361,363(70,25%)**

Theoretical molecular ion: m/z 361.0329 (100%), 363.0299 (32%)
Average MW: 361.70



Herbicide. No longer approved in EU.

Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

Several ester forms (see below). The (R)-isomer of this molecule is named haloxyfop-P

Poor GC transmission unless derivatised.

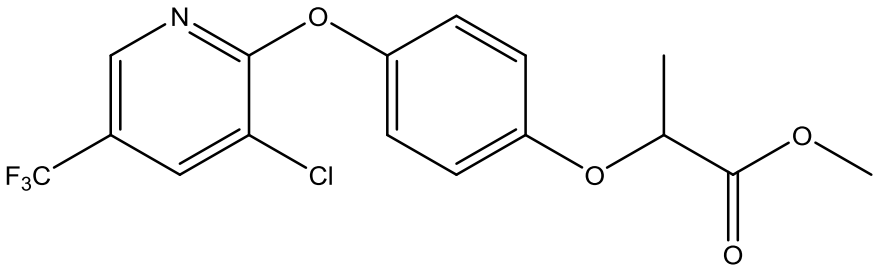
m/z	288	361	289	290	180	316	363	63
%	100	70	60	40	35	30	25	20

361,363 (70,25) – M^+
342,344 (6,2) – [M-19] loss of F to $C_{15}H_{11}ClF_2NO_4^+$ m/z 342.0345 etc.
316,318 (30,10) – [M-45] loss of COOH to $C_{14}H_0ClF_3NO_2^+$ m/z 316.0352 etc.
288,290 (100,40) – [M-73] loss of $CH(CH_3)COOH$ to $C_{12}H_6ClF_3NO_2^+$ m/z 288.0039 etc.
180,182 (35,10) – [M-181] $CF_3(Cl)C_5H_2N^+$ $C_6H_2ClF_3N^+$ m/z 179.9828 etc.
63 (20) – [M-298] C_5H_3+ m/z 63.0235

No NIST spectrum available (but the spectrum of the isomeric herbicide Oxyfluorfen is present.)

Haloxyfop methyl **$C_{16}H_{13}ClF_3NO_4$** **M:375,377(90,30%)**

Theoretical molecular ion: m/z 375.0485 (100%), 377.0456 (32%)
Average MW: 375.73



KI (OV-17) = 23.8

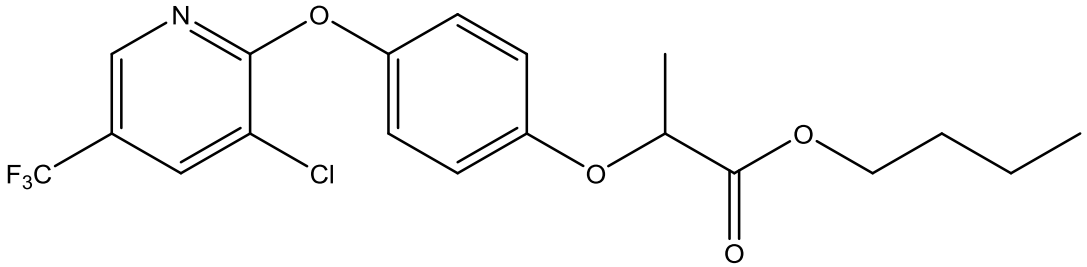
m/z	316	375	288	289	91	290	180	318
%	100	90	85	45	40	35	35	35

375,377 (90,30) – M^+
356,358 (10,3) – [M-19] loss of F to $C_{16}H_{13}ClF_2NO_4^+$ m/z 356.0501 etc.
316,318 (100,35) – [M-59] loss of $COOCH_3$ to $C_{14}H_{10}ClF_3NO_2^+$ m/z 316.0352 etc.

288,290 (85,45) – [M-87] loss of $CHCH_3COOCH_3$ to $C_{12}H_6ClF_3NO_2^+$ m/z 288.0039 etc.
91 (40) – [M-284] $C_6H_3O^+$ m/z 91.0184

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C69806402&Mask=200#Mass-Spec

Haloxyfop n-butyl **$C_{19}H_{19}ClF_3NO_4$** **M:417,419(55,20%)**
Theoretical molecular ion: m/z 417.0955 (100%), 419.0925 (32%)
Average MW: 417.81



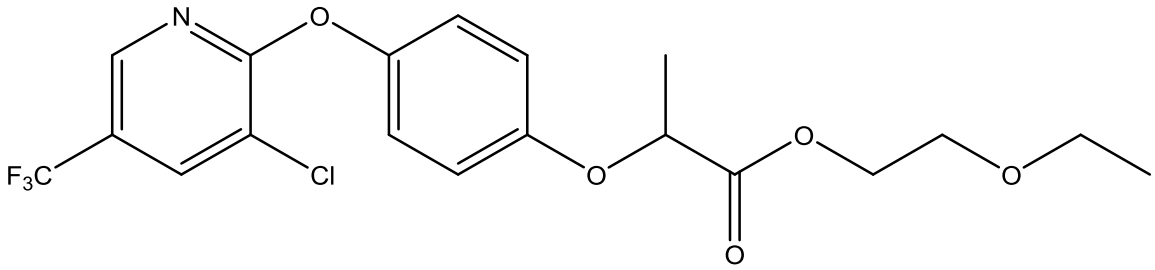
KI (OV-17) = 25.5

m/z	316	417	288	289	318	91	290	272
%	100	55	45	40	35	30	20	20

417,419 (55,20) – M^+
398,400 (5,2) – [M-19] loss of F to $C_{19}H_{19}ClF_2NO_4^+$ m/z 398.0971 etc
316,318 (100,35) – [M-101] loss of C_4H_9OCO to $C_{14}H_{10}ClF_3NO_2^+$ m/z 316.0352 etc.
288,290 (85,45) – [M-129] loss of $C_4H_9OCOCHCH_3$ to $C_{12}H_6ClF_3NO_2^+$ m/z 288.0039 etc.
91 (40) – [M-326] $C_6H_3O^+$ m/z 91.0184

No NIST spectrum available.

Haloxyfop 2-ethoxyethyl / "etolyl" $C_{19}H_{19}ClF_3NO_5$ **M:433,435(60,20%)**
Theoretical molecular ion: m/z 433.0904 (100%), 435.0874 (32%)
Average MW: 433.81



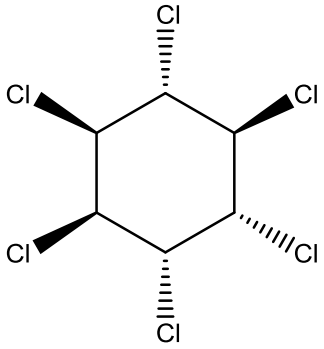
KI (OV-17) = 26.6

m/z	316	45	302	288	433	289	91	318
%	100	85	75	75	60	50	45	35

433,435 (60,20) – M
414,416(5,2) – [M-19] loss of F to $C_{19}H_{19}ClF_2NO_5^+$ m/z 414.0920
361,363 (5,2) – [M-72] loss of $C_2H_3OC_2H_5$ to $C_{15}H_{11}ClF_3NO_4^+$ m/z 361.0329
316,318 (100,35) – [M-117] loss of $COOC_2H_4OC_2H_5$ to $C_{14}H_{10}ClF_3NO_2^+$ m/z 316.0352 etc.
45 (85) – [M-388] $C_2H_5O^+$ m/z 45.0340
91 (40) – [M-342] $C_6H_3O^+$ m/z 91.0184

No NIST spectrum available.

Alpha-HCH **$C_6H_6Cl_6$** **M:288,290,292(0,0,0%)**
Theoretical molecular ion: m/z 287.8601 (52%), 289.8571 (100%), 291.8542 (80%)
Average MW: 290.81



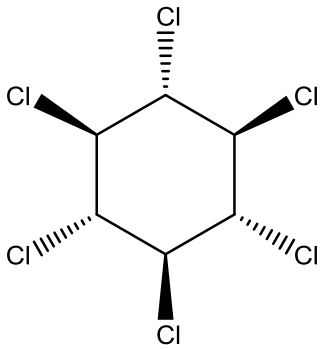
A contaminant of HCH.

m/z	181	183	219	217	109	111	221	185
%	100	90	85	65	55	45	40	30

288,290 (0) – M^+ $C_6H_6Cl_6^+$ absent (different from beta and gamma isomers)
252,254,256 (3,5,3) – [M-36] loss of HCl to $C_6H_5Cl_5^+$ m/z 251.8834 etc.
217,219,221 (65,85,40) – [M-71] loss of HCl_2 to $C_6H_5Cl_4^+$ m/z 216.9145 etc.
181,183,185 (100,90,30) – [M-107] loss of H_2Cl_3 to $C_6H_4Cl_3^+$ m/z 180.9379 etc.
109,111 (55,45) – [M-179] $C_3H_3Cl_2^+$ m/z 108.9612 etc.

Cf. similar (weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C319846&Units=SI&Mask=200#Mass-Spec listed as "α-Lindane"

beta-HCH **$C_6H_6Cl_6$** **M:288,290,292(1,2,1%)**
Theoretical molecular ion: m/z 287.8601 (52%), 289.8571 (100%), 291.8542 (80%)
Average MW: 290.81



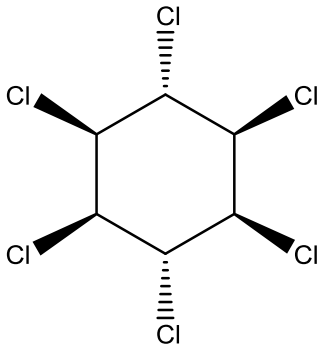
A contaminant of HCH. As a residue, beta-HCH is the most persistent of the HCH isomers because its stereochemistry disfavours hydrolysis. Sometimes poor GC transmission.

m/z	109	181	183	219	111	217	221	185
%	100	90	85	85	70	65	40	25

288,290,292 (1,2,1) – weak M^+ $C_6H_6Cl_6^+$
252,254,256 (6,8,6) – [M-36] loss of HCl to $C_6H_5Cl_5^+$ m/z 251.8834 etc.
217,219,221 (65,85,40) – [M-71] loss of HCl_2 to $C_6H_5Cl_4^+$ m/z 216.9145 etc.
181,183,185 (90,85,25) – [M-107] loss of H_2Cl_3 to $C_6H_4Cl_3^+$ m/z 180.9379 etc.
109,111 (100,70) – [M-179] $C_3H_3Cl_2^+$ m/z 108.9612 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C319857&Units=SI&Mask=200#Mass-Spec
listed as "β-Hexachlorocyclohexane"

gamma-HCH / BHC or lindane $C_6H_6Cl_6$ M:288,290,292(1,2,1%)
Theoretical molecular ion: m/z 287.8601 (52%), 289.8571 (100%), 291.8542 (80%),
Average MW: 290.81



Organochlorine insecticide. Banned under the Stockholm Convention on persistent organic pollutants in 2009. An estimated 600,000 tonnes have been manufactured, mostly for use in agriculture.

Acute oral LD50 for rat approx. 160 mg/kg (moderate toxicity).

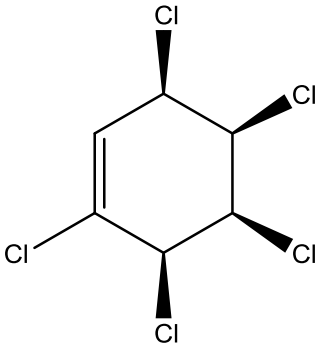
Technical gamma-HCH contains low levels of other isomers (mainly alpha and beta). However, technical "BHC", which has been used in and exported from China for some years, comprises mainly beta- and alpha-HCH. Gamma-HCH may undergo dehydrochlorination, via gamma-PCCH, to trichlorobenzene (see below).

m/z	181	183	219	109	217	111	221	185
%	100	90	90	75	65	60	40	30

288,290,292 (1,2,1) – weak M^+ $C_6H_6Cl_6^+$
252,254,256 (8,12,8) – [M-36] loss of HCl to $C_6H_5Cl_5^+$ m/z 251.8834 etc.
217,219,221 (65,90,40) – [M-71] loss of HCl_2 to $C_6H_5Cl_4^+$ m/z 216.9145 etc.
181,183,185 (100,90,30) – [M-107] loss of H_2Cl_3 to $C_6H_4Cl_3^+$ m/z 180.9379 etc.
109,111 (55,45) – [M-179] $C_3H_3Cl_2^+$ m/z 108.9612 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C58899&Units=SI&Mask=200#Mass-Spec
(The NIST WebBook contains 12 mass spectra with empirical formula $C_6H_6Cl_6$ of which 8 appear to be HCH related.)

HCH related, gamma-PCCH **$C_6H_5Cl_5$** **M:252,254,256(2,3,2%)**
Theoretical molecular ion: m/z 251.8834 (63%), 253.8804 (100%), 255.8775 (64%)
Average MW: 254.36



gamma-PCCH

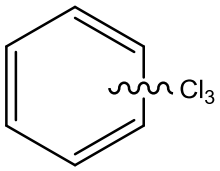
Pentachlorocyclohexenes (PCCHs) are metabolic dehydrochlorination products of HCH isomers:

m/z	181	183	185	111	146	147	145	219
%	100	90	30	25	25	25	25	20

252,254,256 (2,3,2)
217,219,221 (17,21,11)
181,183,185 (100,90,30)

No NIST spectrum available for comparison.

HCH related, trichlorobenzene **$C_6H_3Cl_3$** **M:180,182,184(100,95,30%)**
Theoretical molecular ion: m/z 179.9300 (100%), 181.9271 (96%), 183.9241 (31%)
Average MW: 181.44



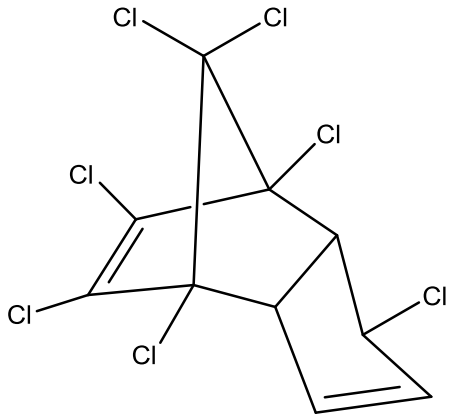
Dehydrochlorination of gamma-HCH with a strong base produces a mixture of trichlorobenzenes, with similar mass spectra; Typical GC elution order 1,3,5- , 1,2,4- , 1,2,3- with peak area ratios of ca 1:10:1

m/z	180	182	74	145	109	184	147	75
%	100	95	45	40	35	30	25	25

180,182,184 (100,95,30) – M^+
145,147 (40,25) – [M-35] loss of Cl to $C_6H_3Cl_2^+$ m/z 144.9612 etc.
109,111 (35,10) – [M-71] loss of HCl_2 to $C_6H_2Cl^+$ m/z 108.9845
74 (45) – [M-106] loss of HCl_3 to $C_6H_2^+$ m/z 74.0157

Cf. generally similar NIST spectra for 1,2,4-, 1,3,5- and 1,2,3- trichlorobenzenes.
E.g. 1,2,4- isomer http://webbook.nist.gov/cgi/cbook.cgi?ID=C120821&Units=SI&Mask=200#Mass-Spec

Heptachlor **$C_{10}H_5Cl_7$** **M:370,372,374,376(2,6,7,3%)**
Theoretical molecular ion: m/z 369.8211 (54%), 371.8181 (70%), 373.8152 (100%), 375.8122 (53%)
Average MW: 373.30



Organochlorine insecticide. One of the "dirty dozen" persistent organic pollutants banned at the Stockholm Convention in 2001.

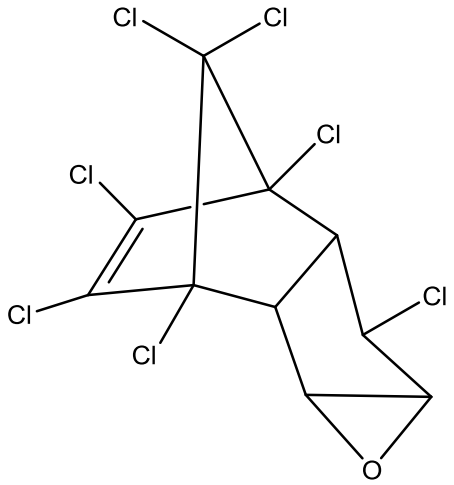
Acute oral LD50 for rat >150 mg/kg (moderate toxicity).

m/z	100	272	274	65	102	270	237	135
%	100	60	45	35	30	30	20	15

370,372,374,376 (2,6,7,3) - M^+
335,337,339,341 (8,15,10,5) – [M-35] loss of Cl
299,301,303 (2,4,2) – [M-71] loss of HCl_2
270,272,274,276 (30,60,45,15) – [M-100] loss of C_5H_5Cl to $C_5Cl_6^+$
100 (100) – [M-270] $C_5H_5Cl^+$ m/z 100.0798
65 (35) – [M-305] $C_5H_5^+$ m/z 65.0391

Cf. similar (but weak/noisy) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C76448&Mask=200#Mass-Spec

Heptachlor epoxide **$C_{10}H_5Cl_7O$** **M:386,388,390,392(3,6,8,4%)**
Theoretical molecular ion: m/z
Average MW: 389.32



KI(CPSil19) = 21.1 (very close to oxychlordane)

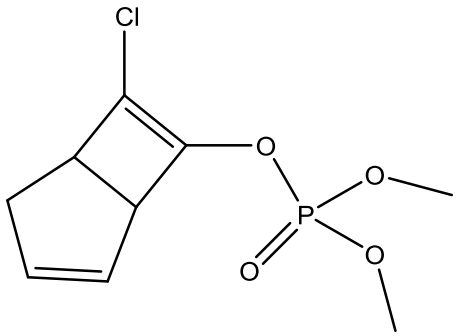
m/z	353	81	355	351	357	263	237	151
%	100	90	80	50	35	25	25	20

386,388,390,392(3,6,8,4) – M^+
351,353,355,357 (50,100,80,35) – [M-35] loss of Cl
81 (90) – [M-305] $C_5H_5O^+$ m/z 81.0340

Cf. Similar (but weak/noisy) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1024573&Mask=200#Mass-Spec

Heptenophos **$C_9H_{21}ClO_4P$** **M:250,252(15,5%)**

Theoretical molecular ion: m/z 250.0162 (100%), 252.0132 (32%)
Average MW: 250.632



Organophosphorus insecticide. No longer approved for use in EU.

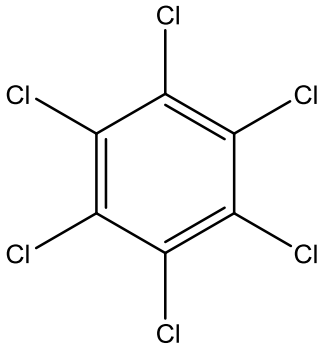
Acute oral LD50 for rat approx. 100 mg/kg (high toxicity).

m/z	124	89	126	127	215	250	109	252
%	100	35	35	20	15	15	10	5

250,252 (15,5) – M^+
215 (15) – [M-35] loss of Cl to $C_9H_{12}O_4P^+$ m/z 215.0473
127 (20) – [M-123] $(CH_3O)_2(HO)_2P^+$ m/z 127.0106
124,126 (100,35) – [M-126] $C_7H_6Cl^+$ m/z 124.0080 etc.
109 (10) – [M-141] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
89 (35) – [M-161] $C_7H_5^+$ m/z 89.0391

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C23560590&Mask=200#Mass-Spec filed under "Phosphoric acid, 7-chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl ester"

Hexachlorobenzene **C_6Cl_6** **M:282,284,286,288(55,100,80,40%)**
Theoretical molecular ion: m/z 281.8131 (52%), 283.8102 (100%), 285.8072 (80%)
Average MW: 284.77



Organochlorine fungicide. One of the "dirty dozen" persistent organic pollutants banned at the Stockholm Convention in 2001.

Acute oral LD50 for rat >10,000 mg/kg (low toxicity).

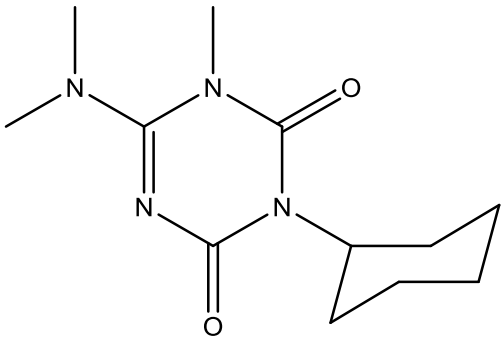
KI (SE-30) =16.5

m/z	284	286	282	288	142	249	106	144
%	100	80	55	35	30	25	20	15

282,284,286,288 (55,100,80,40) – M^+
247,249,251 (10,15,10) – [M-35] loss of Cl to $C_6Cl_5^+$ m/z 246.8443 etc.
142,144 (30,15) – [M-140] loss of Cl_4 to $C_6Cl_2^+$ m/z 141.9377 etc.
141,143 (10,10) – [M-141] $C_3Cl_3^+$ m/z 140.9067 - overlapping ion clusters
107,109 (10) – [M-175] C_6Cl^+ m/z 106.9689 etc.
106,108 (20,5) – [M-176] $C_3Cl_2^+$ m/z 105.9377 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C118741&Mask=200#Mass-Spec apart from more abundant m/z 107 (30%) due to C_6Cl^+ and m/z 71 (15%) due to C_3Cl^+.

Hexazinone **$C_{12}H_{20}N_4O_2$** **M:252(20%)**
Theoretical molecular ion: m/z 252.1586 (100%), 253.1620 (13%)
Average MW: 252.32



Herbicide. No longer approved for use in EU.

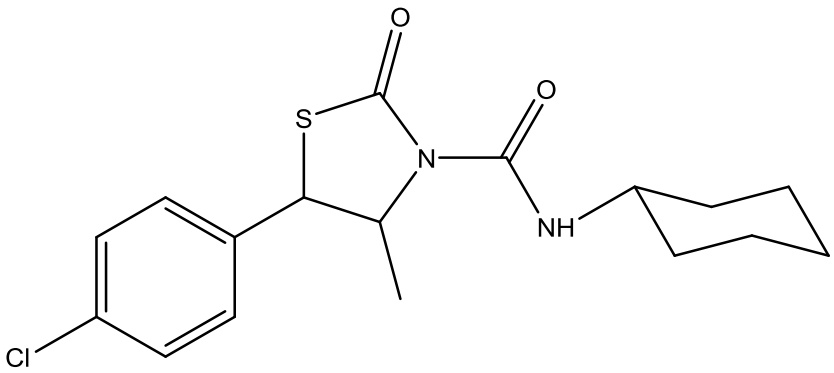
Acute oral LD50 for rat 1,500 mg/kg (moderate toxicity).

m/z	171	44	83	71	128	98	252	127
%	100	65	55	45	45	25	20	20

252 (20) – M^+ $C_{12}H_{20}N_4O_2$
171 (100) – [M-81] loss of cyclohexyl C_6H_9 moiety to $C_6H_{11}N_4O_2^+$ m/z 171.0882
128 (100) – [M-124] loss of $C_6H_{11}NCO$ to $C_5H_{10}N_3O^+$ m/z 128.0824
44 (65) – [M-208] $(CH_3)_2N^+$ $C_2H_6N^+$ m/z 44.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C51235042&Mask=200#Mass-Spec other than some weaker ions (e.g. M^+ m/z 252 at 5% rather than 20%, and m/z 44 at 5% rather than 65%).

Hexythiazox **$C_{17}H_{21}ClN_2O_2S$** **M:352,354 (5,2%)**
Theoretical molecular ion: m/z 352.1012 (100%), 354.0983 (32%)
Average MW: 352.88



Acaricide. Used to control phytophagous mites. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

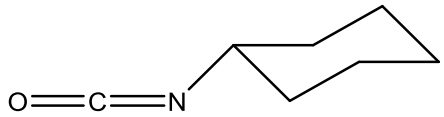
Very susceptible to GC degradation.

m/z	98	271	184	157	156	125	82	309
%	100	30	30	25	25	20	15	15

352,354 (5,2) – M^+
309,311 (15,5) – [M-43] loss of C_3H_7 from cyclohexyl to $C_{41}H_{14}ClN_2O_2S^+$ m/z 309.0465 etc.
271,273 (30,10) – [M-81] loss of cyclohexyl moiety C_6H_9 to $C_{11}H_{12}ClN_2O_2S^+$ m/z 271.0308 etc.
184,186 (30,10) – [M-168] $ClC_6H_4.CHSCO^+$ $C_8H_5ClOS^+$ m/z 183.9750 etc.
98 (100) – [M-254] cyclohexylamine $C_6H_{11}NH^+$ $C_6H_{12}N^+$ m/z 98.0970
82 (15) – [M-260] cyclohexene $C_6H_{10}^+$ m/z 82.0783

No NIST spectrum available.

Hexythiazox related, i) **$C_7H_{11}NO$** **M:125(20%)**
Cyclohexyl isocyanate
Theoretical molecular ion: m/z 125.0841 (100%), 126.0874 (7.6%)
Average MW: 125.17



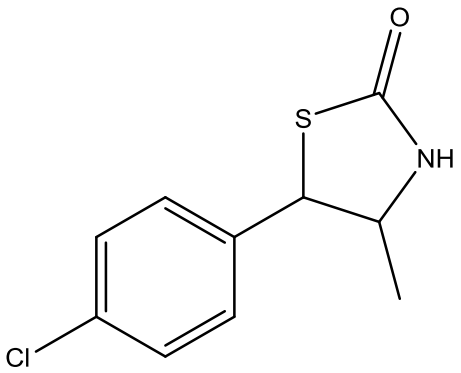
Hexythiazox may decompose entirely on capillary GC (using CPSil19) to produce cyclohexyl isocyanate which is observed as a broad GC peak:

m/z	67	82	97	41	54	56	69	125
%	100	90	75	70	50	50	30	20

125 (20) – M^+
69 (30) – [M-60] $C_5H_9^+$ m/z 69.0704
67 (100) – [M-58] $C_5H_7^+$ m/z 67.0548
56 (50) – [M-69] $OCN\text{-}CH_2^+$ $C_2H_2NO^+$ m/z 56.0440

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C3173533&Mask=200#Mass-Spec

Hexythiazox related, ii) **$C_{10}H_{10}ClNOS$** **M:227,229(70,25%)**
5-(4-chlorophenyl)-4-methyl-2-oxo-3-thiazolidine
Theoretical molecular ion: m/z 227.0172 (100%), 229.0142 (32%)
Average MW: 227.71



Hexythiazox appears to decompose entirely on capillary GC (using CPSil19), to produce 5-(4-chlorophenyl)-4-methyl-2-oxo-3-thiazolidine which is observed as a broad GC peak:

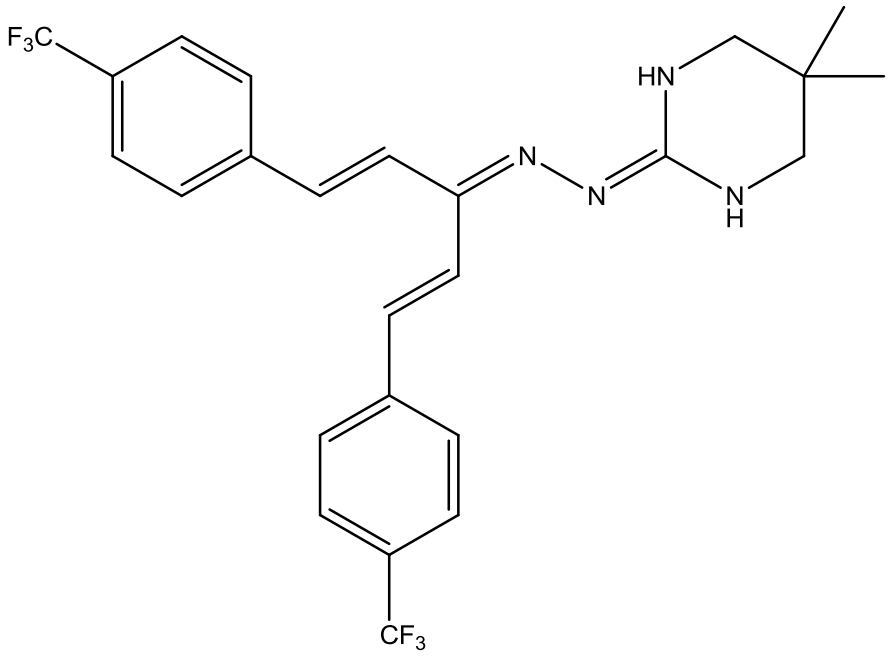
m/z	156	227	184	157	155	44	158	117
%	100	70	65	60	60	40	40	35

227,229 – M^+
156,158 (100,40) – [M-71] $ClC_6H_4CHS^+$ $C_7H_5ClS^+$ m/z 155.9801 etc.

No NIST spectrum available.

Hydramethylnon $C_{25}H_{24}F_6N_4$ **M:494(40%)**

Theoretical molecular ion: m/z 494.1905 (100%), 495.1939 (27%)
Average MW: 494.48



Trifluoromethyl aminohydrazone insecticide. Used in baits to control ants and cockroaches. No longer approved for use in EU.

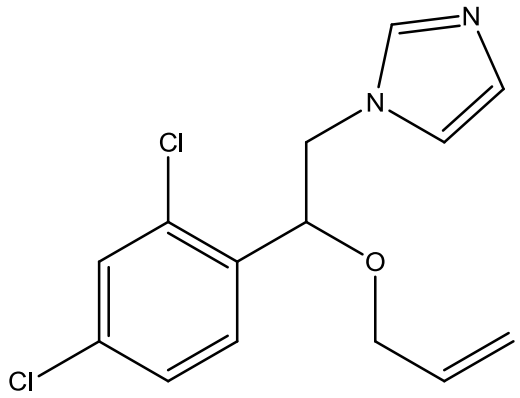
Acute oral LD50 for rat >1,000 mg/kg (moderate toxicity).

m/z	349	297	494	30	350	296	55	475
%	100	60	40	25	25	15	15	5

494 (40) – M^+
475 (5) – [M-19] loss of F to $C_{25}H_{24}F_5N_4^+$ m/z 475.1921
383 (5) – [M-111] loss of $C_6H_{11}N_2$ (surprising scission of hydrazone C=N bond) to
$C_{19}H_{13}F_6N_2^+$ m/z 383.0983
349 (100) – [M-145] loss of F & $C_6H_{12}N_3$ to $C_{19}H_{12}F_5N^+$ m/z 349.0890
297 (60) – [M-197] $C_{15}H_{18}F_3N_3^+$ m/z 297.1453
due to cyclisation and loss of $C_{10}H_6F_3N$ (see m/z 197 below)
197 (5) – [M-297] $CF_3C_6H_4CH{=}CH.CN^+$ $C_{10}H_6F_3N^+$ m/z 197.04523
55 (15) – [M-439] $C_4H_7^+$ m/z 55.0548
30 (25) – [M-464] $CH_2NH_2^+$ CH_4N^+ m/z 30.0344

Cf. Very different spectra at http://webbook.nist.gov/cgi/cbook.cgi?ID=C67485294&Mask=200 and http://www.restek.com/compound/view/67485-29-4/Hydramethylnon
which both exhibit base: peak at m/z 297; weaker m/z 349 (<5%); stronger m/z 383; and weaker M^+ m/z 494 (ca. 10%). It is not obvious why the spectrum reported here appears so different. It could be that the fragmentation processes of hydramethylnon are particularly sensitive to MS ionisation conditions (ion source temperature, source contamination etc.).

Imazalil **$C_{14}H_{14}Cl_2N_2O$** **M:296,298(2,1%)**
Theoretical molecular ion: m/z 296.0483 (100%), 298.0454 (64%), 300.0424 (10%)
Average MW: 297.18



Conazole fungicide. Used to control a wide range of fungi including *Tilletia* (smut) and *Helminthosporium spp*. on fruit, vegetables and ornamentals. Approved for use in EU.

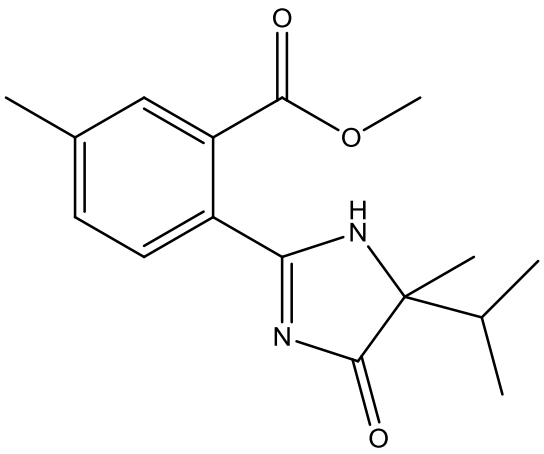
Acute oral LD50 for rat approx. 200 mg/kg (moderate toxicity).

m/z	41	215	173	217	175	81	159	54
%	100	25	15	15	10	10	5	5

296,298 (2,1) – M^+
240,242 (2,1) – [M-56] loss of CH_2=CHCHO to $C_{11}H_{10}Cl_2N_2O^+$ m/z 240.0221 etc.
215,217 (25,15) – [M-81] loss of $(C_3H_3N_2)CH_2$ to $C_{10}H_9Cl_2O$+ m/z 215.0031 etc.
173,175 (15,10) – [M-123] $Cl_2C_6H_4CHCH_2^+$ $C_8H_7Cl_2^+$ m/z 172.9925 etc.
81 (10) – [M-215] $(C_3H_3N_2)CH_2^+$ $C_4H_5N_2^+$ m/z 81.0453
41 (100) – [M-255] CH_2=$CHCH_2^+$ $C_3H_5^+$ m/z 41.0391

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C35554440&Mask=200#Mass-Spec

Imazamethabenz-methyl **$C_{16}H_{20}N_2O_3$** **M:288(10%)**
Theoretical molecular ion: m/z 288.1474 (100%), 289.1507 (17%)
Average MW: 288.34



Imazamethabenz-methyl, main isomer (ca. 60%, 3-methyl benzoic acid form).
(40% 4-methyl benzoic acid form)

Imidazolinone herbicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. >5,000 mg/kg (low toxicity).

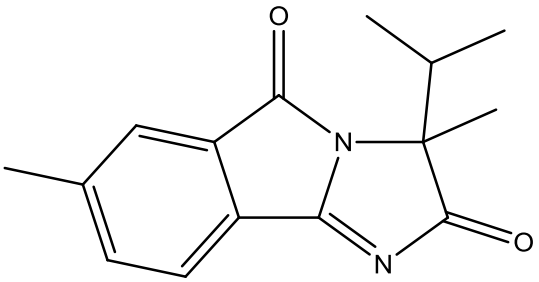
Mixture of 2 isomers, easily separated on capillary GC. May degrade on GC.

m/z	144	245	176	246	117	89	116	214
%	100	65	60	35	30	25	25	25

288 (10) – M^+
256 (15) – [M-32] loss of CH_3OH to $C_{15}H_{16}N_2O_2^+$ m/z 256.1212 - see related compound below
144 (100) – [M-144] [$CH_3.C_6H_4.CO.CN$ minus H]$^+$ $C_9H_6NO^+$ m/z 144.0449

No NIST spectrum available.

Imazamethabenz-methyl related **$C_{15}H_{16}N_2O_2$** **M:256(85%)**
3-isopropyl-3,7-dimethyl-2H-imidazo[2,1-a]isoindole-2,5(3H)-dione
Theoretical molecular ion: m/z 256.1212 (100%), 257.1245 (16%)
Average MW: 256.30



Tentative structure

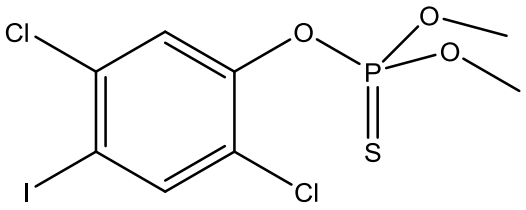
GC degradation product isomers (notional loss of methanol), with shorter RT than parent.

m/z	187	256	144	117	89	116	214	41
%	100	85	80	55	50	40	35	30

256 (85) – M^+
187 (15) – [M-69] loss of C5H9 to $C_{10}H_7N_2O_2^+$ m/z 187.0508
144 (100) – [M-112] "$CH_2.C_6H_4.CO.CN+$" $C_9H_6NO^+$ m/z 144.0449

No NIST spectrum available.

Iodofenphos **$C_8H_8Cl_2IO_3PS$** **M:412,414(2,1%)**
Theoretical molecular ion: m/z 411.8353 (100%), 413.8324 (64%), 415.8294 (10%)
Average MW: 413.00



Organophosphorus (phenyl organothiophosphate) insecticide, previously used for the protection of stored products, and against livestock pests and in public health applications including cockroaches, lice, bugs, flies, fleas and mosquitoes. No longer approved for use in EU.

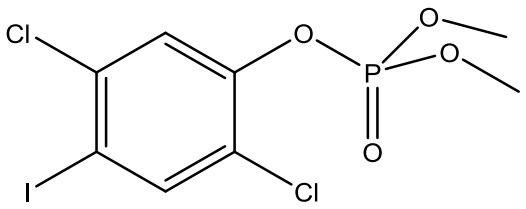
Acute oral LD50 for rat approx. 2,500 mg/kg (low toxicity).

m/z	377	379	125	93	79	109	47	250
%	100	40	35	20	20	20	15	10

412,414 (2,1) – M^+ weak
377,379 (100,40) – [M-35] loss of Cl to $C_8H_8ClIO_3PS^+$ m/z 376.8665
250,252 (10,3) – [M-162] loss of Cl & I to $C_8H_8ClO_3PS^+$ m/z 259.9620
125 (35) – [M-287] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (20) – [M-303] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055 [O/S swap]
93 (20) – [M-319] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (20) – [M-333] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
47 (15) – [M-365] PO^+ m/z 46.9687

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C18181709&Units=SI&Mask=FFFF

Iodofenphos oxon **$C_8H_8Cl_2IO_4P$** **M:396,398(25,15%)**
Theoretical molecular ion: m/z 395.8582 (100%), 397.8552 (64%), 399.8523 (10%)
Average MW: 396.93



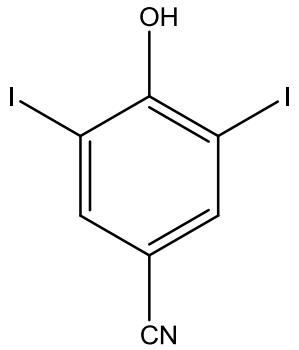
m/z	361	109	363	396	398	79	97	93
%	100	55	35	25	15	15	10	5

396,398 (25,15) – M^+ C8H8Cl2IO4P
361,363 (100,35) – [M-35] loss of Cl to $C_8H_8ClIO_4P^+$ m/z 360.8894 etc.
109 (55) – [M-287] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (15) – [M-317] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
97 (10) – [M-299] $(HO)_2PO_2^+$ $H_2O_4P^+$ m/z 96.9691
93 (5) – [M-303] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105

No NIST spectrum available.

Ioxynil **$C_7H_3I_2NO$** **M:371(100%)**

Theoretical molecular ion: m/z : 370.8304 (100%), 371.8338 (8%)
Average MW: 370.91



Herbicide. Used for post-emergence control of annual broad-leaved weeds. Also pesticide transformation product. (See octanoate ester below.) Approved for use in EU.

Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

Sometimes poor GC transmission.

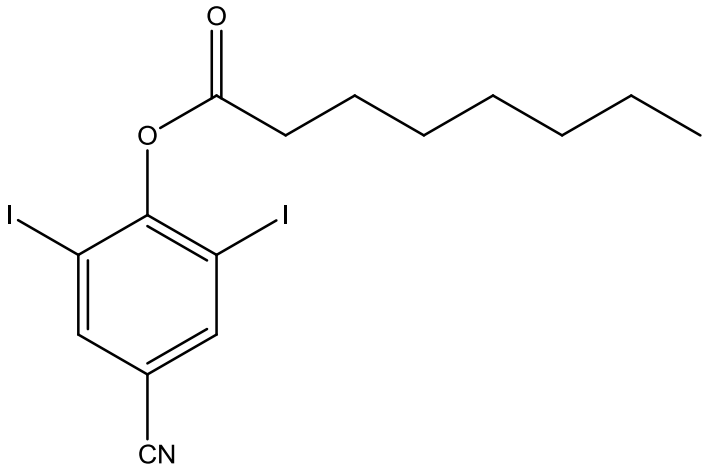
m/z	371	117	88	62	89	61	372	216
%	100	50	15	15	10	10	5	5

371(100) – M^+
117 (50) – [M-254] loss of I_2 to $C_7H_3NO^+$ m/z 117.0215

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1689834&Units=SI&Mask=200#Mass-Spec
Listed under "Loxynil" (perhaps a typo?).

Ioxynil octanoate **$C_{15}H_{17}I_2NO_2$** **M:497(0.5%)**

Theoretical molecular ion: m/z 496.9349 (100%), 497.9382 (16%)
Average MW: 497.11



m/z	127	57	43	41	29	128	88	371
%	100	90	30	15	10	10	5	5

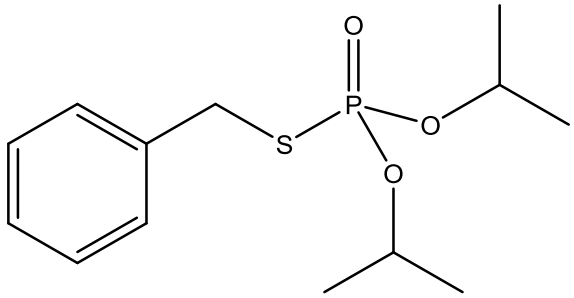
497 (0.5) – M^+ weak

371 (5) – [M-126]
243 (5) – [M-254]
127 (100) – [M-370] $C_7H_{15}CO^+$ $C_8H_{15}O^+$ m/z 127.1123 (*cf.* bromoxynil octanoate).
N.B. Not I^+ which has similar nominal atomic weight (m/z 126.9045).

No NIST spectrum available.

Iprobenfos / Kitazin **$C_{13}H_{21}O_3PS$** **M:288(5%)**

Theoretical molecular ion: m/z 288.0949 (100%), 289.0983 (14%), 290.0907 (4.5%)
Average MW: 288.34



Organophosphorus fungicide. Used on rice to control leaf and ear blast, stem rot and sheath blight. Not approved for use in EU.

Acute oral LD50 for rat approx 500 mg/kg (moderate toxicity)

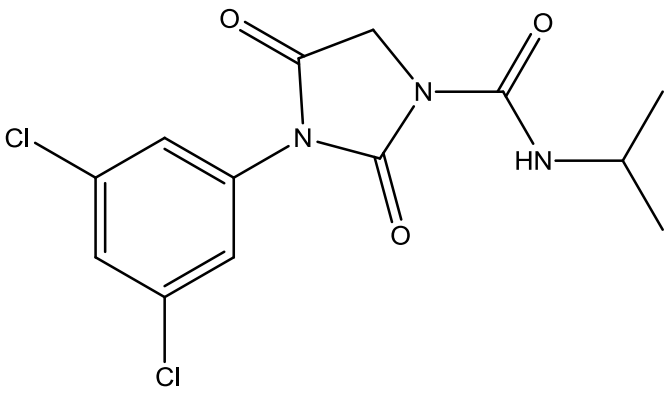
m/z	91	204	41	123	122	107	246	45
%	100	35	25	15	15	10	10	10

288 (5) – M^+
246 (10) – [M-42] loss of C_3H_6 to $C_{10}H_{15}O_3PS^+$ m/z 246.0480
204 (35) – [M-48] loss of $2C_3H_6$ to $C_7H_9O_3PS^+$ m/z 204.1798
123 (15) – [M-165] $C_6H_5CH_2S^+$ $C_7H_7S^+$ m/z 123.0269
107 (10) – [M-181] $C_6H_5CH_2O^+$ $C_7H_7O^+$ m/z 107.0497
91 (100) – [M-197] $C_7H_7^+$ m/z 91.0548
65 (10) – [M-223] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C26087478&Units=CAL&Mask=6EF

Iprodione **$C_{13}H_{13}Cl_2N_3O_3$** **M:329,331(4,3%)**

Theoretical molecular ion: m/z .329.0334 (100%), 331.0304 (64%), 333.0275 (10%)
Average MW: 330.17



Imidazole fungicide. Used to control *Botrytis*, *Minilia*, *Sclerotinia* and other diseases in a wide range of crops. Approved for use in EU.

Acute oral LD50 for rat approx >2,000 mg/kg (moderate toxicity)

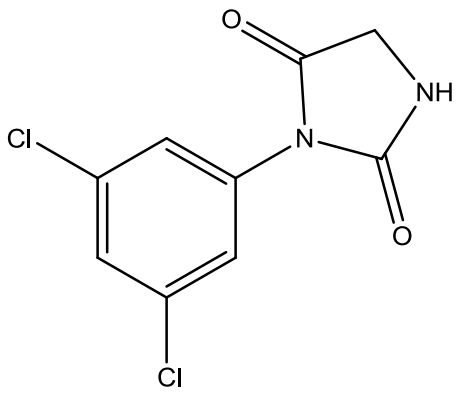
Prone to GC degradation, particularly with phenylmethylsilicone stationary phases (such as OV-17): best transmission obtained with methylsilicones (e.g. SE-30) or fluoroalkylsilicones (OV-210). KI (OV-210) = 31.4

m/z	314	43	56	58	316	187	70	189
%	100	90	70	65	65	45	35	25

329,331 (4,3) – M^+ $C_{13}H_{13}Cl_2N_3O_3$
314,316,318 (100,65,10) – [M-15] loss of CH_3 to $C_{12}H_{10}Cl_2N_3O_3^+$ m/z 314.0099 etc.
271,273 (10,7) – [M-58] loss of $NHCH(CH_3)_2$ to $C_{10}H_5Cl_2N_2O_3^+$ m/z 270.9677 etc.
245,247 (23,16) – [M-84] loss of $CONHCH(CH_3)_2$(-2H) to $C_8H_7Cl_2N_2O_2^+$ m/z 244.9885 etc.
187,189 (45,25) – [M-142] dichlorophenyl isocyanate $Cl_2C_6H_3NCO^+$ $C_7H_3Cl_2NO^+$ m/z 186.9592 etc.
58 (65) – [M-271] $C_3H_8N^+$ m/z 58.0657
56 (70) – [M-273] $C_3H_6N^+$ m/z 56.0500
43 (90) – [M-286] $C_3H_7^+$ m/z 43.0548

Cf. very poor spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C36734197&Mask=200#Mass-Spec with weak high mass ions, e.g. m/z 314 ca. 40%.

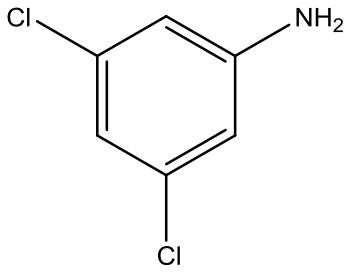
Iprodione related, i) **$C_9H_6Cl_2N_2O_2$** **M:244,246(65,45%)**
3(3,5-dichlorophenyl)imidazolidine-2,4-dione
Theoretical molecular ion: m/z 243.9806 (100%), 245.9777 (64%), 247.9747 (10%)
Average MW: 245.06



GC degradation product.

m/z	187	244	189	246	188	124	56	190
%	100	65	60	45	35	30	20	20

Iprodione related, ii) **$C_6H_5Cl_2N$** **M:161,163(100,50%)**
3,5-dichloroaniline
Theoretical molecular ion: m/z 160.9799 (100%), 162.9770 (64%), 164.9740 (10%)
Average MW: 162.0130

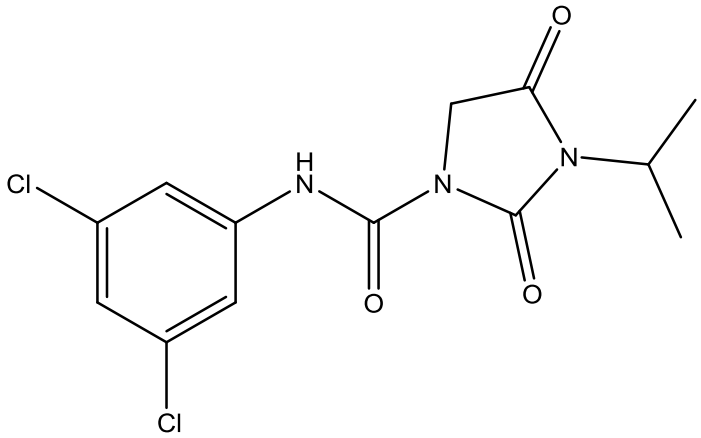


An important degradation product of iprodione and several other compounds (e.g. chlozolinate, procymidone and vinclozolin). Sometimes included in MRLs.
KI (OV-210) = 17

m/z	161	163	90	63	99	126	165	125
%	100	70	25	25	20	20	10	10

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C626437&Mask=200#Mass-Spec

Iprodione related, iii) **$C_{13}H_{13}Cl_2N_3O_3$** **M:329,331(60,35%)**
Iprodione isomer (longer GC RT)
Theoretical molecular ion: m/z
Average MW: 329



Isomer of iprodione which may be formed in methanol or ethanol solutions by opening and re-closing of imidazolidine ring onto adjacent amide (Cooke 1979).
KI (OV-210) = 32.0 (longer retention time than iprodione)

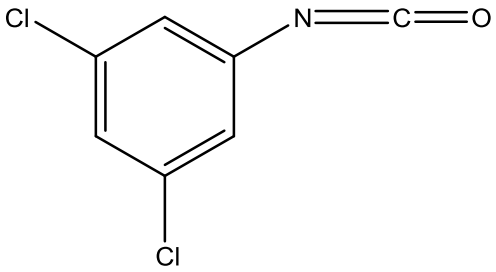
m/z	142	127	329	43	99	331	187	56
%	100	85	60	40	40	35	30	30

329,331 (60,35) – M^+ (over 10x stronger molecular ion than iprodione's, at 4%)
187,189 (30,20) – [M-142] dichlorophenyl isocyanate $C_7H_3Cl_2NO^+$ m/z 186.9592
142 (100) – [M-187] loss of dichlorophenyl isocyanate to $C_6H_{10}N_2O_2^+$ m/z 142.0742

No NIST spectrum available.

Iprodione related, iv) **$C_7H_3Cl_2NO$** **M:187,189(100,65%)**
3,5-dichlorophenyl isocyanate
Theoretical molecular ion: m/z 186.9592 (100%), 188.9562 (64%), 190.9533 (10%)

Average MW: 188.01



GC degradation product of iprodione isomer. KI (OV-17) = 14.0

m/z	187	189	124	159	126	161	191	88
%	100	65	50	20	15	15	15	10

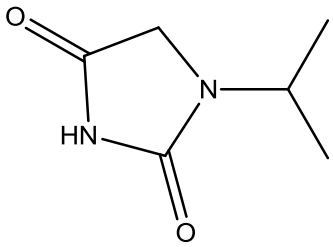
187,189,191 (100,65,15) – M^+
159,161 (20,15) – [M-28] loss of CO to $C_6H_3Cl_2N^+$ m/z 158.9643 etc
124,126 (50,15) – [M-63] loss of CO & Cl to $C_6H_3ClN^+$ m/z $C_6H_3ClN^+$ m/z 123.9954 etc.
88 (10) – [M-99] $C_6H_2N^+$ m/z 88.0187

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C34893920&Mask=200#Mass-Spec

Iprodione related, v) **$C_6H_{10}N_2O_2$** **M:142(45%)**

3-isopropyl imidazolidine-2,4-dione

Theoretical molecular ion: m/z 142.0742 (100%), 143.0776 (6.5%)
Average MW: 142.16

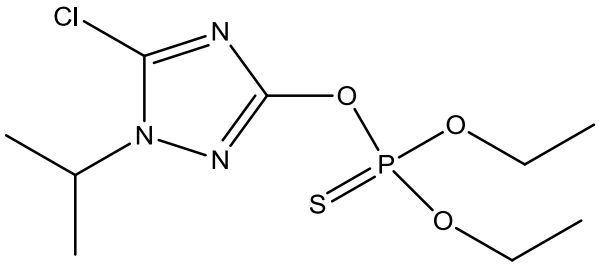


GC degradation product of iprodione isomer.
KI (OV-17) = 16.3

m/z	30	101	127	44	142	99	70	56
%	100	80	80	50	45	45	40	30

142 (50) – M^+
101 (80) – [M-41] loss of C_3H_5 to $C_3H_5N_2O_2^+$ m/z 101.0351
30 (100) – [M-112] CH_2NH_{2+} CH_4N^+ m/z 30.0344

Isazofos **$C_9H_{17}ClN_3O_3PS$** **M:313,315(15,5%)**
Theoretical molecular ion: m/z 313.0417 (100%), 315.0387 (32%), 314.0450 (9.7%)
Average MW: 314.04



Triazole organophosphorus insecticide. Used to control soil insects on turf and some crops. No longer approved for use in EU.

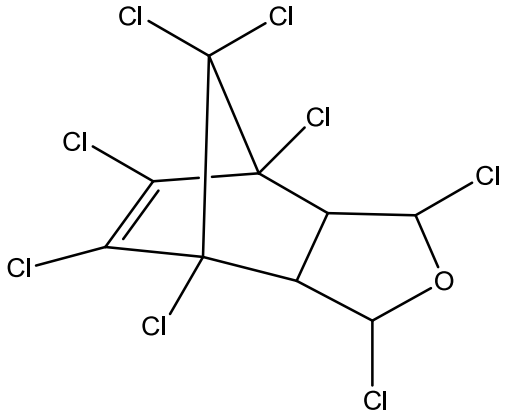
Acute oral LD50 for rat approx. 20 mg/kg (high toxicity).

m/z	161	119	162	97	257	163	172	285
%	100	75	60	50	35	30	30	30

313,315 (15,5) – M^+ $C_9H_{17}ClN_3O_3PS$
285,287 (30,10) – [M-28] loss of C_2H_4 to $C_7H_{13}ClN_3O_3PS^+$ m/z 285.0104
257,259 (35,10) – [M-56] loss of $2C_2H_4$ to $C_5H_9ClN_3O_3PS^+$ m/z 256.9791
161,163 (100,30) – [M-152] $(CH_3)_2CH(C_2N_3Cl)OH^+$ $C_5H_8ClN_3O^+$ m/z 161.0356 etc.
119,121 (75,25) – [M-194] $H(C_2N_3Cl)OH^+$ $C_2H_2ClN_3O^+$ m/z 118.9886
97 (50) – [M-216] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
65 (25) – [M-248] $(HO)_2P^+$ m/z 64.9792

Cf. similar spectra at http://webbook.nist.gov/cgi/cbook.cgi?ID=C42509808&Mask=200#Mass-Spec
& http://www.t3db.ca/spectra/spectra/ei_ms/1177

Isobenzan / Telodrin **$C_9H_4Cl_8O$** **M:408,410,412,414(2,5,5,3%)**
Theoretical molecular ion: m/z 407.7770 (35%), 409.774 (89%), 411.7711 (100%), 413.7682 (64%)
Average MW: 411.75



Banned organochlorine insecticide. Manufactured during the early 1960s. Persistent organic pollutant.

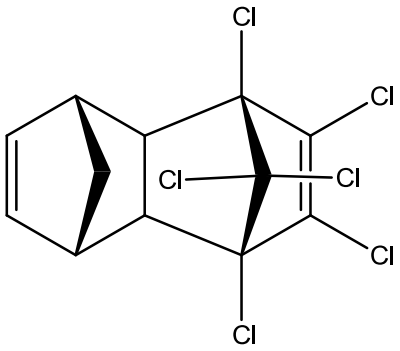
Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

m/z	103	311	313	309	105	375	377	275
%	100	65	50	30	30	25	25	25

408,410,412,414(2,5,5,3) – M^+
373,375,377,379(10,25,25,10) – [M-35] loss of Cl
309,311,313,315(30,65,50,20) – [M-99] loss of $HCCl_2O$ to $C_8H_3Cl_6^+$ m/z 308.8366 etc.
103,105 (100,30) – [M-305] $C_4H_4ClO^+$ m/z 102.9951

Cf. similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C297789&Mask=200#Mass-Spec

Isodrin **$C_{12}H_8Cl_6$** **M:362,364,366,368(5,10,10,3%)**
Theoretical molecular ion: m/z 361.8757 (52%),363.8728 (100%), 365.8698 (80%), 367.8669 (34%)
Average MW: 346.91



Banned organochlorine insecticide. Used to control malarial mosquitoes.
A persistent organic pollutant.

Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

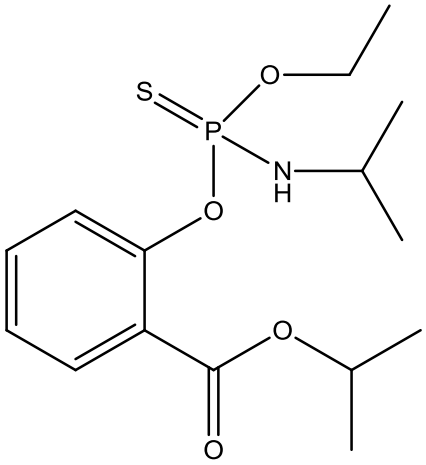
m/z	193	195	66	263	147	197	261	265
%	100	95	80	40	35	35	25	25

362,364,366,368 (5,10,10,3) – M^+ $C_{12}H_8Cl_6^+$
327,329,331(5,7,5) – [M-35] loss of Cl to $C_{12}H_8Cl_5^+$ m/z 326.9069 etc.
291,293,295 (7,10,5) – [M-71] loss of HCl_2 to $C_{12}H_7Cl_4^+$ m/z 290.9302 etc.
261,263,265 (25,40,25) – [M-101] loss of C_5H_6 & Cl to $C_7H_2Cl_5^+$ m/z 260.8599 etc.
193,195 (100,95) – [M-169] $C_7H_4Cl_3^+$ m/z 192.9379
147,149 (35,20) – [M-215] $C_6H_5Cl_2$ m/z 146.9768
66 (80) – [M-296] cyclopentadiene $C_5H_6^+$ m/z 66.0470

Cf. weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C465736&Mask=200

Isofenphos **$C_{15}H_{24}NO_4PS$** **M:345(5%)**

Theoretical molecular ion: m/z 345.1164 (100%), 346.1197 (16%), 347.1122 (4.5%)
Average MW: 345.39



Organophosphorus phosphoramidothioate insecticide. Used to control soil-dwelling insects such as white grubs, cabbage root flies, corn roundworms and wireworms. No longer approved for use in EU.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

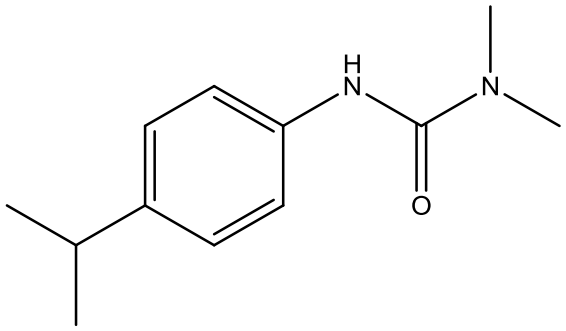
m/z	58	213	121	185	255	96	43	138
%	100	60	55	40	40	40	30	20

Assignments confirmed by accurate mass study (GCT Cardiff)
345 (0) – M^+ absent (but present in NIST spectrum) $C_{15}H_{24}NO_4PS^+$ m/z 345.1164
286 (5) – [M-59] loss of $(CH_3)_2CHO$ to $C_{12}H_{17}NO_3PS^+$ m/z 286.0667
255 (40) – [M-90] loss of C_3H_8NS to $C_{12}H_{16}O_4P^+$ m/z 255.0786
Not possible to assign before accurate mass study
213 (60) – [M-132] loss of $C_6H_{14}NS$ to $C_9H_{10}O_4P^+$ m/z 213.0317
NOT loss of $(CH_3)_2CHOCO$ & CH_3CH_2O to $C_9H_{12}NOPS^+$ m/z 213.0377
185 (40) – [M-160] loss of $C_8H_{18}NS$ to $C_7H_6O_4P^+$ m/z 185.0037
Not assigned before accurate mass study
138 (20) – [M-207] $(C_3H_7NH)(HO)P{=}S^+$ $C_3H_9NOPS^+$ m/z 138.0143
121 (40) – [M-224] $C_6H_5CO_2^+$ $C_7H_5O_2^+$ m/z 121.0290
NOT $C_3H_7NH.P{=}S^+$ $C_3H_8NPS^+$ m/z 121.0115
96 (40) – [M-249] $(HO)(NH_2)P{=}S^+$ H_3NOPS^+ m/z 95.9673
58 (100) – [M-287] $(CH_3)_2CHNH^+$ $C_3H_8N^+$ m/z 58.0657

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C25311711&Mask=200#Mass-Spec which has weaker ions at m/z 213 (30%) and 255 (15%) etc. but curiously it exhibits molecular ion at m/z 345 (5-10%), though this was not detected here.

Isoproturon **$C_{12}H_{18}N_2O$** **M:206(30%)**

Theoretical molecular ion: m/z 206.1419 (100%), 207.1453 (13.0%)
Average MW: 206.28



Herbicide. Approved for use in EU.

Acute oral LD50 for rat approx. 1,800 mg/kg (moderate toxicity).

Not amenable to GC analysis.

m/z	72	146	206	191	161	128	91	57
%	100	50	30	20	15	15	10	10

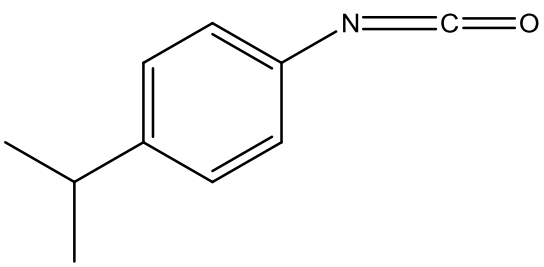
206 (30) – M^+
191 (20) – [M-15] loss of CH_3 to $C_{11}H_{15}N_2O^+$ m/z 191.1184
161 (15) – [M-45] loss of $(CH_3)_2NH$ to isopropylphenyl isocyanate $C_{10}H_{11}NO^+$ m/z 161.0841
146 (50) – [M-60] loss of CH_3 & $(CH_3)_2NH$ to $C_9H_8NO^+$ m/z 146.0606
72 (100) – [M-134] $(CH_3)_2NCO^+$ m/z 72

Cf. weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C34123596&Mask=200#Mass-Spec lacking low abundance ions <5% rel. abundance.

Isoproturon related **$C_{10}H_{11}NO$** **M:161(35%)**

4-isopropyl phenyl isocyanate

Theoretical molecular ion: m/z 161.0841 (100%), 162.0874 (11%)
Average MW: 161.20



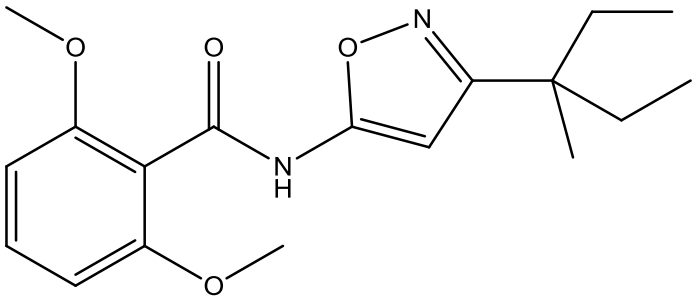
4-isopropyl phenyl isocyanate, GC degradation product :

m/z	146	161	128	91	77	103	147	118
%	100	35	30	15	10	10	10	10

161 (35) – M+
146 (100) – [M-15] loss of CH_3 to $C_9H_8NO^+$ m/z 146.0606
128 (30) – [M-33] loss of CH_3 & H_2O to $C_9H_6N^+$ m/z 128.0500

Isoxaben $C_{18}H_{24}N_2O_4$ **M:332(1%)**

Theoretical molecular ion: m/z
Average MW:



Amide herbicide. Previously called benzamizole. Approved for use in EU.

Acute oral LD50 for rat > 10,000 mg/kg (low toxicity).

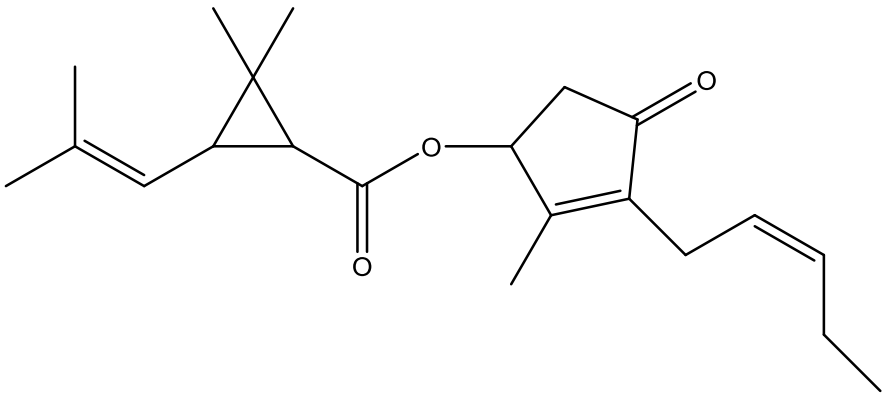
m/z	165	68	163	96	150	41	164	162
%	100	20	15	10	10	10	10	10

332 (1) – M^+ weak
286 (3) – [M-46] loss of CH_3 & CH_3O to $C_{16}H_{18}N_2O_3^+$ m/z 286.1317
221 (5) – [M-111] loss of $(C_2H_5)_2(CH_3)C.CN$ to $C_{11}H_{11}NO_4^+$ m/z 221.0688
165 (100) – [M-167] $(CH_3O)_2C_6H_3.CO^+$ $C_9H_9O3^+$ m/z 165.0552
96 (10) – [M-236] $(C_3HNO)CHCH3^+$ $C_5H_6NO^+$ m/z 96.0449
68 (20) – [M-264] $(C_3HNO)H^+$ $C_3H_2NO^+$ m/z 68.0136

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C82558507&Mask=200#Mass-Spec which also exhibits an m/z 165 base peak, but the other ions reported here are much weaker or absent.

Jasmolin I (a pyrethrin) $C_{21}H_{30}O_3$ **M:330(1%)**

Theoretical molecular ion: m/z 330.2195 (100%), 331.22285 (23%)
Average MW: 330.47



(Z)-(S)-jasmolone (1R)-*trans*-chrysanthemate

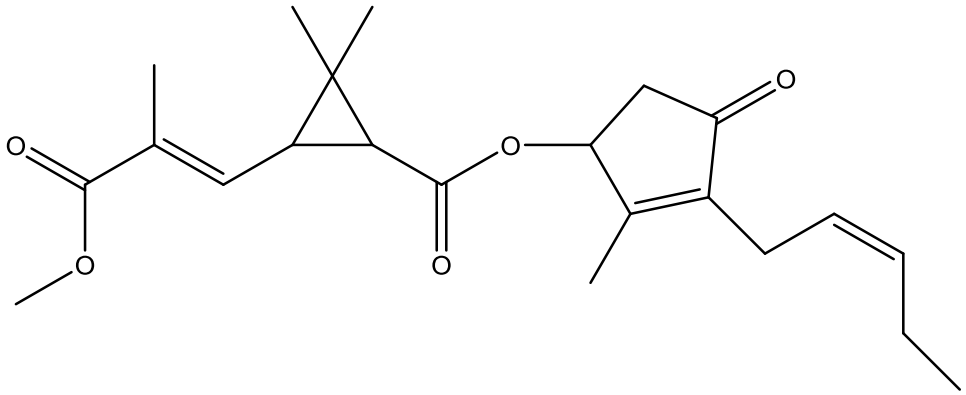
A natural pyrethrin insecticide (see also cinerin I and II and pyrethrin I and II).

m/z	123	164	81	93	55	41	107	135
%	100	30	20	20	20	20	15	15

330 (1) – M^+
164 (30) – [M-166] $H/C_5H_3(CH_3)(O).CH_2CH=CHCH_2CH3^+$ $C_{11}H_{16}O^+$ m/z 164.1201
123 (100) – [M-207] $(CH_3)_2C=CH.C_3H_2(CH_3)_2^+$ $C_9H_{15}^+$ m/z 123.1174
135 (15) – [M-195] $C_{10}H_{15}^+$ m/z 135.1174
107 (15) – [M-223] $C_8H_{11}^+$ m/z 107.0861

Cf. weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C4466142&Mask=200#Mass-Spec

Jasmolin II (a pyrethrin) **$C_{22}H_{30}O_5$** **M:374(1%)**
Theoretical molecular ion: m/z 374.2093 (100%), 375.2127 (24%)
Average MW: 374.48



(Z)-(S)-jasmolone (E)-(1R)-*trans*-pyrethrate

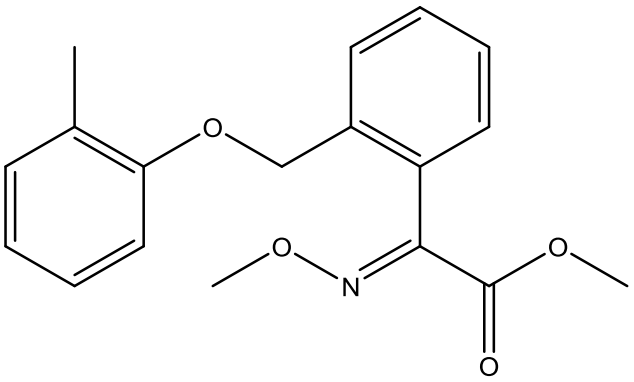
A natural pyrethrin insecticide (see also cinerin I and II and pyrethrin I and II).

m/z	163	107	135	166	121	93	55	164
%	100	85	75	70	60	55	55	50

374 (1) – M^+
212 (5) – [M-162] $CH_3OOC.(CH_3)C=CH.C_3H_2(CH_3)_2COOH^+$ $C_{11}H_{15}O_4^+$ m/z 212.1049
163 (70) – [M-211] $-C_5H_3(CH_3)(O).CH_2CH=CHCH_2CH3^+$ $C_{11}H_{15}O^+$ m/z 163.1123
135 (75) – [M-239] $C_{10}H_{15}^+$ m/z 135.1174
107 (85) – [M-267] $C_8H_{11}^+$ m/z 107.0861

Cf. rather weak, noisy NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1172630&Mask=200#Mass-Spec with no M^+ and much weaker m/z 163 and 166 and with more abundant low mass ions (m/z 29, 41, 43, 55).

Kresoxim-methyl **$C_{18}H_{19}NO_4$** **M:313(3%)**
Theoretical molecular ion: m/z 313.1314 (100%), 314.1348 (20%)
Average MW: 313.35



Methoxyiminoacetate strobilurin fungicide. Used to control scab on apples and pears and a range of other fungal diseases on a wide range of crops. Approved for use in EU.

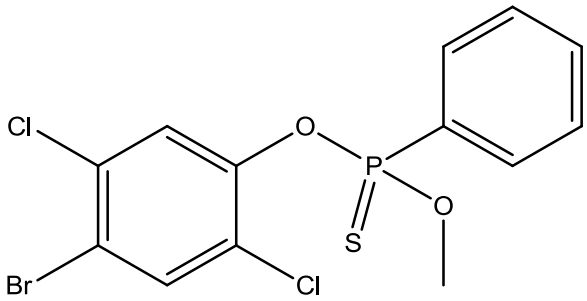
Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

m/z	116	131	206	59	132	89	117	77
%	100	55	50	20	20	15	15	15

313 (3) – M^+ weak $C_{18}H_{19}NO_4^+$
282 (3) – [M-31] loss of CH_3O to $C_{18}H_{19}NO_4^+$ m/z 282.1130
223 (2) – [M-90] loss of C_7H_6 to alcohol $C_{11}H_{13}NO_4^+$ m/z 223.0845
206 (50) – [M-107] loss of $CH_3C_6H_4O$ to $C_{11}H_{12}NO_3^+$ m/z 206.0817
131 (55) – [M-255] $CHC_6H_4CNO^+$ $C_8H_5NO^+$ m/z 131.0371
116 (100) – [M-197] $CH_2C_6H_4CN^+$ $C_8H_6N^+$ m/z 116.0500
59 (45) – [M-254] $COOCH_3^+$ $C_2H_3O_2^+$ m/z 59.0133

Data taken from NIST spectrum, http://webbook.nist.gov/cgi/cbook.cgi?ID=C143390890&Mask=200#Mass-Spec

Leptophos **$C_{13}H_{10}BrCl_2O_2PS$** **M:410,412,414(0,0,0%)**
Theoretical molecular ion: m/z 409.8700 (100%), 411.8679 (97%), 413.8650 (62%)
Average MW: 412.07



Organophosphorus phenyl phosphonothioate insecticide. No longer approved for use in EU or US.

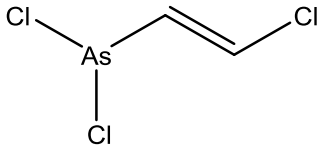
Acute oral LD50 for rat approx. 40 mg/kg (high toxicity). May cause delayed neurotoxicity.

m/z	171	377	375	77	155	109	63	124
%	100	50	40	35	25	20	20	15

410,412,414 (0,0,0) – M^+ absent
375,377,379 (40,50,15) – [M-35] loss of Cl to $C_{13}H_{10}BrClO_2PS^+$ m/z 374.9011 etc.
171 (100) – [M-239] $(C_6H_5)(CH_3O)P{=}S^+$ $C_7H_8OPS^+$ m/z 171.0034
155 (25) – [M-255] $(C_6H_5)(CH_3O)P{=}O^+$ $C_7H_8O_2P^+$ m/z 155.0262 [O/S swap]
124 (15) – [M-286] $C_6H_5PO^+$ $C_6H_5OP^+$ m/z 124.0078
109 (20) – [M-301] $C_6H_5PH^+$ $C_6H_6P^+$ m/z 109.0207
77 (35) – [M-333] $C_6H_5^+$ m/z 77.0391
63 (20) – [M-347] PS^+ m/z 62.9458 or PO_2^+ m/z

Cf. NIST http://webbook.nist.gov/cgi/cbook.cgi?ID=C21609905&Mask=200 with some differences: molecular ion observed (approx. 5%), and m/z 155 weaker (<2%).

Lewisite **$C_2H_2AsCl_3$** **M:206,208,210(75,70,30%)**
Theoretical molecular ion: m/z 205.8438 (100%), 207.8409 (96%), 209.8379 (31%),
Average MW: 207.31



Lewisite, 2-chlorovinyldichloroarsine

Organoarsenic chemical warfare agent. Synthesised in 1904, it is named for Winford Lee Lewis, American soldier and chemist.

Acute oral LD50 for rat approx. 50 mg/kg (high toxicity). Vesicant (blistering agent) and lung irritant. The technical (impure) material has a scent of geraniums (the pure material is odourless).

British anti-Lewisite (BAL) or dimercaprol ($HSCH_2.CH(SH).CH_2OH$) was developed as an antidote to Lewisite during WWII. It complexes the toxic arsenic.

m/z	145	110	206	208	147	180	182	171
%	100	90	75	70	60	40	40	35

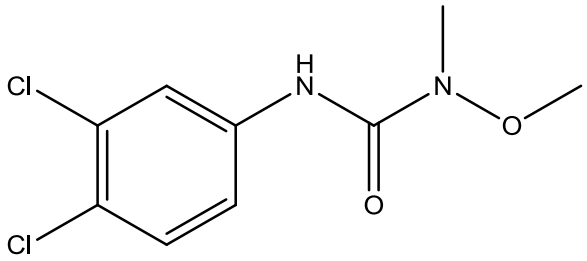
206,208,210 (75,70,30) – M^+
180,182,184 (40,40,15) – [M-26] loss of acetylene C_2H_2 to $AsCl_3^+$ m/z 179.8282 etc.
171,173,175 (35,25,5) – [M-35] loss of Cl to $C_2H_2AsCl_2^+$ m/z 170.8750 etc.
145,147,149 (100,60,10) – [M-61] loss of C_2H_2Cl to give $AsCl_2^+$ m/z 144.8593 etc.
110,112 (90,30) – [M-96] $AsCl^+$ m/z 109.8905 etc.
100 (15) – [M-106] C_2HAs^+ m/z 99.9294
75 (20) – [M-131] As^+ m/z 74.9216
61,63 (30,10) – [M-145] loss of $AsCl_2$ to $C_2H_2Cl^+$ m/z 60.9845 etc.

Data from NIST spectrum http://webbook.nist.gov/cgi/cbook.cgi?ID=C541253&Mask=200

Lindane, see HCH

Linuron $C_9H_{10}Cl_2N_2O_2$ **M:248,250(10,6%)**

Theoretical molecular ion: m/z 248.0119 (100%), 250.0090 (64%), 252.0060 (10%)
Average MW: 249.09



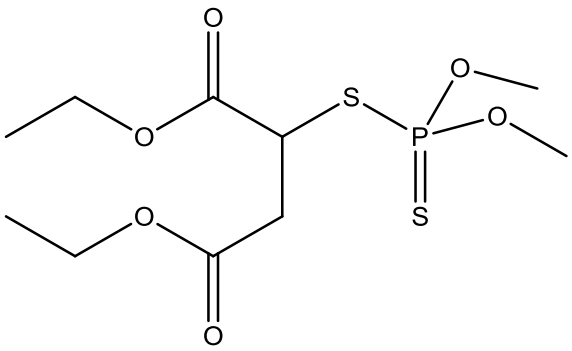
m/z	61	248	46	250	187	200	189	202
%	100	10	10	5	5	5	2	2

248,250 (10,6) – M^+
200,202 (5,2) – [M-48]
187,189 (5,2) – [M-61] dichlorophenyl isocyanate $Cl_2C_6H_3NCO^+$ $C_7H_3Cl_2NO^+$ m/z 186.9592 etc.
61 (100) – [M-187] CH_3ONCH_3+H $C_2H_7NO^+$ m/z 61.0528
46 (10) – [M-202] CH_3ONH^+ CH_4NO^+ m/z 46.0293

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C330552&Mask=200#Mass-Spec which has some differences, e.g. lacks m/z 200, 202 and exhibits m/z 160, 162.

Malathion $C_{10}H_{19}O_6PS_2$ **M:330(1%)**

Theoretical molecular ion: m/z 330.0361 (100%), 331.0394 (11%), 332.0319 (9%)
Average MW: 330.36



Organophosphorus thiophosphate insecticide and acaricide used to control a wide range of crop pests (including *Coleoptera*, *Diptera*, *Hemiptera* and *Lepidoptera*), in public health campaigns, and medically for treatment of head lice and scabies.

Acute oral LD50 for rat approx. 1,500 m/kg (moderate toxicity).

Chiral molecule.

Malathion is readily oxidised to malaoxon, which is 20-50x more toxic to mammals.

m/z	173	127	125	93	158	99	143	79
%	100	90	85	85	45	35	20	15

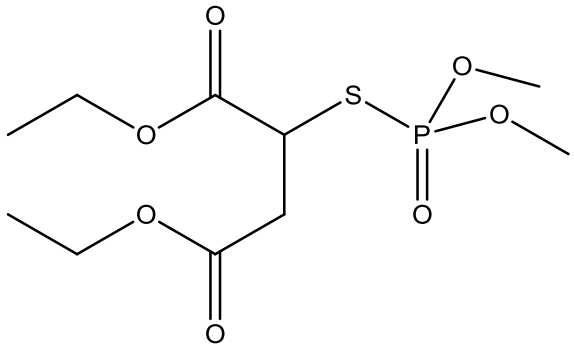
330 (0.5) – M^+ weak

285 (5) – [M-45] loss of CH_3CH_2O to $C_8H_{14}O_5PS_2^+$ m/z 285.0020
284(4) – [M-46] loss of CH_3CH_2OH to $C_8H_{13}O_5PS_2^+$ m/z 283.9942
256 (6) – [M-74] loss of CH_3CH_2OCOH to $C_7H_{13}O_4PS_2^+$ m/z 255.9993
211 (5) – [M-119] $(CH_3O)_2PS.SCH.(CH)(CO)^+$ $C_5H_8O_3PS_2^+$ m/z 210.9653
173 (100) – [M-157] $C_2H_3(COOCH_2CH_3)_2^+$ $C_8H_{13}O_4^+$ m/z 173.0814
158 (45) – [M-172] $(CH_3O)_2(HS)P{=}S^+$ $C_2H_7OPS_2^+$ m/z 157.9625
127 (90) – [M-203] $C_2H_2(COOCH_2CH_3)(CO)^+$ $C_6H_7O_3^+$ m/z 127.0395
125 (85) – [M-205] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
99 (35) – [M-231] $C_2H_2(COOH)(CO)^+$ $C_4H_3O_3^+$ m/z 99.0082
93 (85) – [M-237] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (15) – [M-251] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (10) – [M-267] PS^+ m/z 62.9458

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C121755&Mask=200#Mass-Spec with strong m/z 29 (80%).

Malathion oxon / Malaoxon $C_{10}H_{19}O_7PS$ M:314(1%)

Theoretical molecular ion: m/z 314.0589 (100%), 315.0623 (11%), 316.0547 (4.5%)
Average MW: 314.29



An oxidative metabolite of malathion with higher toxicity.

Acute oral LD50 for rat approx. 100 mg/kg (high toxicity).

Shorter GC retention time than malathion.

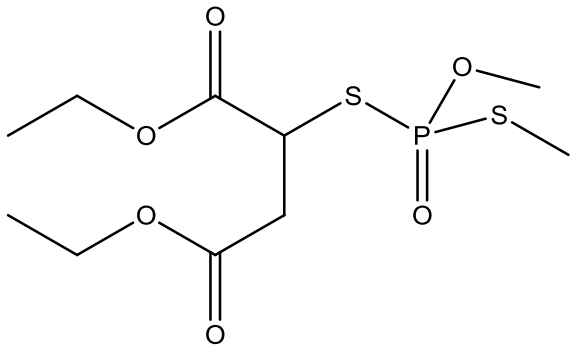
m/z	127	99	109	55	142	195	268	79
%	100	45	25	20	15	15	15	15

314 (1) – M^+ weak
268 (15) – [M-46] loss of CH_3CH_2OH to $C_8H_{13}O_6PS^+$ m/z 268.0171
240 (6) – [M-74] loss of CH_3CH_2OCOH to $C_7H_{13}O_5PS^+$ m/z 240.0221
195 (15) – [M-119] $(CH_3O)_2PO.SCH.(CH)(CO)^+$ $C_5H_8O_4PS^+$ m/z 194.9881
127 (100) – [M -187] $C_2H_2(COOCH_2CH_3)(CO)^+$ $C_6H_7O_3^+$ m/z 127.0395
125 (10) – [M-189] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (25) – [M-205] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
99 (45) – [M-215] $C_2H_2(COOH)(CO)^+$ $C_4H_3O_3^+$ m/z 99.0082
55 (20) – [M-259] $C_3H_3O^+$ m/z 55.0184

Cf. similar but weak and noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1634782&Mask=200

Malathion isomer, Isomalathion $C_{10}H_{19}O_6PS_2$ **M:330(1%)**

Theoretical molecular ion: m/z 330.0361 (100%), 331.0394 (11%), 332.0319 (9%)
Average MW: 330.36



A toxicologically significant isomer and technical contaminant of malathion

$(CH_3O)_2PS\text{-}SR \rightarrow (CH_3O)(CH_3S)PO\text{-}SR$

with approx. 20x higher mammalian toxicity. Formed on storage or heating. Levels in malathion formulations may be 1 to >3% of nominal malathion content.

Longer GC retention time than malathion.

Two chiral centres, so four stereoisomers are present with different toxicities. Diastereomeric pairs may be resolved into two GC peaks.

Acute oral LD50 for rat approx. 90 m/kg (high toxicity).

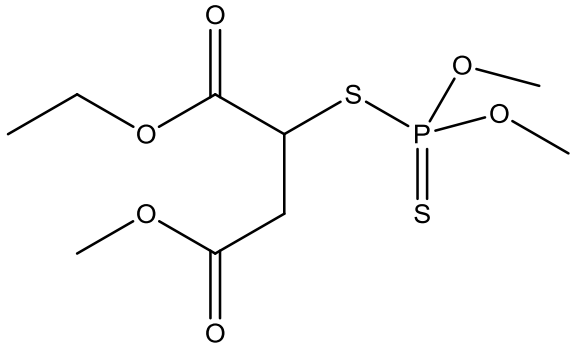
m/z	127	99	55	128	173	47	283	79
%	100	50	30	25	20	20	20	15

330 (1) – M^+
283 (20) – [M-47] loss of CH_3S to $C_9H_{16}O_6PS^+$ m/z 283.0405
209 (5) – [M-121] loss of CH_3S & CH_3CH_2OCOH to $C_6H_{10}O_4PS^+$ m/z 209.00375
181 (5) – [M-149] loss of CH_3S & CH_3CH_2OCOH & C_2H_4 to $C_4H_6O_4PS^+$ m/z 180.97245
173 (20) – [M-157] $C_2H_3(COOCH_2CH_3)_2^+$ $C_8H_{13}O_4^+$ m/z 173.0814
127 (100) – [M-203] $C_2H_2(COOCH_2CH_3)(CO)^+$ $C_6H_7O_3^+$ m/z 127.0395
99 (50) – [M-231] $C_2H_2(COOH)(CO)^+$ $C_4H_3O_3^+$ m/z 99.0082
79 (15) – [M-251] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
55 (30) – [M-255] $C_3H_3O^+$ m/z 55.0184
47 (20) – [M-283] PO^+ m/z 46.9687 (and/or CH_3S^+ m/z 46.9955)

No NIST spectrum available.

Malathion "mixed ester" I **$C_9H_{17}O_6PS_2$** **M:316(1%)**

Theoretical molecular ion: m/z 316.0204 (100%), 317.0238 (10%), 318.0162 (9%)
Average MW: 316.33



Malathion mixed ester I (major, *alpha*-ethyl/*beta*-methyl succinate isomer)

Malathion "mixed ester" compounds are found as contaminants of technical malathion, following transesterification of the one of the two succinate ethyl ester groups with methanol (Wilkins 1987).

Malathion Mixed Ester I is the major, *beta*-methyl substituted isomer, with shorter RT than II. The transesterification is catalysed by acidic conditions, and occurs most rapidly at the less sterically hindered beta position.

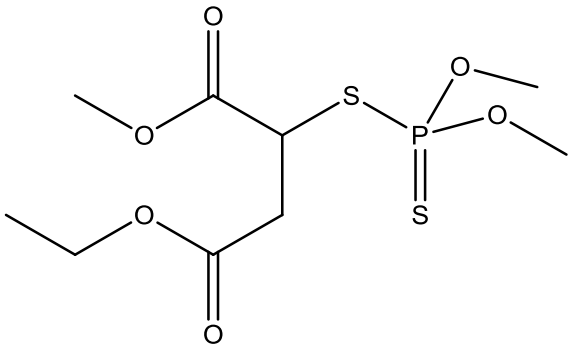
The mass spectra of the mixed ester isomers are rather similar, but a minor difference is evident in the relative abundance of the minor m/z 270 and 271 ions:
- in Malathion Mixed Ester I the m/z 270 ion is more abundant.
- In Malathion Mixed Ester II the m/z 271 ion is more abundant

The isomer with both ethyl groups replaced by methyl groups may also be detected (empirical formula $C_8H_{15}O_6PS_2$ and molecular weight 316, see ref. above).

m/z	159	125	93	113	158	127	99	143
%	100	90	80	55	55	35	20	20

316 (1)
284,285 (2,2) – [M-32/31] loss of CH_3OH/CH3O) to $C_8H_{13}O_5PS_2^+$ m/z 283.9942 etc.
270,271 (6,3) – [M-46/45] loss of C_2H_5OH/ C2H5O to $C_7H_{11}O_5PS_2^+$ m/z 269.9786 etc.
242 (10) – [M-74]
211(6) ()– [M-105]
159 (100) – [M-
125 (90) – [M-
93 (80) – [M-

Malathion "mixed ester" II **$C_9H_{17}O_6PS_2$** **M:316(1%)**
Theoretical molecular ion: m/z
Average MW:



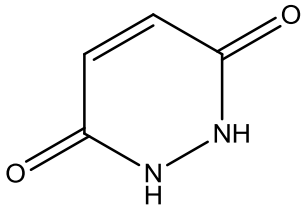
Malathion mixed ester II (minor, *alpha*-methyl/*beta*-ethyl succinate isomer)

Slightly longer GC RT than mixed ester I

m/z	159	125	93	113	158	127	99	143
%	100	90	80	55	55	35	20	20

316(1)
284,285 (2,2) – [M-
270,271 (3,6) – [M-
256(6) – [M-
211(6) – [M-
159 (100) – [M-
125 (90) – [M-
93 (80) – [M-

Maleic hydrazide **$C_4H_4N_2O_2$** **M:112(100%)**
Theoretical molecular ion: m/z : 112.0273 (100%), 113.0306 (4.3%)
Average MW: 112.09



Plant growth regulator. Used to suppress grass growth on lawns and to induce dormancy in citrus fruit.

Not directly amenable to GC analysis but may be determined by LCMS (EURL 2015).

m/z	112	82	55	26	54	27	29	41
%	100	80	40	25	25	20	20	10

112 (100) – M^+
82 (80) – [M-30] loss of diazene N_2H_2 to $C_4H_2O_2^+$ m/z 82.0055

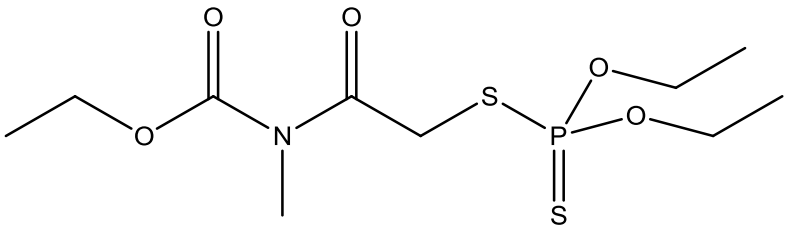
Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C123331&Mask=200#Mass-Spec

Mancozeb, see Dithiocarbamates

Maneb, see Dithiocarbamates

Mecarbam $C_{10}H_{20}NO_5PS_2$ **M:329(35%)**

Theoretical molecular ion: m/z 329.0521 (100%), 330.0554 (11%), 331.0478 (9.0%)
Average MW: 329.37



Organophosphorus insecticide and acaricide. Used to control aphids, whiteflies, scale insects, mites, mealybugs and other bugs.

Acute oral LD50 for rat is approx. 36 mg/kg (high toxicity).

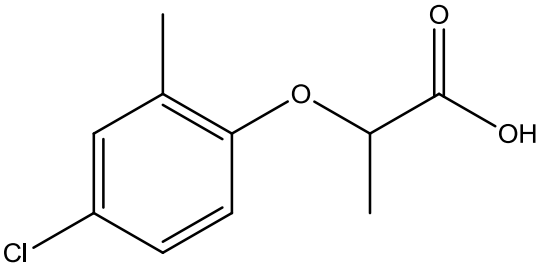
m/z	131	159	97	160	125	329	116	121
%	100	70	60	50	45	35	35	35

329 (35) – M^+
296 (15) – [M-33] loss of SH to $C_{10}H_{19}NO_5PS^+$ m/z 296.0722
227 (15) – [M-102] loss $CH_3CH_2OCON(CH_3)$ to $C_6H_{12}O_3PS_2^+$ m/z 226.9966
160 (50) – [M-169] $CH_3CH_2O.CON(CH_3)CO.CH_2O^+$ $C_6H_{10}NO_4^+$ m/z 160.0610 [O/S swap]
159 (70) – [M-168] $CH_3CH_2O.CON(CH_3)CO.CHO^+$ $C_6H_9NO_4^+$ m/z 159.0532 [O/S swap]
153 (30) – [M-174] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.1039
131 (100) – [M-198] $CH_3CH_2O.CO.N(CH_3)COH^+$ $C_5H_9NO_3^+$ m/z 131.0582
125 (45) – [M-204] $(CH_3CH_2O)(HO)PS_2^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121 (35) – [M-208] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
116 (35) – [M-213] $HO.CON(CH_3)CO.CH_2^+$ $C_4H_6NO_3^+$ m/z 116.0348
97 (60) – [M-232] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
93 (30) – [M-236] $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105
65 (30) – [M-] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2595542&Mask=200 which has less abundant m/z 159 and 121, and more abundant low mass ions e.g. m/z 65 and 58.

Mecoprop acid $C_{10}H_{11}ClO_3$ **M:214,216(65,20%)**

Theoretical molecular ion: m/z 214.0397 (100%), 216.0367 (32%)
Average MW: 214.65



Phenoxypropionic Herbicide. Used post-emergence for control of broad-leaved weeds. Approved for use in EU.

Acute oral LD50 for rat approx. 1,000 mg/kg (moderate toxicity)

Chiral molecule. The (R)-isomer is most active herbicidally ("mecoprop-P").

Poor transmission on GC unless derivatised.

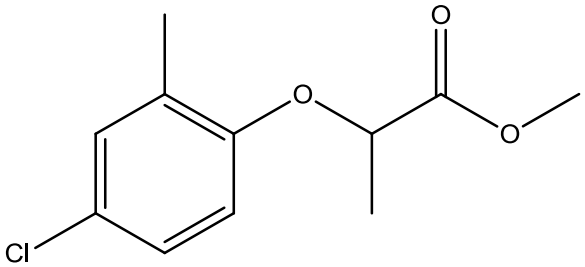
m/z	142	214	107	141	169	144	77	216
%	100	65	50	35	35	35	25	20

214,216 (65,20) – M^+
142,144 (100,35) – [M-72] loss of C_2H_3COOH to phenol $(Cl)(CH_3)C_6H_3OH^+$ $C_7H_7ClO^+$ m/z 142.0185 etc.
107 (50) – [M-107] $(CH_3)C_6H_3OH^+$ $C_7H_7O^+$ m/z 107.0497

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C93652&Mask=200#Mass-Spec though noisy and weaker M^+

Mecoprop-methyl **$C_{11}H_{13}ClO_3$** **M:228,230(90,30%)**

Theoretical molecular ion: m/z 228.0553 (100%), 230.0524 (32%)
Average MW: 228.67



Methyl ester of Mecoprop acid.

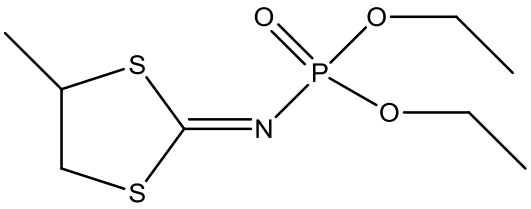
m/z	142	169	228	107	144	171	230	141
%	100	95	90	45	35	30	30	25

228,230 (90,30) – M^+
169,171 (95,30) – [M-59] loss of COOCH3 to $C_9H_{10}ClO^+$ m/z 169.0420 etc.
142,144 (100,35) – [M-114] loss of $C_2H_3COOCH_3$ to phenol $Cl(CH_3)C_6H_3OH^+$ $C_7H_7ClO^+$ m/z 142.0185 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C23844566&Mask=200#Mass-Spec though lacks low intensity ions at higher mass (> m/z 150)

Mephosfolan $C_8H_{16}NO_3PS_2$ **M:269(10%)**

Theoretical molecular ion: m/z 269.0309 (100%), 271.0267 (9.0%), 270.0343 (8.7%)
Average MW: 269.32



Organophosphorus (phosphoramidate) insecticide used to control many Lepidopterous species and other pests, especially in aquatic situations.

Acute oral LD50 for rat approx. 10 mg/kg (high toxicity).

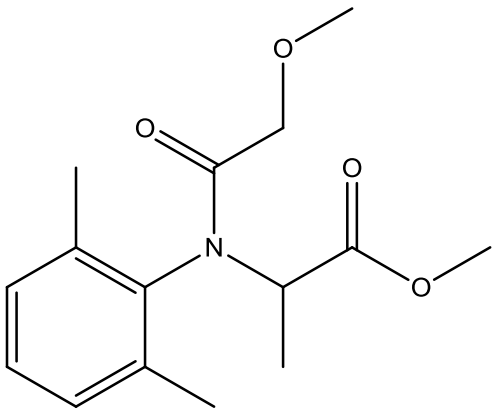
m/z	196	140	106	74	41	168	227	81
%	100	95	90	90	70	60	45	35

269 (10) – M^+
227 (45) – [M-42] loss of C_3H_6 to $S_2CN\text{-}PO(OCH_2CH_3)_2^+$ $C_5H_{10}O_3PNS_2^+$ m/z 226.9840
196 (100) – [M-73] loss of C_3H_5S to $SCN\text{-}P(OH)(OCH_2CH_3)_2^+$ $C_5H_{11}NO_3PS^+$ m/z 196.0197
168 (60) – [M-101] loss of $C_3H_5S+C_2H_4$ to $SCN\text{-}P(OH)_2(OCH_2CH_3)^+$ $C_3H_7NO_3PS^+$ m/z 167.9884
140 (95) – [M-129] loss of $C_3H_5S+2C_2H_4$ to $SCN\text{-}P(OH)_3^+$ $CH_3NO_3PS^+$ m/z 139.9571
106 (90) – [M-163] $SCN\text{-}P(OH)^+$ m/z 105.9517
81 (35) – [M-188] $(HO)_2PO^+$ $H_2O_3P^+$ m/z 80.9742
74 (90) – [M-195] $C_3H_6S^+$ m/z 74.0190
41 (70) – [M-228] $C_3H_5^+$ m/z 41.0391

No NIST spectrum available.

Metalaxyl $C_{15}H_{21}NO_4$ **M:279(10%)**

Theoretical molecular ion: m/z 279.1471 (100%), 280.1504 (16%)
Average MW: 279.33



Fungicide. Used to control diseases caused by air- and soil-borne Peronosporales. Approved for use in EU.

Acute oral LD50 for rat approx. 600 mg/kg (moderate toxicity).

Chiral molecule. The more active (-)-isomer is sold as metalaxyl-M.

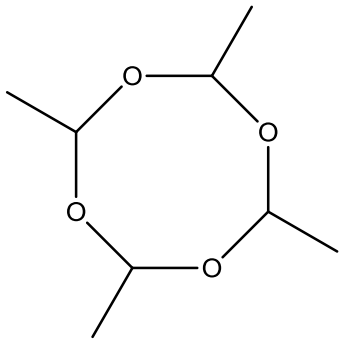
m/z	45	206	192	220	249	234	146	160
%	100	35	25	20	20	15	15	15

279 (10) – M^+ $C_{15}H_{21}NO_4^+$
249 (20) – [M-30] loss of CH_2O to $C_{14}H_{19}NO_3^+$ m/z 249.1365
234 (15) – [M-45] loss of CH_2OCH_3 to isocyanate $C_{13}H_{16}NO_3^+$ m/z 234.1130
206 (35) – [M-73] $COCH_2OCH_3$ to $C_{12}H_{16}NO_2^+$ m/z 206.1181
45 (100) – [M-234] $CH_2OCH_3^+$ $C_2H_5O^+$ m/z 45.0340

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C57837191&Mask=200#Mass-Spec

Metaldehyde **$C_8H_{16}O_4$** **M:176(0%)**

Theoretical molecular ion: m/z 176.1049 (100%), 177.1082 (8.7%)
Average MW: 176.21



Molluscicide. Used in baits to control slugs and snails. Approved for use in EU.

Acute oral LD50 for rat approx. 250 mg/kg (moderate toxicity).

Not amenable to GC analysis (decomposes to acetaldehyde).

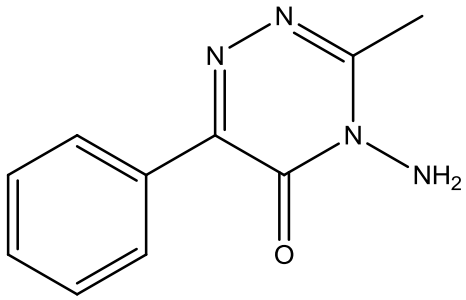
m/z	29	44	43	45	42	26	89	27
%	100	85	55	45	15	10	10	5

176 (0) – M^+ absent $C_8H_{16}O_4^+$
131 (1) – [M-45] loss of CH_3CHOH to $C_6H_{11}O_3^+$ m/z 131.0708
117 (2) – [M-57] C_2HO_2 or C_3H_5O or C_4H_9 – all require rearrangement
89 (10) – [M-85] $C_4H_9O_2^+$ m/z 89.0603
44 (85) – [M-130] acetaldehyde CH_3CHO^+ $C_2H_4O^+$ m/z 44.0262
29 (100) – [M-145] $C_2H_5^+$ m/z 29.0391

Cf. very different (over-enhanced ?) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C108623&Mask=200#Mass-Spec (filed under "Acetaldehyde tetramer") with base peak at m/z 45.

Metamitron **$C_{10}H_{10}N_4O$** **M:202(60%)**

Theoretical molecular ion: m/z 202.0855 (100%), 203.0888 (11%)
Average MW: 202.21



Triazinone herbicide. Used to control grass and broad-leaved weeds in beet crops. Approved for use in EU.

Acute oral LD50 for rat approx. >1,000 mg/kg (moderate toxicity).

Poor GC transmission.

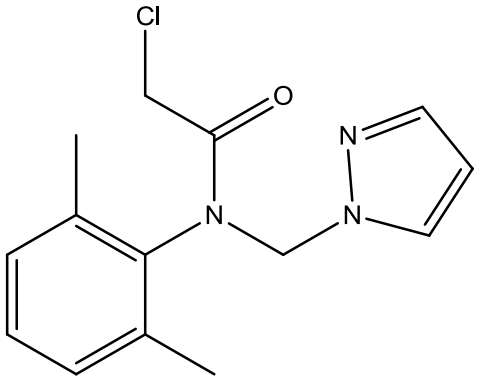
m/z	104	42	202	77	30	174	63	89
%	100	65	60	40	40	35	25	90

202 (60) – M^+
174 (35) – [M-28] loss of CO to $C_9H_{10}N_4^+$ m/z 174.09055 and/or loss of N_2 to $C_{10}H_{10}N_2O^+$ m/z 174.0793
104 (100) – [M-98] $C_6H_5CNH^+$ $C_7H_6N^+$ m/z 104.0500
77 (40) – [M-125] $C_6H_5^+$ m/z 77.0391
42 (65) – [M-260] NCO^+ CNO^+ m/z 41.9980

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C41394052&Mask=200#Mass-Spec

Metazachlor **$C_{14}H_{16}ClN_3O$** **M:277,279(15,5%)**

Theoretical molecular ion: m/z 277.0982 (100%), 279.0952 (32%)
Average MW: 277.75



Herbicide. Used to control a wide range of cereal foliar diseases. Approved for use in EU.

Acute oral LD50 for rat approx. 3,000 mg/kg (low toxicity).

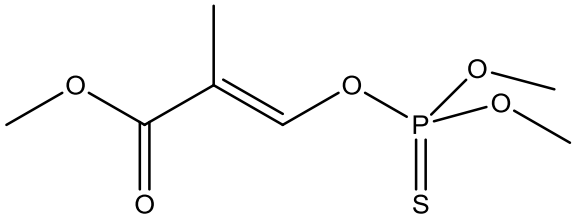
m/z	81	133	209	132	134	211	117	277
%	100	90	75	65	45	25	15	15

277,279 (15,5) – M^+

228 (10) – [M-49] loss of CH_2Cl to $C_{14}H_{16}ClN_3O^+$
209,211 (75,25) – [M-68] loss of ($C_3H_3N_2$+H) to $C_{14}H_{16}ClN_3O^+$
133 (90) – [M-144] $(CH_3)_2C_6H_3\text{-}NCH_2^+$ $C_9H_{11}N^+$ m/z 133.08915
81 (100) – [M-196] $C_3H_3N_2\text{-}CH_2^+$ $C_4H_5N_2^+$ m/z 81.0453

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C67129082&Mask=200#Mass-Spec though M^+ weaker.

Methacrifos **$C_7H_{13}O_5PS$** **M:240(55%)**
Theoretical molecular ion: m/z 240.0221 (100%), 241.0255 (7.6%), 242.0179 (4.5%)
Average MW: 240.21



Organophosphorus (thiophosphate) insecticide and acaricide. Broad spectrum activity used to control grain pests in storage. No longer approved for use in EU.

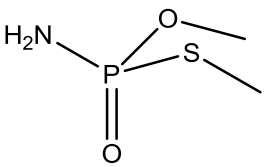
Acute oral LD50 for rat approx. 700 mg/kg (moderate toxicity).

m/z	125	180	93	208	240	110	79	209
%	100	60	60	55	55	35	30	20

240 (55) – M^+
208 (55) – [M-32] loss of CH_3OH to $C_6H_9O_4PS^+$ m/z 207.9959
180 (60) – [M-60] loss of $C_2H_4O_2$ to $C_5H_9O_4PS^+$ m/z 180.0010
131 (15) – [M-109] loss of $(CH_3O)_2PO$ to $C_5H_7O_2S^+$ m/z 131.0167
125 (100) – [M-115] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
110 (35) – [M-130] $(CH_3O)_2P(OH)^+$ $C_2H_7O_3P^+$ m/z 110.0133
93 (60) – [M-147] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ at m/z 93.0105
79 (30) – [M-161] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
47 (20) – [M-193] PO^+ m/z 46.9687

Cf. Similar spectrum at NIST MS http://webbook.nist.gov/cgi/cbook.cgi?ID=C62610779&Mask=200

Methamidophos **$C_2H_8NO_2PS$** **M:141(40%)**
Theoretical molecular ion: m/z 141.0013 (100.0%), 142.0047 (2.2%), 142.9971 (4.5%)
Average MW: 141.13



Organophosphorus (phosphoramidothioate) insecticide and acaricide, used to control chewing and sucking pests. Also a pesticide transformation product of acephate.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

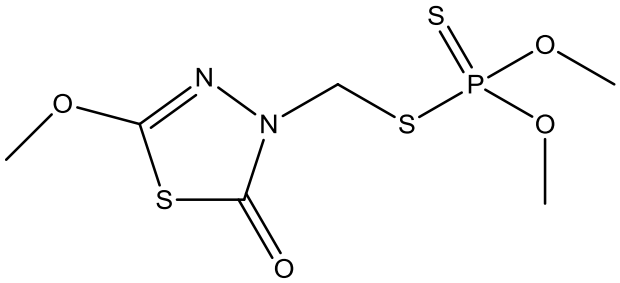
m/z	94	95	141	64	47	79	46	110
%	100	60	40	20	20	10	10	5

141 (40) – M^+
126 (5) – [M-15] loss of CH_3 to $CH_5NO_2PS^+$ m/z 125.9779
110 (5) – [M-31] loss of CH_3O to CH_5NOPS^+ m/z 109.9829
95 (60) – [M-46] loss of CH_2S to $NH_2P(OH)(OCH_3)^+$ $CH_6NO_2P^+$ m/z 95.0136
94 (100) – [M-47] loss of CH_3S to $NH_2P{=}O(OCH_3)^+$ $CH_5NO_2P^+$ m/z 94.0058
79 (10) – $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
64 (20) – [M-76] SO_2^+ m/z 63.9619
47 (20) – [M-94] PO^+ m/z 46.9687 and/or CH_3S^+ 46.9955

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C10265926&Mask=200
listed under "Phosphoramidothioic acid, O,S-dimethyl ester"

Methidathion **$C_6H_{11}N_2O_4PS_3$** **M:302(5%)**

Theoretical molecular ion: m/z 301.9619 (100%), 303.9577 (14%)
Average MW: 302.33



Organophosphorus insecticide and acaricide. Used to control a wide range of chewing and sucking pests. Not approved for use in EU.

Acute oral LD50 for rat approx. 25 mg/kg (high toxicity).

Sometimes poor GC transmission/peak shape.

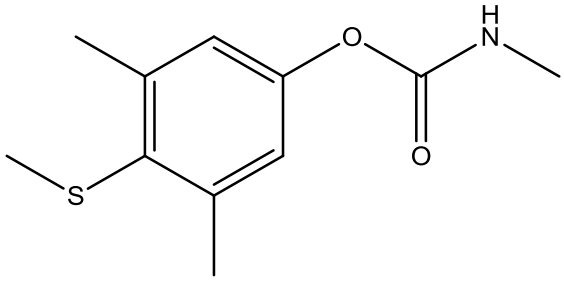
m/z	145	85	125	93	58	47	63	302
%	100	85	25	15	15	10	10	5

302 (5) – M^+
157 (5) – [M-145] $(CH_3O)_2PS_2^+$ $C_2H_6O_2PS_2^+$ m/z 156.9547
145 (100) – [M-157] $CH_2(C_2N_2OS)OCH_3^+$ $C_4H_5N_2O_2S^+$ m/z 145.0072
125 (25) – [M-177] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
93 (15) – [M-209] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
85 (85) – [M-217] loss of SCO from m/z 145 [$CH_2(C_2N_2OS)OCH_3^+$] to $C_3H_5N_2O^+$ m/z 85.0402
63 (10) – [M-239] PS^+ m/z 62.9458
58 (15) – [M-244[$HN{=}C{-}OCH_3^+$ $C_2H_4NO^+$ m/z 58.0293
47 (10) – [M-255] PO^+ m/z 46.9687 and/or CH_3S^+ m/z 46.9956

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C950378&Mask=200#Mass-Spec
but listed with incorrect empirical formula and molecular weight – "$C_6H_{11}N_2O_3PS_2$, 254.257")

Methiocarb $C_{11}H_{15}NO_2S$ **M:225(10%)**

Theoretical molecular ion: m/z 225.0823 (100%), 226.0857 (12%), 227.0781 (4.5%)
Average MW: 225.31



Carbamate molluscicide and insecticide for control of slugs, snails and many other pests. Also used as a pheasant repellent. Approved for use in EU.

Acute oral LD50 for rat approx. 20 mg/kg (high toxicity).

N.B. Sulphoxide and sulphone oxidative metabolites are included in MRLs.
May degrade to 3,5-dimethyl(4-methylthio)phenol ($C_9H_{12}OS$, mw 168).

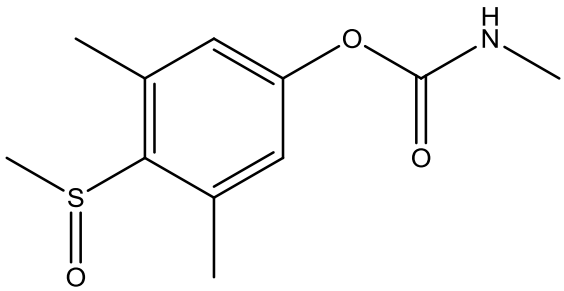
m/z	168	153	109	45	57	91	225	77
%	100	60	25	20	15	15	10	5

225 (10) – M^+
168 (100) – [M-57] loss of CH_3NCO to phenol $C_9H_{12}OS^+$ m/z 168.0609
153 (60) – [M-72] loss of CH_3NCO & CH_3 to $C_8H_9OS^+$ m/z 153.0374
109 (25) – [M-116] $(CH_3)(C_6H_3)OH^+$ $C_7H_7O^+$ m/z
45 (20) – [M-180]

Cf. similar (weak) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2032657&Mask=200#Mass-Spec

Methiocarb sulphoxide $C_{11}H_{15}NO_3S$ **M:241(10%)**

Theoretical molecular ion: m/z 241.0773 (100.0%), 242.0806 (11.9%), 243.0731 (4.5%)
Average MW: 241.31



Prone to decomposition on GC (to phenol, by loss of methyl isocyanate).

The appearance of the spectrum of methiocarb sulphoxide may be modified by reduction of some or all of it to methiocarb (i.e. sulphide) in the MS ion source, giving rise to apparently "mixed" sulphoxide/sulphide spectra.

Compare the data obtained using two different MS systems (both using GC introduction):
(A) a VG 7070 MS, which exhibits mainly sulphoxide ions, and

(B) a JEOL DX-300 MS, which exhibits mixed sulphoxide/sulphide ions.

A)	m/z	169	107	184	108	57	168	123	153
	%	100	80	75	55	35	30	20	20

241 (10) – M^+
184 (75) – [M-57] loss of CH_3NCO to phenol $C_9H_{12}O_2S^+$ m/z 184.0558
169 (100) – [M-72] loss of CH_3NCO & CH_3 to $C_8H_9O_2S^+$ m/z 169.0323
N.B. m/z 57 and 56 distinguishes from phenol degradation product

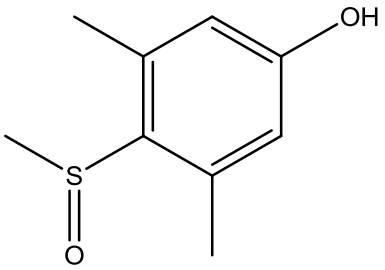
B)	m/z	168	153	109	169	107	57	184	91
	%	100	65	45	35	30	25	20	20

241 (3) – M^+
225 (5) – [M-16] molecular ion of methiocarb sulphide (reduction product)

Cf. NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2635101&Mask=200#Mass-Spec (listed as "Mesurol sulfoxide"), which displays mainly the expected sulphoxide ions:

m/z	169	107	184	168	108	153	184	241
%	100	70	50	50	35	35	20	20

Methiocarb sulphoxide related **$C_9H_{12}O_2S$** **M:184(85%)**
3,5-dimethyl(4-methylsulphinyl)phenol
Theoretical molecular ion: m/z 184.0558 (100.0%), 185.0592 (9.7%), 186.0516 (4.5%)
Average MW: 184.26



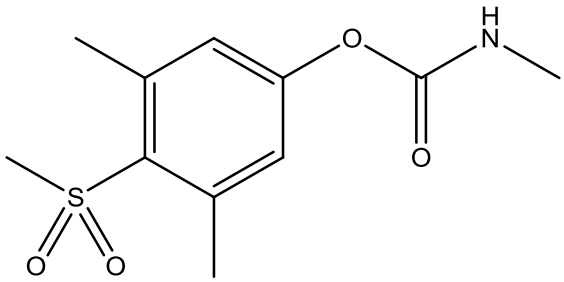
Phenolic GC degradation product (loss of methyl isocyanate).

m/z	169	107	184	108	168	153	123	79
%	100	95	85	70	40	25	20	20

Assignments confirmed by accurate mass study (GCT Cardiff)
184 (75) – M^+ $C_9H_{12}O_2S^+$ m/z 184.0558
169 (100) – [M-15] loss of CH_3 to $C_8H_9O_2S^+$ m/z 169.0323
168 (40) – [M-16] loss of O to $C_9H_{12}OS^+$ m/z 168.0609
153 (25) – [M-31] loss of CH_3 & O to $C_8H_9OS^+$ m/z 153.0374
123 (20) – [M-61] $C_7H_7S^+$ m/z 123.0269
107 (95) – [M-77] $C_7H_7O^+$ m/z 107.0497
79 (20) – [M-105] $C_6H_7^+$ m/z 79.0548

Methiocarb sulphone **$C_{11}H_{15}NO_4S$** **M:257(0%)**

Theoretical molecular ion: m/z 257.0722 (100%), 258.0755 (12%), 259.0680 (4.5%)
Average MW: 257.31



Susceptible to GC degradation to phenol (see below).

m/z	121	200	57	137	185	91	56	77
%	100	80	75	45	40	30	25	20

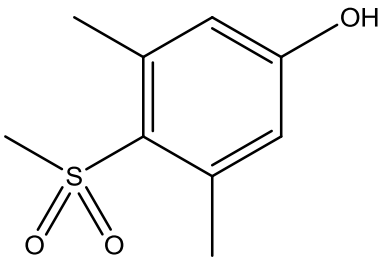
257 (0) – M^+ absent
200 (80) – [M-57] loss of CH_3NCO to phenol $C_9H_{12}O_3S^+$ m/z 200.0507
185 (40) – [M-72] loss of CH_3NCO & CH_3 to $C_8H_9O_3S^+$ m/z 185.0272
137 (45) – [M-120] loss of CH_3NCO & CH_3 & SO to $C_8H_9O_2^+$ m/z 137.0603
121 (100) – [M-136] loss of CH_3NCO & CH_3 & SO_2 to $C_8H_9O^+$ m/z 121.0653
57 (75) – [M-200] CH_3NCO^+ $C_2H_3NO^+$ m/z 57.0215

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2179251&Units=CAL&Mask=200#Mass-Spec which also exhibits a weak M^+ at m/z 257 (1%).

Methiocarb sulphone related **$C_9H_{12}O_3S$** **M:200(90%)**

3,5-dimethyl(4-methylsulphonyl)phenol

Theoretical molecular ion: m/z 200.0507 (100%), 201.0541 (9.7%), 202.0465 (4.5%)
Average MW: 200.25



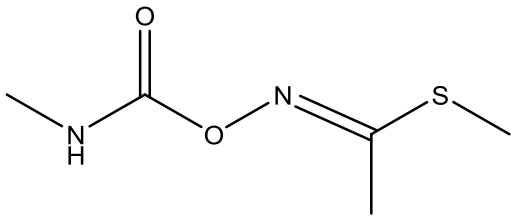
Phenolic GC degradation product (loss of methyl isocyanate).

m/z	121	200	185	137	91	77	39	65
%	100	90	60	55	35	25	10	10

200 (90) – M^+
185 (60) – [M-15] loss of CH_3
137 (55) – [M-63] loss of CH_3SO to $C_8H_9O_2^+$ m/z 137.0603
121 (100) – [M-79] loss of CH_3SO_2 to $C_8H_9O^+$ m/z 121.0653

No NIST spectrum available

Methomyl **$C_5H_{10}N_2O_2S$** **M:162(1%)**
Theoretical molecular ion: m/z 162.0463 (100%), 163.0497 (5.4%), 164.0421 (4.5%)
Average MW: 162.21



Oxime carbamate insecticide. Used to control a wide range of insects including Lepidoptera, Coleoptera and Diptera.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

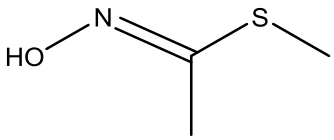
Poor transmission on GC. Degrades to **methomyl oxime** (by loss of methyl isocyanate), which, apart from the weak molecular ion (m/z 162) has a largely similar spectrum:

m/z	58	105	42	88	47	45	57	59
%	100	80	35	30	30	25	15	15

162 (1) – M^+
115 (5) – [M-47] loss of CH_3S to $C_4H_7N_2O_2^+$ m/z 115.0508
105 (80) – [M-57] loss of methylisocyanate CH_3NCO to $HONC(CH_3)SCH_3^+$ $C_3H_7NOS^+$ m/z 105.0248
88 (35) – [M-74] loss of CH_3NHCOO to $N=C(CH_3)SCH_3^+$ $C_3H_6NS^+$ m/z 88.0221
58 (100) – [M-112] CH_3NHCO^+ $C_2H_4NO^+$ m/z 58.0293
42 (35) – [M-120] NCO+ m/z 41.9980

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C16752775&Mask=200 but which has weaker m/z 42 and stronger m/z 88.

Methomyl oxime **C_3H_7NOS** **M:105(55%)**
Theoretical molecular ion: m/z 105.0248 (100%), 107.0206 (4.5%), 106.0282 (3.2%)
Average MW: 105.16



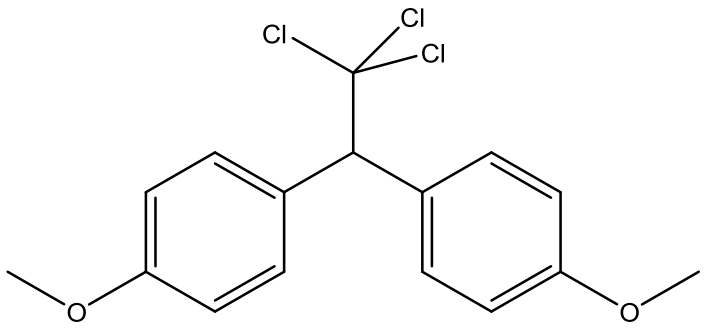
Poor GC transmission/peak shape.

m/z	58	105	47	45	42	88	31	59
%	100	55	45	45	45	35	35	20

105 (55) – M^+
88 (35) – [M-17] loss of HO to $N=C(CH_3)SCH_3^+$ $C_3H_6NS^+$ m/z 88.0221
58 (100) – [M-47] loss of SCH3 to CH_3NCOH^+ $C_2H_4NO^+$ m/z 58.0293
47 (45) – [M-58] CH_3S^+ m/z 46.99555

No NIST spectrum available.

Methoxychlor **$C_{16}H_{15}Cl_3O_2$** **M:344,346,348(5,5,2%)**
Theoretical molecular ion: m/z 344.0138 (100%), 346.0108 (64%), 348.0079 (31%)
Average MW: 345.64



Banned organochlorine insecticide.

Acute oral LD50 for rat >6,000 mg/kg (low toxicity)

m/z	227	228	114	212	152	141	344	346
%	100	20	10	5	5	5	5	5

344,346,348 (5,5,2) – M^+
227 (100) – [M-117] loss of CCl_3 to $C_{15}H_{15}O_2^+$ m/z 227.1072
analogous to dimethoxy analogue of dichloro m/z 235 ion of DDT
114 (10) – [M-230]

Cf. weak and incomplete spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C72435&Mask=200#Mass-Spec which only exhibits ions > m/z 115 and > 2% abundance.

Methyl bromide **CH_3Br** **M:94,96(100,95%)**
Theoretical molecular ion: m/z 93.9418 (100%), 95.9398 (97.5%)
Average MW: 94.94

CH_3-Br

Fumigant. Not approved for use in EU.

Acute oral LD50 for rat approx. 200 mg/kg (moderate toxicity)

Highly toxic and irritant. Very volatile (boiling point 3.5°C) so it is stored in pressurised containers. Previously widely used as a soil sterilant (before Montreal Protocol ban). Rapidly hydrolysed to methanol and hydrobromic acid.

Fumigant residues of inorganic bromide in soil and crops may be determined by several methods, e.g. GC determination of **2-bromoethanol** generated by reaction with ethylene oxide (Roughan & Wilkins 1983).

Methyl isothiocyanate **C_2H_3NS** **M:73(100%)**
Theoretical molecular ion: m/z 72.9986 (100%)
Average MW: 73.12

CH_3-N=C=S

Multipurpose soil fumigant used to control nematodes, soil insects, fungi and weed seeds. Also a pesticide transformation product. Very volatile.

Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

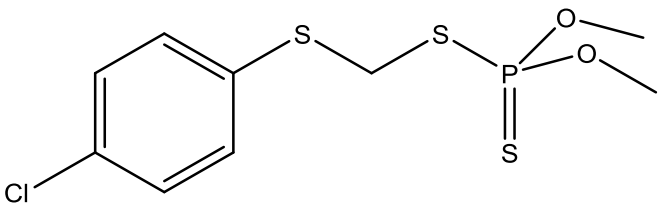
N.B. may be confused with isobaric m/z 73 ion of methylsilicones, though m/z 72 is helpful diagnostically. Acquisition at 1,500 resolution easily resolves m/z 72.9986 of $C_2H_3NS^+$ from m/z 73.04735 of $(CH_3)_3Si^+$

m/z	73	72	45	35	44	70	74	75
%	100	50	25	10	10	5	5	5

73 (100) – M^+
72 (50) – [M-1] loss of H
45 (25) – [M-28] loss of CH_2N to CHS+ m/z
35 (10) – [M-38] H_3S m/z 34.9955 (?)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C556616&Mask=200#Mass-Spec

Methyl-trithion / Methyl Carbophenothion $C_9H_{12}ClOPS_3$ **M:314,316(15,5%)**
Theoretical molecular ion: m/z 313.9426 (100%), 315.9396 (32%)
Average MW: 314.80



Organophosphorus insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 50 mg/kg (moderate toxicity).

N.B. Several oxidative metabolites (oxon, and sulphoxides and sulphones)

m/z	157	125	45	93	159	314	171	108
%	100	45	40	40	35	15	10	10

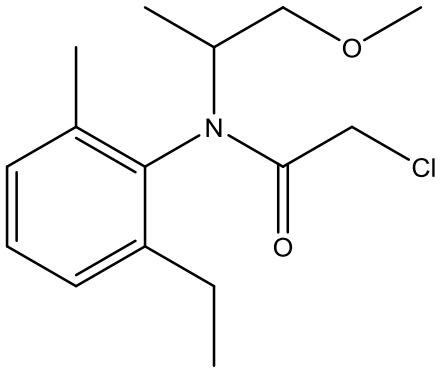
314,315 (15,5) – M^+
171 (10) – [M-143] $(CH_3O)_2PS.SCH_2^+$ $C_3H_8O_2PS_2^+$ m/z 170.9703
157,159 (100,35) – [M-157] Cl-C_6H_4-SCH_2^+ $C_7H_6ClS^+$ m/z 156.9879
125 (45) – [M-189] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
93 (40) – [M-221] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105

Cf. Weak and noisy but generally similar spectrum (apart from m/z 172 instead of m/z 171) at
http://webbook.nist.gov/cgi/cbook.cgi?ID=C953173&Mask=200#Mass-Spec

Metiram, see Dithiocarbamates

Metolachlor **$C_{15}H_{22}ClNO_2$** **M:283,285(0,0%)**

Theoretical molecular ion: m/z 283.1339 (100%), 285.1310 (32%)
Average MW: 283.80



Herbicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 1,200 mg/kg (moderate toxicity).

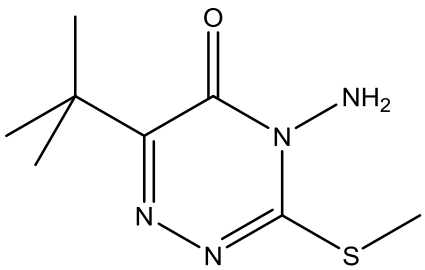
m/z	162	238	146	77	73	211	240	117
%	100	55	20	15	15	15	15	10

283,285 (0,0) – M^+ absent
238,240 (55,15) – [M-45] loss of CH_2OCH_3 to $C_{13}H_{17}ClNO^+$ m/z 238.0999 etc.
162 (100) – [M-121] loss of CH_2OCH_3 & $COCH_2Cl$ to $C_{11}H_{16}N^+$ m/z 162.1283

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C51218452&Mask=200#Mass-Spec

Metribuzin **$C_8H_{14}N_4OS$** **M:214(10%)**

Theoretical molecular ion: m/z 214.0888 (100%), 215.0922 (8.7%), 216.0846 (4.5%)
Average MW: 214.29



Herbicide. Approved for use in EU.

Acute oral LD50 for rat approx. 30 mg/kg (high toxicity).

Poor GC transmission. N.B. Sulphoxide and sulphone metabolites.

m/z	198	199	57	41	103	144	214	182

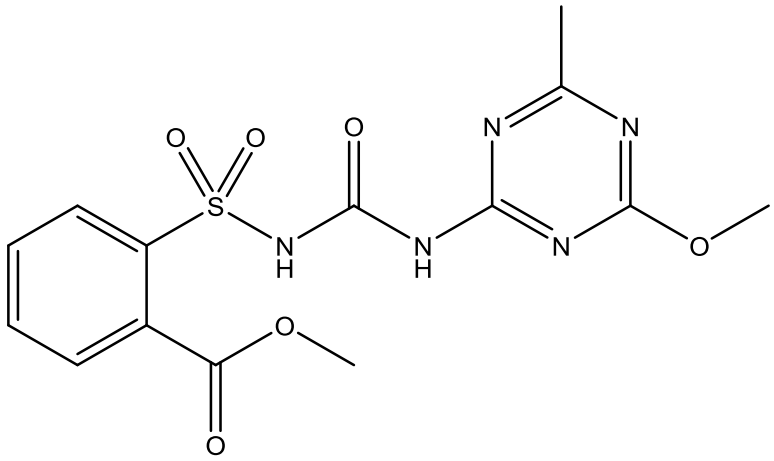
%	100	20	20	20	20	15	10	10

214 (0) – M^+ absent $C_8H_{14}N_4OS^+$ m/z
198 (100) – [M-16] uncommon loss of NH_2 to $C_8H_{14}N_4OS^+$ m/z 198.0701

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C21087649&Mask=200#Mass-Spec

Metsulfuron-methyl **$C_{14}H_{15}N_5O_6S$** **M:381(0%)**

Theoretical molecular ion: m/z 381.0743 (100%), 382.0777 (15%), 383.07010 (4.5%)
Average MW: 381.36



Sulphonylurea herbicide. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

Not amenable to GC analysis.

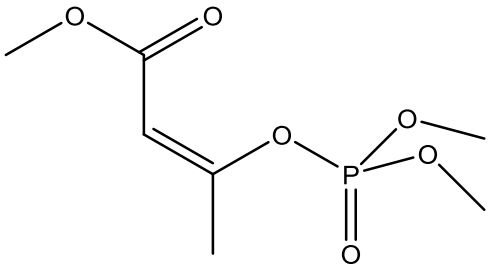
m/z	210	69	140	42	110	90	77	199
%	100	65	50	40	40	35	30	30

381 (0) – M^+
241 (15) – [M-140] loss of triazine moiety $C_5H_8N_4O$ to $C_9H_7NO_5S^+$ m/z 241.0045
210 (100) – [M-171] $C_6H_4(SO_2NCO)(CO)^+$ $C_8H_4NO_4S^+$ m/z 209.9861
140 (50) – [M-241] triazine amine $NH_2(C_3N_3)(CH_3)(OCH_3)^+$ $C_5H_8N_4O^+$ m/z
(probably not due to $C_6H_4.SO_2^+$ $C_6H_4O_2S^+$ m/z 139.9932)
110 (40) – [M-271] $C_4H_6N_4^+$ m/z 110.05925
69 (65) – [M-312] triazine ring opening to CH3.C=$NCNH_2^+$ $C_3H_5N_2^+$ m/z 69.0453 [see chlorsulfuron related i)]

Compare spectrum of **chlorsulfuron related i)** 2-amino-4-methoxy-6-methyl-1,3,5-triazine which shares several ions.

No NIST spectrum available.

Mevinphos / Phosdrin **$C_7H_{13}O_6P$** **M:224(2%)**
Theoretical molecular ion: m/z
Average MW: 224.15



Mevinphos (E)/(cis)-isomer (>60%)

Organophosphorus insecticide and acaricide. Used to used to control a broad spectrum of insects including aphids, grasshoppers, leafhoppers and caterpillars. No longer approved for use in EU.

Acute oral LD50 for rat <5 mg/kg (high toxicity).

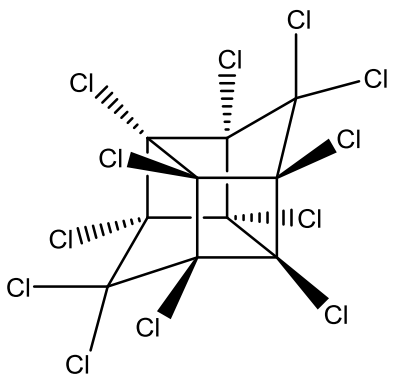
Technical mevinphos contains >60% (E)/cis (with shorter GC retention time) and ca. 20% (Z)/trans isomer, with similar mass spectra:

m/z	127	192	109	67	164	193	141	79
%	100	30	20	15	10	5	5	5

224 (2) – M^+
192 (30) – [M-32] loss of CH_3OH to $C_6H_9O_5P^+$ m/z 192.0188
164 (10) – [M-60] loss of CH_3OCOH to $C_5H_9O_4P^+$ m/z 164.0238
127 (100) – [M-97] $(CH_3O)_2(HO)_2P^+$ $C_2H_6O_4P^+$ m/z 127.0160
109 (20) – [M-115] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (5) – [M-145] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
67 (15) – [M-157] $C_4H_3O^+$ m/z 67.0184

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C7786347&Mask=200

Mirex **$C_{10}Cl_{12}$** **M:540,542,544,546(1,2,2,1%)**
Theoretical molecular ion: m/z 539.62623 (15.8%), 541.62328 (60.6%), 543.62033 (100.0%), 545.61738 (93.8%), 547.61443 (57.0%), 549.61148 (23.5%)
Average MW: 545.51



Organochlorine insecticide. Dimer of hexachlorocyclopentadiene.

Mirex is one of the "dirty dozen" Persistent Organic Pollutants (POPs).

Approximately 250,000kg was applied in the south-eastern US to control invasive “red imported fire ants” (e.g. *Solenopsis invicta*), but had several other, non-pesticide uses (e.g. fire retardant in plastics). Its persistence in the environment, tendency to bio-accumulate and toxicity to humans and marine life, resulted in its being banned in 1978 at the Stockholm Convention.

Acute oral LD50 for rat >235 mg/kg (moderate acute toxicity).

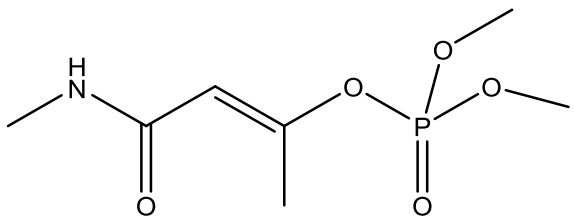
m/z	272	274	270	237	276	239	235	332
%	100	80	50	50	35	30	30	10

540,542,544,546 (1,2,2,1) – M^+
505,507,509,511,513 (0.5,1,2,2,1) – [M-35] loss of Cl to $C_{10}Cl_9^+$
400,402,404,406 (2,5,5,3) – [M-140] loss of Cl_4 to $C_{10}Cl_6^+$
330,332,334 (3,7,5,2) – [M-210] loss of Cl6 to $C_{10}Cl_4^+$
270,272,274,276,278 (50,100,80,35,10) – [M-270] $C_5Cl_6^+$
235,237,239,241 (30,50,30, 10) – [M-305] $C_5Cl_5^+$

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C2385855&Mask=200

Monocrotophos **$C_7H_{14}NO_5P$** **M:223(5%)**

Theoretical molecular ion: m/z 223.0610 (100%), 24.0643 (7.6%), 225.0652 (1.0%)
Average MW: 223.165



Organophosphorus insecticide. Used to control sucking, chewing pests and common mites, ticks and spiders, typically on cotton, citrus, olives and many other crops. No longer approved for use in EU or US.

Acute oral LD50 for rat approx. 10 mg/kg (high toxicity).

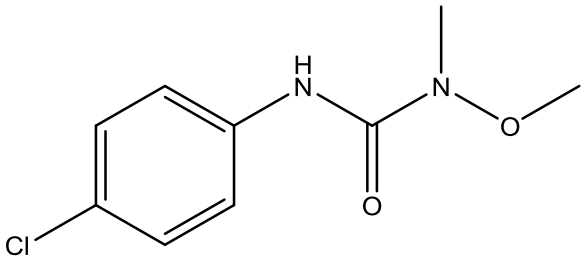
m/z	127	67	97	192	109	58	193	223
%	100	35	20	15	15	15	10	5

223 (5) – M^+
192 (15) – [M-31] loss of CH_3O to $C_6H_{11}NO_4P^+$ m/z 192.0426
127 (100) – [M-96] $(CH_3O)_2(HO)_2P^+$ $C_2H_8O_4P^+$ m/z 127.0160
109 (15) – [M-114] $(CH_3O)_2P{=}O^+$ $C_2H_6O_2P^+$ m/z 109.0055
97 (20) – [M-126] loss of (CH3O)2(HO)PO to $C_5H_7NO^+$ m/z 97.0528 (not OP ion!)
67 (35) – [M-156] $C_4H_3O^+$ m/z 67.0184
58 (15) – [M-165] CH_3NHCO^+ $C_2H_4NO^+$ m/z 58.0293

Cf. similar data at http://webbook.nist.gov/cgi/cbook.cgi?ID=C6923224&Mask=200

Monolinuron $C_9H_{11}ClN_2O_2$ **M:214,216(15,5%)**

Theoretical molecular ion: m/z 214.0509 (100%), 216.0480 (32%)
Average MW: 214.65



Herbicide. No longer approved for use in EU. (Cf. **linuron**.)

Acute oral LD50 for rat approx. 2,000 mg/kg (low toxicity).

Poor GC transmission.

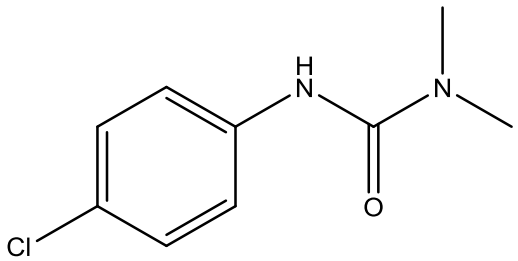
m/z	61	214	46	153	127	126	99	90
%	100	15	15	15	15	15	10	5

214 (15) – M^+
153,155 (15,5) – [M-61] isocyanate $C_7H_4ClNO^+$ m/z 152.9981
61 (100) – [M-153] CH_3ONCH_3+H $C_2H_7NO^+$ m/z 61.0528
46 (10) – [M-168] CH_3ONH^+ CH_4NO^+ m/z 46.0293

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1746812&Mask=200#Mass-Spec

Monuron $C_9H_{11}ClN_2O$ **M:198,200(50,15%)**

Theoretical molecular ion: m/z 198.0560 (100%), 200.0530 (32%)
Average MW: 198.65



Herbicide. No longer approved for use in EU. (Cf. **linuron**.)

Acute oral LD50 for rat approx. 1,000 mg/kg (low toxicity). Suspected carcinogen.

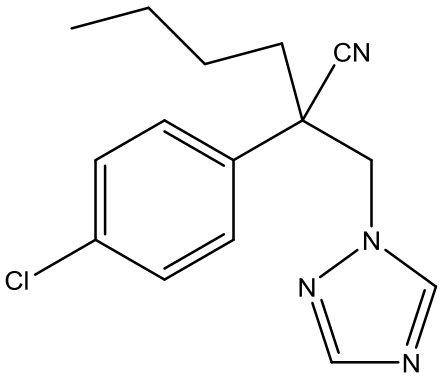
Poor GC transmission.

m/z	72	198	153	45	200	44	125	155
%	100	50	20	15	15	10	5	5

198,200 (50,15) – M+
153,155 (20,50) – [M-45] chlorophenyl isocyanate $C_7H_4ClNO^+$ m/z 152.9981 etc.
72 (100) – [M-126] dimethyl isocyanate $(CH_3)_2NCO^+$ $C_3H_6NO^+$ m/z 72.0449

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C150685&Mask=200#Mass-Spec

Myclobutanil **$C_{15}H_{17}Cl_4N$** **M:288,290(25,10%)**
Theoretical molecular ion: m/z 318.1611 (100%), 320.1582(32%)
Average MW: 318.85



Triazole fungicide. Approved for use in EU.

Acute oral LD50 for rat approx. 1,600 mg/kg (moderate toxicity).

m/z	179	82	150	181	55	206	288	152
%	100	55	45	35	35	30	25	25

288,290 (25,10) – M^+
179,181 (100,35) – [M-109] rearrangement $ClC_6H_4.(C_3H_2N_3)^+$ $C_8H_6ClN_3^+$ m/z 179.0250 etc.
82 (55) – [M-206] $C_2H_2N_3.CH_2^+$ $C_5H_4N_3^+$ m/z 82.0405

No NIST spectrum available, but very similar spectrum in Flamini (2010), page 300.

Mustard gas / Sulphur mustard **$C_4H_8Cl_2S$** **M:158,160,162(25,15,5%)**
Theoretical molecular ion: m/z 157.9724 (100%), 159.9694 (65%), 161.9665 (10%)
Average MW: 159.08

Cl-CH2CH2-S-CH2CH2-Cl
Mustard Gas, bis(2-chloroethyl) sulphide

Chemical warfare agent. Synthesised in the nineteenth century, its potential as a chemical weapon was first exploited by the German army in WWI at Ypres. It is named for its characteristic odour of mustard, garlic or horseradish when in an impure form.

Acute oral LD50 for rat approx. 10 mg/kg (high toxicity). Cytotoxic, vesicant (blistering agent) and lung irritant.

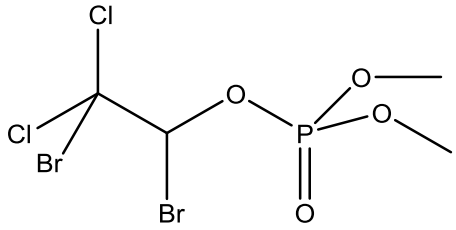
m/z	109	111	63	158	27	47	65	160
%	100	40	35	25	25	20	15	15

158,160,162 (25,15,5) – M^+
123,125 (5,2) – [M-35] loss of Cl to $C_4H_8ClS^+$ m/z 123 etc.
109,111 (100,40) – [M-49] loss of CH_2Cl to $C_3H_6ClS^+$ m/z 108.9879 etc.
63,65 (35,15) – [M-95] $CH_2CH_2Cl^+$ $C_2H_4Cl^+$ m/z 63.0002 etc.
47,49 (20,5) – [M-111] CCl^+ m/z 46.9689 etc.
27 (25) – [M-131] $C_2H_3^+$ m/z 27.0235

Data from NIST spectrum http://webbook.nist.gov/cgi/cbook.cgi?ID=C505602&Mask=200#Mass-Spec

Naled **$C_4H_7Br_2Cl_2O_4P$** **M:378,380,382(0%)**

Theoretical molecular ion: m/z 377.7826 (51%), 379.7805 (100%), 381.7776 (64%), 383.7755 (31%)
Average MW: 380.76



Organophosphorus insecticide and acaricide. Used to control aphids, mites, mosquitoes, flies and many other pests in non-food applications. Not approved for use in EU.

Acute oral LD50 for rat approx. 80 mg/kg (high toxicity).

Naled may decompose on GC (-Br_2) to produce **dichlorvos**. (Several ions in the spectrum of naled are similar to those in that of dichlorvos.)

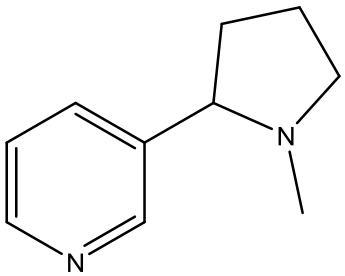
m/z	109	145	79	147	185	301	47	189
%	100	40	20	15	10	10	10	10

378,380,382 (0) – M^+ absent
299,301,303 (5,10,5) – [M-79] loss of Br to $C_4H_7BrClO_4P^+$ m/z 298.8642 etc.
220,222 (5,2) – [M-158] loss of Br_2 to dichlorvos, $C_4H_7Cl_2O_4P^+$ m/z 219.9459 etc.
185,187 (10,3) – [M-193] loss of Br2Cl to $C_4H_7ClO_4P^+$ m/z 184.9771 etc.
145,147 (40,10) – [M-233] $(CH_3O)_2(HO)PCl^+$ $C_2H_7ClO_3P^+$ m/z 144.9821 etc. [rearrangement]
109 (100) – [M-269] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (15) – [M-141] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
47 (10) – [M-173] PO^+ m/z 46.9687

Cf. similar but poor quality spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C300765&Mask=200

Nicotine **$C_{10}H_{14}N_2$** **M:162(20%)**

Theoretical molecular ion: m/z 162.1157 (100%), 163.1191 (10.8%)
Average MW: 162.24



Insecticide. No longer used.

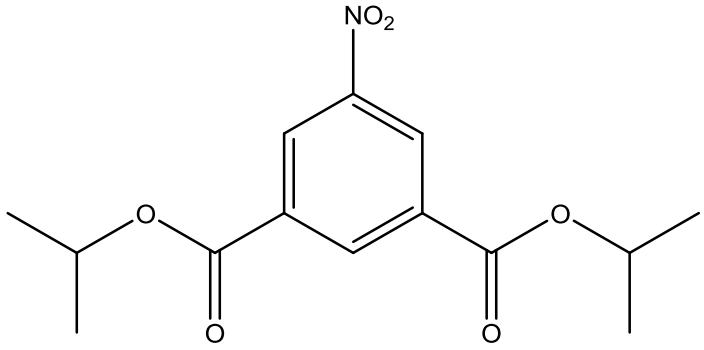
Acute oral LD50 for rat approx. 50 mg/kg (high toxicity)

m/z	84	162	133	161	85	42	-	-
%	100	20	15	10	5	5	-	-

162 (20) – M^+
133 (15) – [M-29] loss of NCH_3 to $C_5H_4N.C_4H_7^+$ $C_9H_{11}N^+$ m/z 133.0892
84 (100) – [M-78] loss of pyridine C_5H_4N moiety to $C_4H_7N(CH_3)^+$ $C_5H_{10}N^+$ m/z 84.0813

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C54115&Mask=200#Mass-Spec

Nitrothal-isopropyl **$C_{14}H_{17}NO_6$** **M:295(5%)**
Theoretical molecular ion: m/z 295.10560 (100%), 296.1089 (15%)
Average MW: 295.29



Fungicide. No longer approved for use in EU.

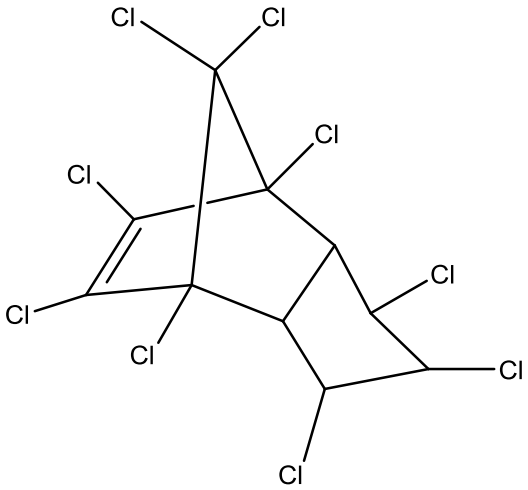
Acute oral LD50 for rat >6,000 mg/kg (low toxicity).

m/z	236	212	194	43	254	59	237	42
%	100	65	60	55	55	35	30	30

295 (5) – M^+ $C_{14}H_{17}NO_6^+$ m/z
254 (55) – [M-41] loss of C_3H_5 to $C_{11}H_{12}NO_6^+$ m/z 254.0665
236 (100) – [M-59] loss of $-OCH(CH_3)_2$ to $C_{11}H_{10}NO_5^+$ m/z 236.0559
212 (65) – [M-83] loss of C_3H_5 & C_3H_6 to $C_8H_6NO_6^+$ m/z 212.0195
194 (60) – [M-101] $HOOC.C_6H_3(NO_2)CO^+$ $C_8H_4NO_5^+$ m/z 194.0090
43 (55) – [M-252] $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C10552746&Mask=200#Mass-Spec

Nonachlor $C_{10}H_5Cl_9$ **M:440,442,444,446,448(2,5,5,3,2%)**
Theoretical molecular ion: m/z 439.7588 (27%), 441.7559 (44%), 443.7529 (100%), 445.7410 (62%), 447.7470 (30%)
Average MW: 444.20



Obsolete organochlorine insecticide related to **chlordane**.

Acute oral LD50 for rat approx. 500 mg/kg (moderate acute toxicity).

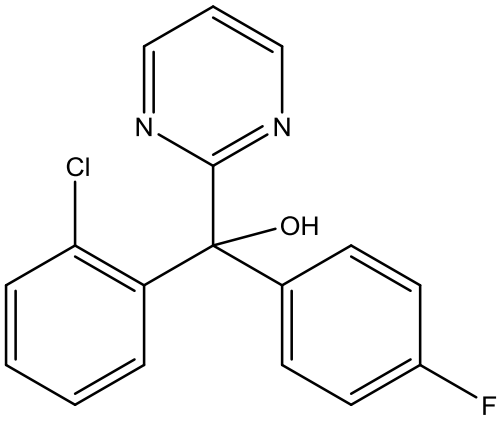
Cis- and *trans*- isomers.

m/z	409	407	411	405	413	237	272	109
%	100	90	65	35	25	20	20	20

440,442,444,446,448 (2,5,5,3,2) – M^+ weak
405,407,409,411,413 (35,90,100,65,25) – [M-35] loss of Cl to $C_{10}H_5Cl_8^+$ m/z 404.7900, 406.7870, 408.7841 etc.
270,272,274,276 (10,20,10,5) – [M-170] $C_5Cl_6^+$ m/z 269.8131, 271.8102, 273.8072 etc.
235,237,239,241 (10,20,10,5) – [M-205] $C_5Cl_5^+$ m/z 234.8443, 246.8413, 238.8384 etc.

Cf. similar NIST spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C39765805&Mask=200#Mass-Spec

Nuarimol $C_{17}H_{12}ClFN_2O$ **M:314,316(40,10%)**
Theoretical molecular ion: m/z 314.0622 (100%), 316.0593 (32%)
Average MW: 314.74



Pyrimidine fungicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 1,000 mg/kg (moderate toxicity).

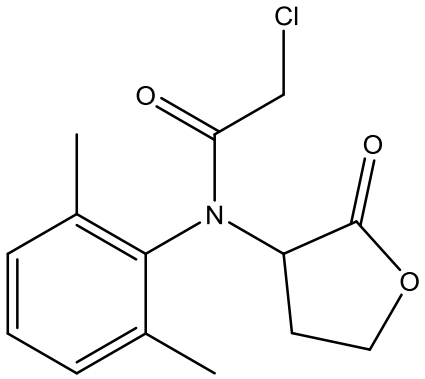
Sometimes poor GC transmission.

m/z	107	235	203	139	123	314	112	237
%	100	80	80	70	40	40	30	25

314,316 (36,12) – M+
297,299 (10,3) – [M-17] loss of OH to $C_{17}H_{11}ClFN_2^+$ m/z 297.0595 etc.
279 (10) – [M-35] loss of Cl to $C_{17}H_{12}FN_2O^+$ m/z 279.0934
235,237 (80,25) – [M-79] loss of ($C_4H_3N_2$) to $C_{13}H_9ClFO^+$ m/z 235.0326 etc.
203 (80) – [M-111] loss of C_6H_4Cl to $C_{11}H_8FN_2O^+$ m/z 203.0621
139,141 (70,25) – [M-175] $C_6H_4Cl.C{=}O^+$ $C_7H_4ClO^+$ m/z 138.9951 etc.
123 (40) – [M-191] $C_6H_4F.C{=}O^+$ $C_7H_4FO^+$ m/z 123.1064
107 (100) – [M-207] $(C_4H_3N_2)C{=}O^+$ $C_5H_3NO^+$ m/z 107.0245

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C63284719&Mask=200#Mass-Spec

Ofurace **$C_{14}H_{16}ClNO_3$** **M:281,283(50,15%)**
Theoretical molecular ion: m/z 281.0819 (100%), 283.0789 (32%)
Average MW: 281.74



Anilide fungicide. Used to control a range of diseases but mainly downy mildew and late blights. Not approved for use in EU.

Acute oral LD50 for rat approx 3,000 mg/kg (low toxicity).

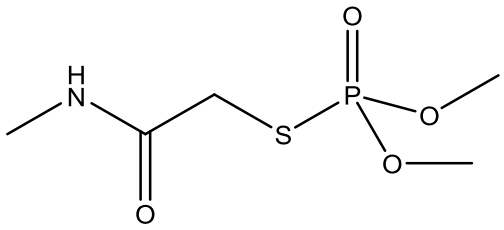
m/z	132	160	232	281	77	146	105	204
%	100	85	70	50	50	45	45	40

281,283 (50,15) – M^+
232 (70) – [M-49] loss of CH_2Cl to $C_{13}H_{14}NO_3^+$ m/z 232.0974
204 (40) – [M-77] loss of $COCH_2Cl$ to $C_{12}H_{14}NO^+$ m/z 204.1025
160 (85) – [M-121] loss of $COCH_2Cl$ & CO_2 to $C_{11}H_{14}N^+$ m/z 160.1126
132 (100) – [M-149] loss of $COCH_2Cl$ & CO_2 & C2H4 to $C_9H_{10}N^+$ m/z 32.0813

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C58810483&Mask=200#Mass-Spec

Omethoate **$C_5H_{12}NO_4PS$** **M:213(2%)**

Theoretical molecular ion: m/z 213.0225 (100%), 214.0258 (5.4%), 215.0183 (4.5%)
Average MW: 213.19



Organophosphorus insecticide. Not approved for use in EU.

Also pesticide transformation product (equivalent to **dimethoate oxon**).

Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

Sometimes poor GC transmission/peak shape.

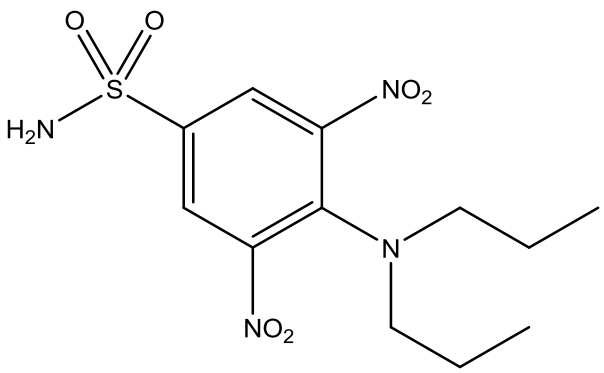
m/z	156	110	79	109	80	126	46	141
%	100	100	30	25	15	15	10	10

213 (2) – M^+ weak
156 (100) – [M-57] loss of CH_3NCO to $CH_2SP(OH)(OCH_3)_2^+$ $C_3H_9O_3PS^+$ m/z 156.0010
141 (10) – [M-72] $(CH_3O)_2P{=}O.S^+$ $C_2H_6O_3PS^+$ m/z 140.9775
126 (15) – [M-87] $(CH_3O)_2(HS)P^+$ $C_2H_7O_2PS^+$ m/z 125.9904
110 (100) – [M-103] $(CH_3O)_2(HO)P^+$ $C_2H_7O_3P^+$ m/z 110.0133 and/or
$(CH_3O)POS^+$ $CH_3O_2PS^+$ m/z 109.9591 (as isotope pattern indicates mono-sulphur)
109 (25) – [M-104] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (30) – [M-134] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
46 (10) – [M-167] CH_2S^+ m/z 45.9877

Cf. similar spectra at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1113026&Mask=200#Mass-Spec and http://www.restek.com/compound/view/1113-02-6/Omethoate

Oryzalin **$C_{12}H_{18}N_4O_6S$** **M:346(5%)**

Theoretical molecular ion: m/z 346.0947 (100%), 347.0981 (13%), 348.0905 (4.5%)
Average MW: 346.36



Dinitroaniline sulphonamide herbicide. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

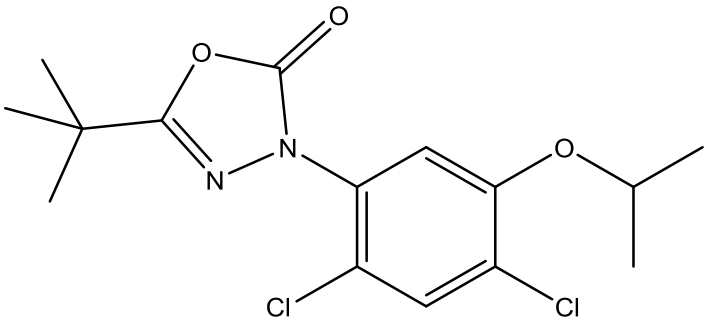
Not amenable to GC.

m/z	317	43	275	41	301	318	258	259
%	100	85	55	25	15	15	10	10

346 (5) – M^+
329 (5) – [M-17] loss of HO from nitro to $C_{10}H_{13}N_4O_6S^+$ m/z 329.0920
317 (100) – [M-29] loss of C_2H_5 to $C_{10}H_{13}N_4O_6S^+$ m/z 317.0556
301 (15) – [M-45] loss of C_2H_5 & NH_2 to $C_{10}H_{11}N_3O_6S^+$ m/z 301.0369
275 (55) – [M-71] loss of C_2H_5 & C_3H_6 to $C_7H_7N_4O_6S^+$ m/z 275.0086
258 (10) – [M-88] loss of C_2H_5 & NH_2 & C_3H_7 to $C_7H_4N_3O_6S^+$ m/z 257.9821
43 (85) – [M-303] $C_3H_7^+$ m/z 43.0890

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C19044883&Mask=200#Mass-Spec though m/z 43 weaker (15%).

Oxadiazon **$C_{15}H_{18}Cl_2N_2O_3$** **M:344,346(20,15%)**
Theoretical molecular ion: m/z 344.0695 (100%), 346.0665 (64%), 348.06355 (10.2%)
Average MW: 345.22



A pre-emergence oxadiazolone herbicide used to control bindweed and annual broad-leaved weeds. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

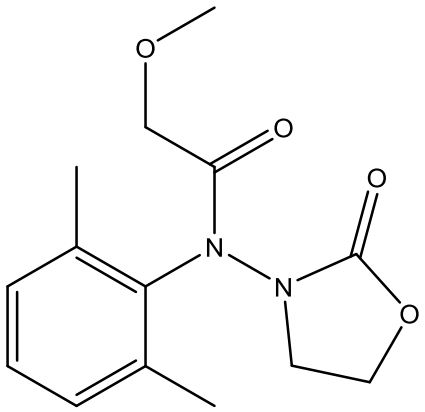
m/z	175	41	177	57	43	258	260	302
%	100	85	65	65	55	50	30	30

344,346 (20,15) – M+ $C_{15}H_{18}Cl_2N_2O_3^+$ m/z
302,304 (30,20) – [M-42] loss of C_3H_6 to $C_{12}H_{12}Cl_2N_2O_3^+$ m/z 302.0225 etc.
258,260 (50,30) – [M-86] loss of C_3H_6 & CO_2 to $C_{11}H_{12}Cl_2N_2O^+$ m/z 258.0327 etc.
175,177,179 (100,65,10) – [M-169] $Cl_2C_6H_2(N)(OH)$ C6H3Cl2NO+m/z 174.9592 etc.
41 (85) – [M-303] $C_3H_5^+$ m/z 41.0391

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C19666309&Mask=200#Mass-Spec

Oxadixyl **$C_{14}H_{18}N_2O_4$** **M:278(10%)**

Theoretical molecular ion: m/z 278.1267 (100%), 279.1300 (15%), 280.1334 (1.1%)
Average MW: 278.31



Anilide oxamyl fungicide. Used to control Peronosporales including downy mildew and late blights. No longer approved for use in EU.

Acute oral LD50 for rat approx.1,500 mg/kg (moderate toxicity).

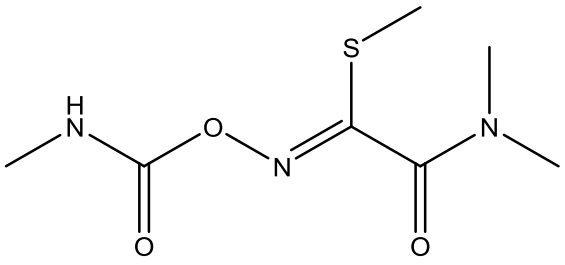
m/z	45	105	163	132	120	77	133	91
%	100	60	55	35	25	20	15	15

278 (10) – M^+ $C_{14}H_{18}N_2O_4^+$ m/z
250 (10) – [M-28] loss of CO to $C_{13}H_{18}N_2O_3^+$ m/z 250.1317
233(7) – [M-45] loss of CH_2OCH_3 to $C_{12}H_{13}N_2O_3^+$ m/z 233.0926
163 (55) – [M-115] $(CH_3)_2C_6H_3.N_2H_2CO^+$ $C_9H_{11}O^+$ m/z 163.0871
132 (35) – [M-146] $(CH_3)_2C_6H_3.NC^+$ $C_9H_{10}N^+$ m/z 132.0813
105 (60) – [M-173] $(CH_3)_2C_6H_3^+$ $C_8H_9^+$ m/z 105.0704
45 (100) – [M-233] $CH_2OCH_3^+$ $C_2H_5O^+$ m/z 45.0340

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C77732093&Mask=200#Mass-Spec

Oxamyl **$C_7H_{13}N_3O_3S$** **M:219(0%)**

Theoretical molecular ion: m/z 219.0678 (100%), 220.0711 (7.6%), 221.0636 (4.5%)
Average MW: 219.26



Oxime carbamate insecticide, acaricide and nematicide. Approved for use in EU.

Acute oral LD50 for rat approx.2 mg/kg (high toxicity).

Not amenable to GC analysis. Incomplete degradation on GC to oxamyl oxime by loss of methyl isocyanate, the spectrum of which is rather similar to oxamyl itself:

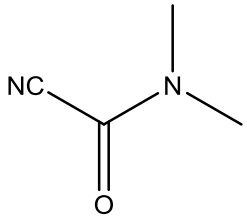
m/z	72	44	162	115	57	145	47	98
%	100	95	55	35	35	25	25	20

219 (0) – M^+ absent
162 (55) – [M-57] loss of CH_3NCO to oxime $C_5H_{10}N_2O_2S^+$ m/z 162.2070
145 (25) – [M-57] loss of CH_3NCO & CH_3 to $C_4H_7N_2O_2S^+$ m/z 1450228
115 (35) – [M-104] loss of CH_3NCO & CH_2S to $C_4H_7N_2O_2^+$ m/z 115.0508
98 (20) – [M-121] loss of CH_3NCO & CH_2S & HO to $C_4H_6N_2O^+$ m/z 98.0480 (see below)
72 (100) – [M-147] $(CH_3)_2NCO^+$ $C_3H_6NO^+$ m/z 72.0449
44 (95) – [M-175] $(CH_3)_2N^+$ $C_2H_6N^+$ m/z 44.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C23135220&Mask=200#Mass-Spec though m/z 44 much less abundant (30%).

Oxamyl metabolite, DMCF **$C_4H_6N_2O$** **M:98(100%)**

Theoretical molecular ion: m/z 98.0480 (100%), 99.0514 (4.3%)
Average MW: 98.11

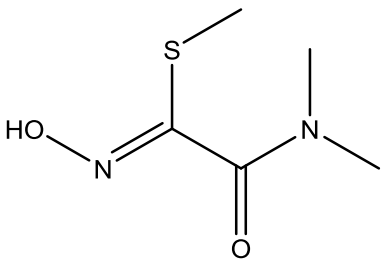


Oxamyl metabolite DMCF, N,N-dimethyl-cyanoformamide
(or dimethylcarbamoyl cyanide)

m/z	98	42	72	69	58	97	83	54
%	100	60	55	50	45	45	30	35

Oxamyl oxime **$C_5H_{10}N_2O_2S$** **M:162(20%)**

Theoretical molecular ion: m/z 162.0463 (100%), 163.0497 (5.4%), 164.0421 (4.5%)
Average MW: 162.21



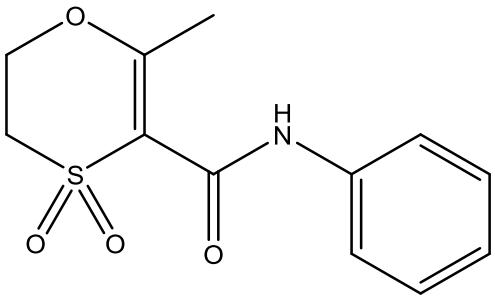
Oxamyl degradation product. N.B. Very similar spectrum to that of oxamyl.

May exhibit poor GC transmission/peak shape.

m/z	72	44	47	98	48	162	115	145
%	100	80	50	50	35	20	20	20

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C30558431&Mask=200#Mass-Spec

Oxycarboxin **$C_{12}H_{13}NO_4S$** **M:267(20%)**
Theoretical molecular ion: m/z 267.0565 (100%), 268.0599 (13.0%), 269.0523 (4.5%)
Average MW: 267.30



Fungicide. Used for control of rust diseases on ornamentals, cereals and nursery trees, and fairy rings on turf. Also a pesticide transformation product (identical to carboxin sulphone). No longer approved for use in EU.

Acute oral LD50 for rat approx. 1,500 mg/kg (moderate toxicity).

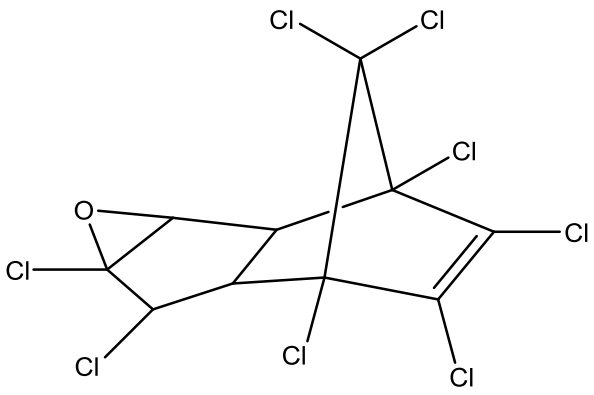
Poor GC transmission/peak shape. N.B. The spectra obtained using different instruments may differ (particularly in abundance of m/z 175 and 119).

m/z	119	175	43	91	93	147	64	267
%	100	90	60	20	20	20	15	20

267 (20) – M^+
250 (5) – [M-17] loss of OH to $C_{12}H_{12}NO_3S^+$ m/z 250.0358
175 (90) – [M-92] $(CH_3)(OC_4H_5SO_2)CO^+$ $C_6H_7O_4S^+$ m/z 175.0065
147 (20) – [M-120] $(CH_3)(OC_4H_5SO_2)^+$ $C_5H_7O_3S^+$ m/z 147.0116
119 (100) – [M-148] phenyl isocyanate $C_6H_5NCO^+$ $C_7H_5NO^+$ m/z 119.0371
93 (20) – [M-174] $C_6H_7N^+$ m/z 93.0579
91 (20) – [M-176] $C_6H_5N^+$ m/z 91.0422
43 (40) – [M-224] $CHNO^+$ m/z 43.0058

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C5259881&Mask=200#Mass-Spec which exhibits several similar ions (in order of abundance: m/z 43, 175, 93, 267, 147, 65, 39, 77) but m/z 119 is only 5%. This highly reactive species must be very sensitive to specific MS ion source conditions.

Oxychlordane **$C_{10}H_4Cl_8O$** **M:420,422,424(2,4,5%)**
Theoretical molecular ion: m/z 419.7770 (45%), 421.7741 (57%), 423.7711 (100%), 425.7682 (70%)



Metabolite, oxidation product, of **chlordane**.

KI (OV-17) = 22.7, (CPSil19) = 21.1 (very close to **heptachlor epoxide**).

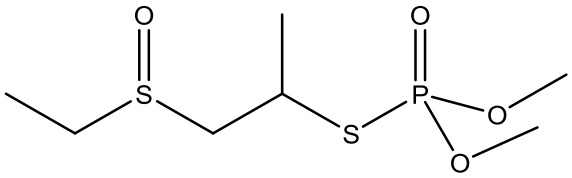
m/z	115	185	187	149	51	387	389	117
%	100	75	70	50	40	40	40	30

420,422,424,426 (2,4,5,3) – M^+
385,387,389,391 (20,40,40,20) – [M-35] C10H4Cl7O+ m/z 384.8182 etc.
115,117 (100,30) – [M-305] $C_5H_4ClO^+$ m/z 114.9951 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C27304138&Mask=200#Mass-Spec
rather unhelpfully listed under "2,5-Methano-2H-indeno[1,2-b]oxirene, 2,3,4,5,6,6a,7,7-octachloro-1a,1b,5,5a,6,6a-hexahydro-, (1aα,1bβ,2α,5α,5aβ,6β,6aα)-"

Oxydeprofos **$C_7H_{17}O_4PS_2$** **M:260(0%)**

Theoretical molecular ion: m/z
Average MW: 260.2



Organophosphorus insecticide and acaricide. Not approved for use in EU.

Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

May be oxidised to the sulphone, or reduced to the sulphide. Poor GC transmission.

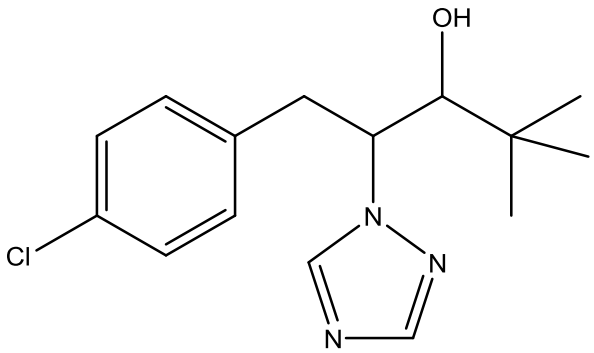
m/z	183	41	125	109	102	143	79	29
%	100	40	35	25	20	10	10	5

260 (0) – M^+
183 (100) – [M-77] loss of CH_3CH_2SO to $C_5H_{12}O_3PS^+$ m/z 183.0245
143 (10) – [M-117] $(CH_3O)_2(HO)(HS)P^+$ $C_2H_8O_3PS^+$ m/z 142.9932
125 (35) – [M-135] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (25) – [M-151] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
102 (20) – [M-158] $CH_3CH_2SCHCHCH_2^+$ $C_5H_{10}S^+$ m/z 102.0503
79 (10) – [M-181] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
41 (40) – [M-219] $C_3H_5^+$ m/z 41
29 (5) – [M-231] $CH_3CH_2^+$ $C_2H_5^+$ m/z 29.0391

No NIST spectrum available

Paclobutrazol **$C_{15}H_{20}ClN_3O$** **M:293(0%)**

Theoretical molecular ion: m/z 293.1295 (100%), 295.1265 (32%)
Average MW: 293.80



Conazole plant growth regulator for ornamentals, fruit and other crops to inhibit vegetative growth. Approved for use in EU.

Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity).

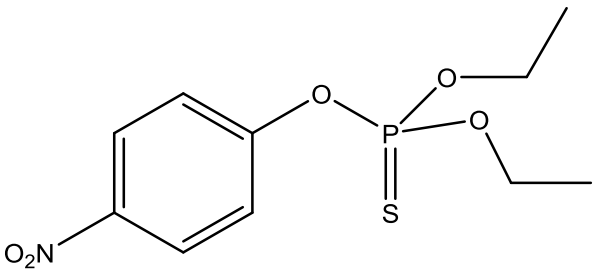
m/z	236	125	82	238	167	57	70	127
%	100	60	35	30	30	25	20	20

293,295 (0) – M^+ $C_{15}H_{20}ClN_3O^+$ m/z
278,280 (1,0.5) – [M-15] loss of CH_3 to $C_{14}H_{17}ClN_3O^+$ m/z 278.1060 etc.
236,238 (100,30) – [M-57] $C_{11}H_{11}ClN_3O^+$ m/z 236.0591 etc.
167,169 (30,10) – [M-126] $ClC_6H_4CH_2CH{=}CHOH^+$ $C_9H_9ClO^+$ m/z 168.0342 etc.
125,127 (60,20) – [M-168] $ClC_6H_4CH_2^+$ $C_7H_6Cl^+$ m/z 125.0158 etc.
82 (35) – [M-211] $(C_2H_2H_3)CH^+$ $C_3H_4N_3^+$ m/z 82.0405
57 (25) – [M-236] $C_4H_9^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C76738620&Mask=200#Mass-Spec

Parathion **$C_{10}H_{14}NO_5PS$** **M:291(100%)**

Theoretical molecular ion: m/z 291.0330 (100%), 292.0364 (11%), 293.0288 (4.5%)
Average MW: 291.26



Organophosphorus insecticide and acaricide. Used to control sucking and chewing insects and mites. Not approved for use in EU. See related oxidative & reductive products below.

Acute oral LD50 for rat 2 mg/kg (high toxicity).

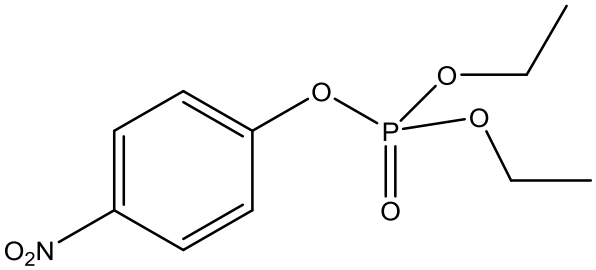
m/z	291	109	97	137	139	125	155	123
%	100	95	95	60	55	45	45	20

Assignments confirmed by accurate mass data (Cardiff GCT)
291 (100) – M^+ $C_{10}H_{14}NO_5PS^+$ m/z 291.0330
275 (5) – [M-16] loss of O to $C_{10}H_{14}NO_4PS^+$ m/z 275.0381
263 (5) – [M-28] loss of C_2H_4 to $C_8H_{10}NO_5PS^+$ m/z 263.0017
235 (10) – [M-56] loss of $2C_2H_4$ to $C_6H_4NO_5PS^+$ m/z 234.9704
218 (5) – [M-73] loss of C_2H_4 & C_2H_5O to $C_6H_5NO_4PS^+$ m/z 217.9677
188 (25) – [M-103] loss of C_2H_4 & C_2H_5O & NO to $C_6H_5O_3PS^+$ m/z 187.9697
186 (20) – [M-105] loss of C_2H_5S & C_2H_5O to $C_6H_5NO_4P^+$ m/z 185.9956
155 (45) – [M-136] $NO_2.C_6H_4.SH^+$ $C_6H_5NO_2S^+$ m/z 155.0041 [O/S swap]
150 (10) – [M-141] $NO_2.C_6H_4.C_2H_4^+$ $C_8H_8NO_2^+$ m/z 150.0555 [unexpected rearrangement/loss of $C_2H_6O_3PS$]
139 (55) – [M-152] $NO_2.C_6H_4.OH^+$ $C_6H_5NO_3^+$ m/z 139.0269
137 (60) – [M-154] $(CH_3CH_2O)_2P{=}O^+$ $C_4H_{10}O_3P^+$ m/z 137.0368 [O/S swap]
125 (45) – [M-166] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
123 (20) – [M-168] $NO_2.C_6H_4/H^+$ $C_6H_5NO_2^+$ m/z 123.0320
109 (95) – [M-182] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (95) – [M-196] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C56382&Mask=200#Mass-Spec

Parathion oxon / Paraoxon $C_{10}H_{14}NO_6P$ M:275(60%)

Theoretical molecular ion: m/z 275.0559 (100%), 276.0592 (11%), 277.0601 (1.2%)
Average MW: 275.20



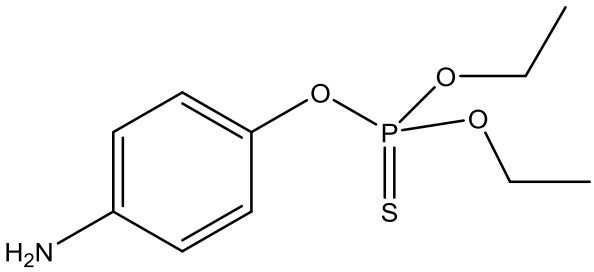
m/z	109	81	149	275	99	139	127	247
%	100	95	95	60	55	45	45	20

275 (60) – M^+
247 (20) – [M-28] loss of C_2H_4 to $C_8H_{10}NO_6P^+$ m/z 247.0246
219 (95) – [M-56] loss of $2C_2H_4$ to $C_6H_4NO_6P^+$ m/z 218.9933
149 (95) – [M-126]
139 (45) – [M-136] $NO_2.C_6H_4.OH^+$ $C_6H_5NO_3^+$ m/z 139.0269
127 (45) – [M-148] $(CH_3CH_2O)(HO)_3P^+$ $C_2H_8O_4P^+$ m/z 127.0160
109 (100) – [M-166] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
99 (55) – [M-176] $(HO)_4P^+$ $H_4O_4P^+$ m/z 98.9847
81 (95) – [M-294] $(HO)_2PO^+$ $H_2O_3P^+$ m/80.9742

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C311455&Mask=200#Mass-Spec
listed under "Diethyl *p*-nitrophenyl phosphate"

Parathion, Amino- **$C_{10}H_{16}NO_3PS$** **M:261(35%)**

Theoretical molecular ion: m/z 261.0589 (100%), 262.0622 (10.8%), 263.0547 (4.5%)
Average MW: 261.28



"Aminoparathion" is a reductive degradation product of parathion. It may be generated in a hot GC injector (300°C) during a slow injection (over several seconds).

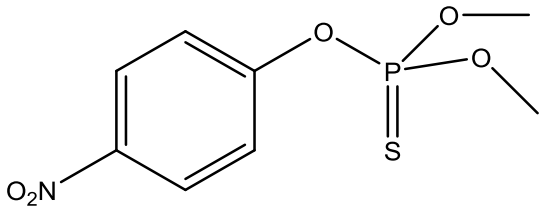
m/z	125	109	108	29	97	80	65	261
%	100	95	85	75	60	55	35	35

261 (35) – M^+
233 (5) – [M-28] loss of C_2H_4 to $C_8H_{12}NO_3PS^+$ m/z 233.0275
205 (10) – [M-56] loss of $2C_2H_4$ to $C_6H_8NO_3PS^+$ m/z 204.99634
153 (10) – [M-108] $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (100) – [M-236] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (95) – [M-252] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
108 (85) – [M-153] $NH_2.C_6H_4.O^+$ $C_6H_6NO^+$ m/z 108.0449
80 (55) – [M-181] $NH_2.C_5H_4^+$ $C_5H_6N^+$ m/z 80.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3735011&Mask=200#Mass-Spec

Parathion-methyl **$C_8H_{10}NO_5PS$** **M:263(65%)**

Theoretical molecular ion: m/z 263.0017 (100%), 264.0051 (8.7%), 264.9975 (4.5%)
Average MW: 263.20



Organophosphorus insecticide and acaricide. Used to control sucking and chewing insects and mites. Not approved for use in EU. See related oxidative & reductive products below.

Acute oral LD50 for rat 3 mg/kg (high toxicity).

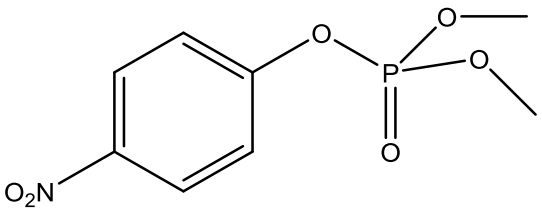
m/z	109	125	263	79	93	47	63	200
%	100	80	65	30	20	20	10	5

N.B. Assignments confirmed by accurate mass data
263 (65) – M^+ $C_8H_{10}NO_5PS^+$ m/z 263.0017
246 (5) – [M-17] loss of OH to $C_8H_9NO_4PS^+$ m/z 245.9990
233 (5) – [M-30] loss of NO to $C_8H_{10}O_4PS^+$ m/z 233.0037
202 (5) – [M-61] loss of NO & CH_3O to $C_7H_7O_3PS^+$ m/z 201.9854
200 (5) – [M-63] loss of CH_3O & S to $C_7H_7NO_4P^+$ m/z 200.0113
125 (80) – [M-138] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826

109 (100) – [M-154] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (20) – [M-170] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (30) – [M-184] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C298000&Mask=200#Mass-Spec

Parathion-methyl oxon, "Paraoxon methyl" $C_8H_{10}NO_6P$ M:247(15%)
Theoretical molecular ion: m/z 247.0246 (100%), 248.0279 (8.7%)
Average MW: 247.14

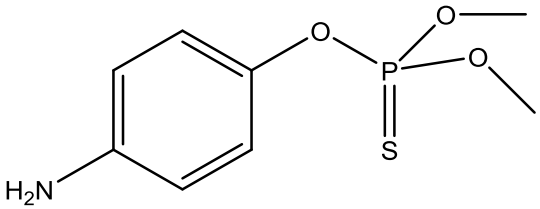


m/z	109	96	79	30	63	230	247	200
%	100	75	35	35	30	20	15	15

247 (15) – M^+ $C_8H_{10}NO_6P^+$ m/z
230 (20) – [M-17] loss of HO to $C_8H_9NO_5P^+$ m/z 230.0218
200 15) – [M-47] loss of HNO2 to $C_8H_9O_4P^+$ m/z 200.0239
109 (100) – [M-138] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
96 (75) – [M-151] $(CH_3O)(HO)2P+$ CH_5O_3P+ m/z 95.9976
79 (35) – [M-168] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (30) – [M-184] PO_2^+ m/z 62.9636
30 (35) – [M-217] NO^+ m/z 29.9980

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C950356&Units=SI&Mask=200#Mass-Spec though some ions missing, e.g. m/z 108 and 95, perhaps because of poor MS resolution.

Parathion-methyl, Amino- $C_8H_{12}NO_3PS$ M:233(100%)
Theoretical molecular ion: m/z 233.0276 (100%), 234.0309 (8.7%), 235.0234 (4.5%)
Average MW: 233.22



"Aminoparathion methyl" is a reductive degradation product. It may be generated in a hot GC injector.

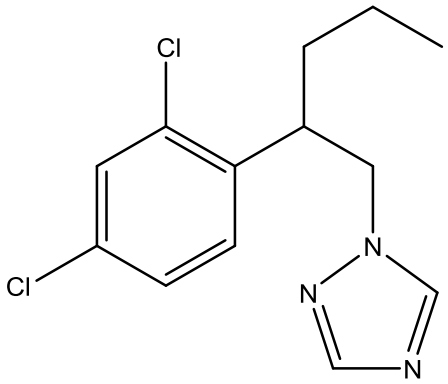
m/z	233	124	108	125	109	106	93	79
%	100	99	44	35	19	7	7	7

233 (100) – M^+
125 (35) – [M-108] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
124 (99) – [M-109] $NH_2C_6H_4S^+$ $C_6H_6NS^+$ m/z 124.0221
109 (19) – [M-124] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
108 (44) – [M-125] $NH_2C_6H_4O^+$ $C_6H_6NO^+$ m/z 108.0449

106 (7) – [M-127] $NC_6H_4O^+$ $C_6H_4NO^+$ m/z 106.02929
93 (7) – [M-140] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (7) – [M-154] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

No NIST spectrum available.

Penconazole **$C_{13}H_{15}Cl_2N_3$** **M:283,285(0%)**
Theoretical molecular ion: m/z 283.0643 (100%), 285.0614 (64%), 287.0584 (10%),
Average MW: 284.18



Conazole fungicide. Used fungicide used to control powdery mildew, scab and other pathogenic *Ascomycetes*, *Basidiomycetes* and *Deuteromycetes*.

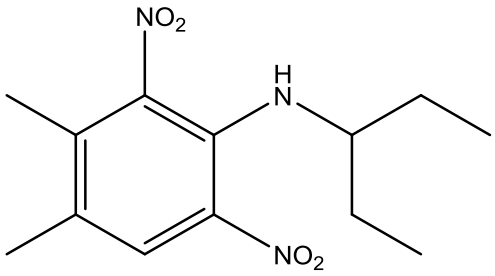
Acute oral LD50 for rat >2,000 (moderate toxicity).

m/z	159	248	161	250	249	83	213	163
%	100	85	65	25	10	10	10	10

283,285 (0) – M^+ absent
248,250 (85,25) – [M-35] loss of Cl to $C_{13}H_{15}ClN_3^+$ m/z 248.0955 etc.
159,161 (100,65) – [M-124] $Cl_2C_6H_3.CH_2^+$ $C_7H_5Cl^+$ m/z 158.9768 etc.

No NIST spectrum available, but very similar spectrum in Flamini (2010), page 300.

Pendimethalin **$C_{13}H_9N_3O_4$** **M:281(10%)**
Theoretical molecular ion: m/z 281.1376 (100%), 282.1409 (14%)
Average MW: 281.37



Herbicide. Approved for use in EU.

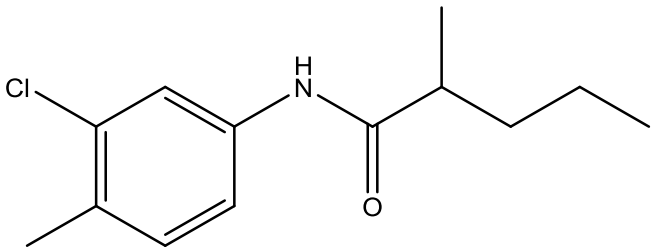
Acute oral LD50 for rat > 3,000 (low toxicity).

m/z	252	162	29	57	253	43	192	119
%	100	15	15	15	15	15	10	10

281 (10) – M^+ $C_{13}H_{19}N_3O_4$
252 (100) – [M-29] loss of C2H5 to $C_{13}H_{19}N_3O_4^+$ m/z 252.2500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C40487421&Mask=200#Mass-Spec

Pentanochlor **$C_{13}H_{18}ClNO$** **M:239,241(15,5%)**
Theoretical molecular ion: m/z 239.1077 (100%), 240.1111 (14%), 241.1047 (32%)
Average MW: 239.74

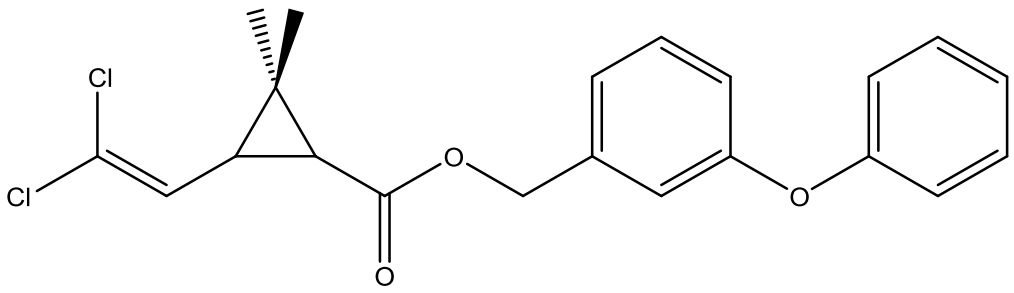


m/z	141	43	71	143	41	140	142	239
%	100	70	65	30	20	15	15	15

239,241 (15,5) – M^+ $C_{13}H_{18}ClNO^+$ m/z
197,199 (10,3) – [M-42] loss of propene C_3H_6 to $C_{10}H_{12}ClNO^+$ m/z 197.0607
168,170 (5,2) – [M-71] isocyanate $CH_3(Cl)C_6H_3NCO^+$ $C_8H_7ClNO^+$ m/z 168.0216 etc.
141,143 (100,30) – [M-98] chlorotoluidine $CH_3(Cl)C_6H_3NH_2^+$ $C_7H_8ClN^+$ m/z 141.0345
71 (65) – [M-168] CH3CHCH2CH2CH3+ C6H11+ m/z 71.0861
43 (70) – [M-197] $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2307688&Units=SI&Mask=200#Mass-Spec listed under "Pentanamide, N-(3-chloro-4-methylphenyl)-2-methyl-"

Permethrin **$C_{21}H_{20}Cl_2O_3$** **M:390,392(2,1%)**
Theoretical molecular ion: m/z 390.07895 (100%), 392.0760 (64%), 394.07305 (10%)
Average MW: 391.29



Synthetic pyrethroid insecticide. No longer approved for use in EU.

Acute oral LD50 for rat >400 mg/kg (moderate toxicity).

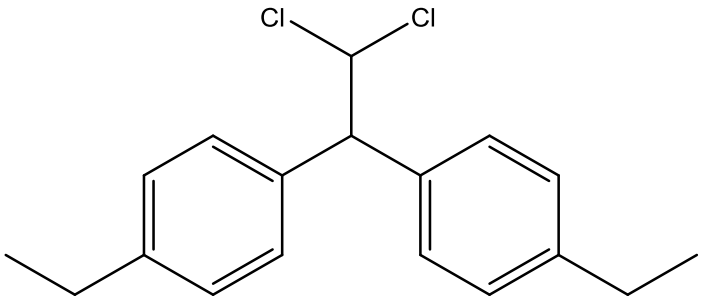
May be resolved into two peaks on capillary GC (*ca* 1:3).

m/z	183	163	165	184	77	91	127	51
%	100	30	20	15	15	15	10	10

390,392 (2,1) – M+
183 (100) – [M-207] $CH_2C_6H_4OC_6H_5^+$ $C_{13}H_{11}O^+$ m/z 183.0810
163,165 (30,20) – [M-227] $Cl_2C{=}C\text{-}C_3H_3(CH_3)_2^+$ $C_7H_9Cl_2^+$ m/z 163.0081 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C52645531&Mask=200#Mass-Spec

Perthane **$C_{18}H_{20}Cl_2$** **M:306,308(2,1%)**
Theoretical molecular ion: m/z 306.0942 (100%), 308.0913 (64%), 307.0976 (20%)
Average MW: 307.26



Organochlorine insecticide. No longer approved for use in EU.

Acute oral LD50 for rat 8,000 mg/kg (low toxicity).

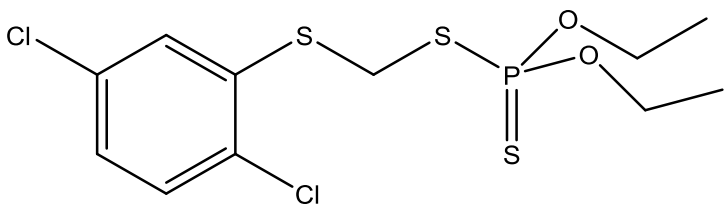
Very simple mass spectrum, dominated by m/z 223 ion (analogous to m/z 235 of DDT).

m/z	223	224	165	179	193	104	115	178
%	100	20	5	5	5	5	5	5

306,308(2,1) – M^+
223 (100) – [M-83] $(CH_3CH_2C_6H_5)_2CH_+$ $C_{17}H_{19}^+$ m/z 223.1287

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C72560&Mask=200#Mass-Spec

Phenkapton **$C_{11}H_{15}Cl_2O_2PS_3$** **M:376,378,380(15,10,3%)**
Theoretical molecular ion: m/z 375.9349 (100%), 377.9319 (64%), 379.9290 (10.2%)
Average MW: 377.39



Organophosphorus insecticide and acaricide. Used to control red spider mite and other insects on a range of crops including fruit. No longer approved for use in EU.

Acute oral LD50 for rat approx. 40 mg/kg (high toxicity).

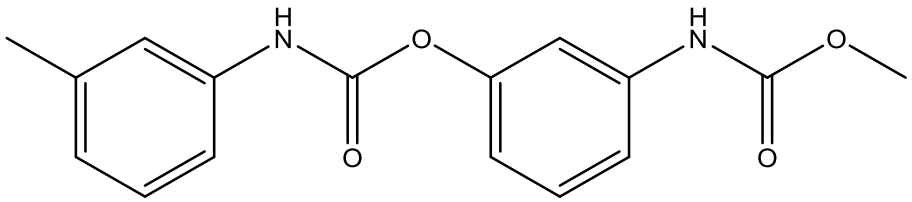
Several oxidative metabolites (oxon, and sulphoxide and sulphone).

m/z	121	97	45	153	191	125	65	199
%	100	80	75	65	50	50	45	40

376,378,380(15,10,3) – M^+
341,343(5,2) – [M-35] loss of Cl to $C_{11}H_{15}ClO_2PS_3^+$ m/z 340.9660 etc.
199 (40) – [M-177] $(C_2H_5O)_2P{=}S.SCH_2^+$ $C_5H_{12}O_2PS_2^+$ m/z 199.0016
191 (50) – [M-185] $Cl_2C_6H_4S^+$ $C_7H_5Cl_2S^+$ m/z 190.0489
153 (65) – [M-223] $(C_2H_5O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (50) – [M-251] $(C_2H_5O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121 (100) – [M-255] $(C_2H_5O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
97 (80) – [M-279] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
65 (45) – [M-311] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
45 (75) – [M-331] $C_2H_5O^+$ m/z 45.0340

No NIST spectrum available.

Phenmedipham **$C_{16}H_{16}N_2O_4$** **M:300(0%)**
Theoretical molecular ion: m/z 300.1110 (100%), 301.1144 (17%)
Average MW: 300.31



Selective systemic carbamate herbicide. Approved for use in EU.

Acute oral LD50 for rat >8,000 mg/kg (low toxicity).

Not amenable to GC.

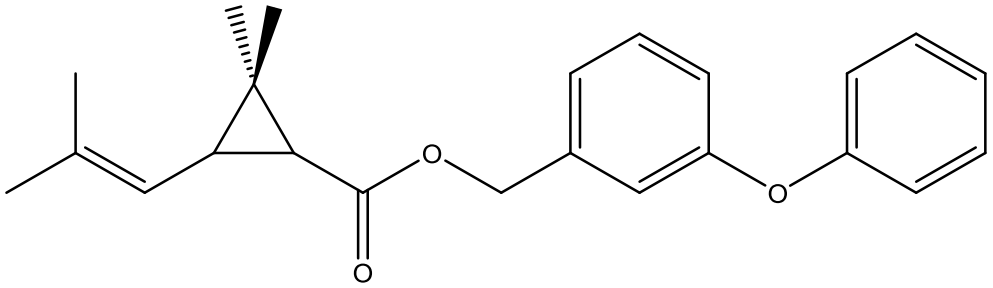
m/z	133	135	167	104	132	78	52	122
%	100	65	50	40	30	20	15	10

300 (0) –M+ absent
167 (50) – [M-133] $OC_6H_4NHCOOCH_3$ $C_8H_9NO_3^+$ m/z 167.0582
133 (100) – [M-167] isocyanate $CH_3C_6H_4NCO_+$ $C_8H_7NO^+$ m/z 133.0527
104 (40) – [M-196]] $C_7H_6N^+$ m/z 104.0500

Cf. similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C13684634&Mask=200#Mass-Spec

Phenothrin $C_{23}H_{26}O_3$ **M:350(5%)**

Theoretical molecular ion: m/z 350.1882 (100%), 351.19155 (25%)
Average MW: 350.45



Synthetic pyrethroid insecticide.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

May be resolved into two peaks on capillary GC (ca 1:3).

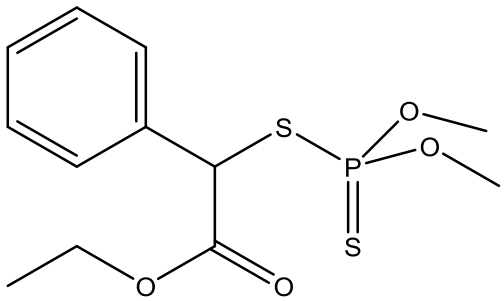
m/z	123	183	81	184	43	124	350	168
%	100	55	20	15	10	10	5	5

350 (5) – M+
183 (55) – [M-167] $CH_2C_6H_4$-O-$C_6H_5^+$ $C_{13}H_{11}O^+$ m/z 183.0810
123 (100) – [M-227] $(CH_3)_2C$=C-$C_3H_3(CH_3)_2^+$ $C_9H_{15}^+$ m/z 123.1174
81 (20) – $CH_3(C_3H_2)CO^+$ $C_5H_5O^+$ m/z 81.0340

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C26002802&Mask=200#Mass-Spec

Phenthoate $C_{12}H_{17}O_4PS_2$ **M:320(5%)**

Theoretical molecular ion: m/z 320.0306 (100%), 321.0339 (13%), 322.0264 (9.0%)
Average MW: 320.36



Organophosphorus insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 200 mg/kg (moderate toxicity).

m/z	274	93	125	121	107	92	79	246
%	100	95	90	70	55	55	55	30

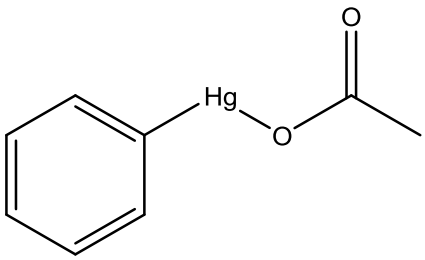
320 (5) – M^+
274 (100) – [M-46] loss of C_2H_5OH to $C_{10}H_{11}O_3PS_2^+$ m/z 273.9887
246 (30) – [M-74] loss of C_2H_5OCO to $C_9H_{11}O_2PS_2^+$ m/z 245.9938
125 (90) – [M-195] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121 (70) – [M-199] $C_6H_5CS^+$ $C_7H_5S^+$ m/z 121.0112

107 (55) – [M-213] $C_7H_7O^+$ (O/S swap) m/z 107.0497
93 (95) – [M-227] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.1054
79 (25) – [M-241] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2597037&Mask=200#Mass-Spec which has more abundant m/z 91 rather than m/z 92.

Phenylmercury acetate **$C_8H_8HgO_2$** **M:338(0%)**

Theoretical molecular ion: m/z 334.0192 (34%), 335.02071 (57%), 336.02076 (78%), 337.02273 (45%), **338.02307 (100%),** 340.02592 (23%)
Average MW: 336.74



Organomercury fungicide and herbicide. Largely obsolete, highly toxic substance once used as a fungicide, herbicide and mildew inhibitor. It also found use in leather processing, eye drops and as a preservative in paints.

Acute oral LD50 for rat approx. 70 mg/kg (high toxicity).

Poor GC transmission.

The mass spectra of mercury compounds are easily recognised because mercury has seven isotopes with significant natural abundance:

196 0.5%
198 34.1%
199 57.3%
200 77.9%
201 44.5%
202 100%
204 22.9%

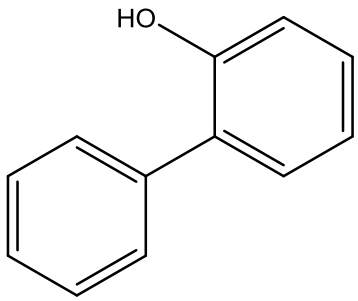
For monoisotopic MS formulae, the most abundant isotope, ^{202}Hg, is used.

m/z	77	51	50	279	277	78	-	-
%	100	35	15	5	5	5	-	-

336,338 (0,0) – M^+ absent
275,276,277,278,279 (1,2,3,2,5) – $[M-59]^+$ loss of acetate to give $C_6H_5Hg^+$ m/z 275.00589 (34%), 276.0074 (57%), 277.00745 (78%), 278.00942 (45%), 279.00976 (100%), 281.01261 (23%)
77 (100) – [M-259] $C_6H_5^+$ m/z 77.0391

2-Phenylphenol **$C_{12}H_{10}O$** **M:170(100%)**

Theoretical molecular ion: m/z 170.0732 (100%), 171.0765 (13%)
Average MW: 170.21



Fungicide and post harvest treatment agent. Used in EU.

Acute oral LD50 for rat approx. 2,500 mg/kg (moderate toxicity).

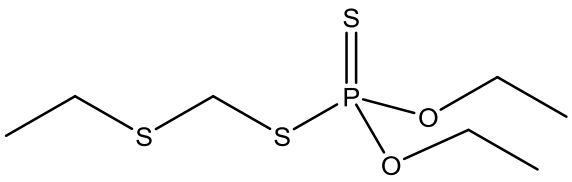
m/z	170	169	141	115	31	171	142	139
%	100	60	35	25	20	15	10	10

170 (100) – M^+
169 (60) – [M-1] loss of H to $C_{12}H_9O^+$ m/z 169.0653
141 (35) – [M-29] loss of CHO to $C_{11}H_9^+$ m/z 141.0704

Cf. similar (but poor quality) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C90437&Mask=200#Mass-Spec

Phorate **$C_7H_{17}O_2PS_3$** **M:260(10%)**

Theoretical molecular ion: m/z 260.0128 (100%), 261.0162 (7.6%), 262.0086 (9.0%)
Average MW: 260.36



Organophosphorus insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 2 mg/kg (high toxicity).

N.B. Five oxidative metabolites, all included in MRLs.

m/z	75	121	97	93	47	260	65	29
%	100	25	10	10	10	10	10	5

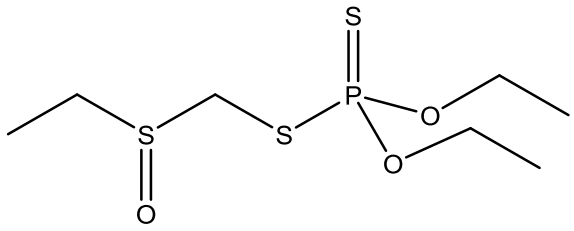
260 (10) – M^+
231 (5) – [M-29] loss of CH_3CH_2 to $C_5H_{13}O_2PS_3^+$ m/z 230.9737
121 (25) – [M-139] $(C_2H_5O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
97 (10) – [M-163] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
93 (10) – [M-167] $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105
75 (100) – [M-185] $CH_3CH_2SCH_2^+$ $C_3H_7S^+$ m/z 75.0269
65 (10) – [M-195] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

47 (10) – [M-213] PO^+ m/z 46.9687

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C298022&Mask=200#Mass-Spec

Phorate sulphoxide **$C_7H_{17}O_3PS_3$** **M:276(0%)**

Theoretical molecular ion: m/z 276.0077 (100%), 277.0111 (7.6%), 278.0035 (9.0%)
Average MW: 276.36



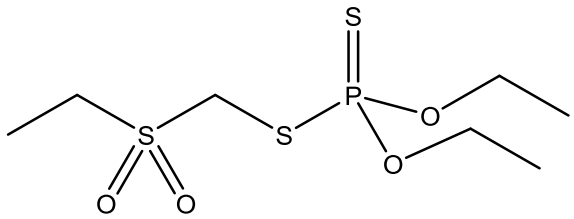
m/z	97	125	153	199	29	65	171	75
%	100	85	80	75	20	15	15	10

276 (0) – M+ absent $C_7H_{17}O_3PS_3^+$ m/z
199 (75) – [M-77] loss of CH_3CH_2SO to $C_5H_{12}O_2PS_2^+$ m/z 199.0016
171 (15) – [M-105] loss of CH_3CH_2SO & C_2H_4 to $C_3H_8O_2PS_2^+$ m/z 170.9703
153 (80) – [M-123] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (80) – [M-151] $(CH_3CH_2O)(HO)PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (100) – [M-179] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2588036&Units=SI&Mask=200#Mass-Spec

Phorate sulphone **$C_7H_{17}O_4PS_3$** **M:292(5%)**

Theoretical molecular ion: m/z 292.0027 (100%), 293.0060 (7.6%), 293.9985 (9.0%)
Average MW: 292.36



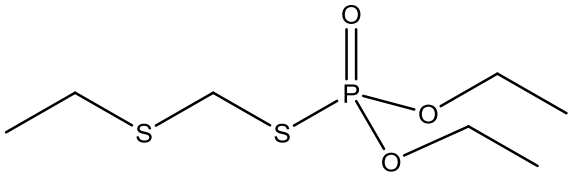
m/z	153	97	199	125	171	65	29	93
%	100	85	80	80	15	15	15	15

292 (5) – M+ $C_7H_{17}O_4PS_3^+$ m/z
199 (80) – [M-93] loss of $CH_3CH_2SO_2$ to $C_5H_{12}O_2PS_2^+$ m/z 199.0016
153 (100) – [M-139] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (80) – [M-167] $(CH_3CH_2O)(HO)PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (85) – [M-195] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
93 (10) – [M-199] $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105
and/or $CH_3CH_2SO_2^+$ $C_2H_5SO_2^+$ m/z 93.0010
65 (15) – [M-227] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
29 (15) – [M-263] CH_3CH_2+ C2H5+ m/z 29.0391

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2588047&Mask=200 which has exaggerated abundances for the lower mass ions (m/z 29, 97, 125, 153, 199 etc. in order of abundance)

Phorate oxon $C_7H_{17}O_3PS_2$ **M:244(15%)**

Theoretical molecular ion: m/z 244.0357 (100%), 245.03903 (7.6%), 246.0315 (9.0%)
Average MW: 244.30



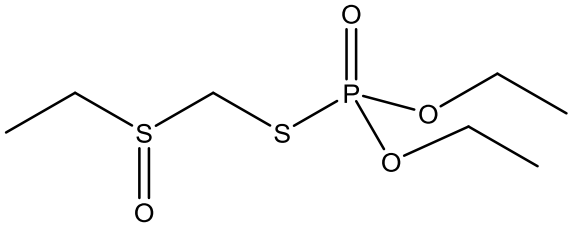
m/z	74	75	171	111	138	109	47	244
%	100	70	45	30	15	15	15	15

244 (15) – M^+
171 (45) – [M-73] $(CH_3CH_2O)_2(HO)(HS)P^+$ $C_4H_{12}O_3PS^+$ m/z 171.0245
138 (15) – [M-106] $(CH_3CH_2O)_2(HO)P^+$ $C_4H_{11}O_3P^+$ m/z 138.0446
111 (30) – [M-133] $(CH_3CH_2O)(HO)2PH^+$ $C_2H_8O_3P^+$ m/z 111.0211
109 (15) – [M-135] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
75 (70) – [M-169] $CH_3CH_2SCH_2^+$ $C_3H_7S^+$ m/z 75.0269
74 (100) – [M-170] $CH_3CH_2SCH^+$ $C_3H_6S^+$ m/z 74.0190
47 (15) – [M-197] PO^+

Cf. similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=U289841&Mask=200

Phorate oxon sulphoxide $C_7H_{17}O_4PS_2$ **M:260(0%)**

Theoretical molecular ion: m/z 260.0306 (100%), 261.0339 (7.6%), 262.0264 (4.5%)
Average MW: 260.30



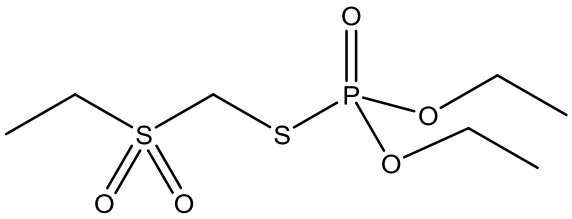
m/z	109	183	75	137	155	139	81	127
%	100	46	35	25	25	25	20	20

260 (0) – M^+
183 (46) – [M-77] $(CH_3CH_2O)_2PO.SCH_2^+$ $C_5H_{12}O_3PS^+$ m/z 183.0245
155 (25) – [M-105] $(CH_3CH_2O)(HO)P{=}O.SCH_2^+$ $C_3H_8O_3PS^+$ m/z 154.9932
139 (25) – [M-121] $(CH_3CH_2O)_2(HO)PH^+$ $C_4H_{12}O_3P^+$ m/z 139.0524
137 (25) – [M-123] $(CH_3CH_2O)_2PO^+$ $C_4H_{10}O_3P^+$ m/z 137.0368
127 (20) – [M-133] $(CH_3CH_2O)(HO)_3P^+$ $C_2H_8O_4P^+$ m/z 127.0160
109 (100) – [M-151] $(CH_3CH_2O)(HO)PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
91 (20) – [M-169] $CH_3CH_2SOCH_2^+$ $C_3H_7OS^+$ m/z 91.0218
81 (20) – [M-179] $(HO)_2PO^+$ $H_2O_3P^+$ m/z 80.9742
75 (35) – [M-185] $CH_3CH_2SCH_2^+$ $C_3H_7S^+$ m/z 75.0269 – following reduction of sulphoxide?

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2588058&Mask=200 (listed under "O,O-Diethyl S-eththionylmethyl phosphorothioate") which has exaggerated abundances for the lower mass ions (in order of abundance: m/z 29, 109, 18, 81, 27, 45, 183, etc.)

Phorate oxon sulphone **$C_7H_{17}O_5PS_2$** **M:276(0%)**

Theoretical molecular ion: m/z 276.0255 (100%), 277.0289 (7.6%), 278.0213 (4.5%)
Average MW: 276.30



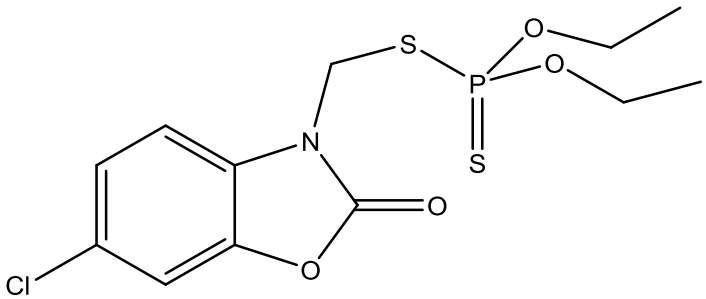
m/z	109	183	139	137	81	75	155	127
%	100	90	40	30	30	30	30	20

276 (0) – M+
183 (90) – [M-93] loss of $CH_3CH_2SO_2$ to $C_5H_{12}O_3PS^+$ m/z 183.0245
155 (30) – [M-121] $(CH_3CH_2O)(HO)P{=}O.SCH_2^+$ $C_3H_8O_3PS^+$ m/z 154.9932
139 (40) – [M-137] $(CH_3CH_2O)_2(HO)PH^+$ $C_4H_{12}O_3P^+$ m/z 139.0524
137 (30) – [M-139] $(CH_3CH_2O)_2PO^+$ $C_4H_{10}O_3P^+$ m/z 137.0368
127 (20) – [M-149] $(CH_3CH_2O)(HO)_3P^+$ $C_2H_8O_4P^+$ m/z 127.0160
109 (100) – [M-167] $(CH_3CH_2O)(HO)PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
81 (30) – [M-195] $(HO)_2PO^+$ $H_2O_3P^+$ m/z 80.9742
75 (30) – [M-201] $CH_3CH_2SCH_2^+$ $C_3H_7S^+$ m/z 75.0269 – following reduction of sulphone?

Cf. noisy and poor resolution spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2588069&Mask=200#Mass-Spec which exhibits ions (by abundance): m/z 29, 27, 109, 81, 45, 46, 183, 47 etc.

Phosalone **$C_{12}H_{15}ClNO_4PS_2$** **M:367,369(20,8%)**

Theoretical molecular ion: m/z 366.9869 (100%), 368.9839 (32.0%)
Average MW: 367.80



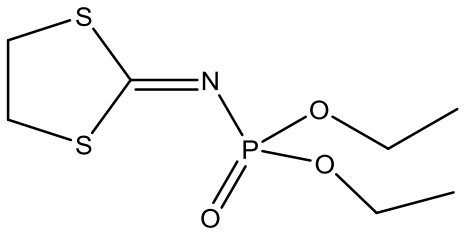
m/z	182	121	97	200	154	111	65	367
%	100	50	40	30	25	25	25	20

367,369 (20,8) – M+
200 (30) – [M-167] $(CH_3CH_2O)_2(\underline{CH_2S})PSH^+$ $C_5H_{13}O_2PS_2^+$ m/z 200.0095 - interesting rearrangement
182,184 (100,30) – [M-185] $Cl.C_6H_4/NCO_2.CH_2^+$ $C_8H_5ClNO_2^+$ m/z 182.0009 etc.
154 (25) – [M-213] $(CH_3CH_2O)_2(HS)P^+$ $C_4H_{11}O_2PS^+$ m/z 154.0217
153 (20) – [M-214] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
121 (50) – [M-246] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
111,113 (25,10) – [M-256] C_6H_4Cl+ m/z 111.0002 etc.
97 (40) – [M-270] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
65 (25) – [M-300] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. weak spectrum missing m/z 200 at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2310170&Mask=200#Mass-Spec
N.B. incorrect empirical formula and MW (omitted P).

Phosfolan $C_7H_{14}NO_3PS_2$ **M:255(35%)**

Theoretical molecular ion: m/z 255.0153 (100%), 256.0186 (7.6%), 257.0111 (9.0%)
Average MW: 255.29



Organophosphorus phosphoramidate insecticide. Not approved for use in EU.

Acute oral LD50 for rat approx. 10 mg/kg (high toxicity).

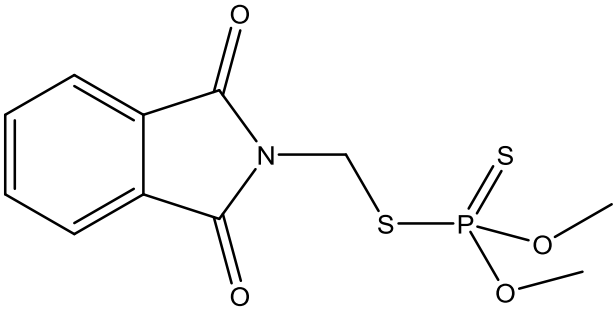
m/z	92	140	196	60	168	255	81	227
%	100	65	55	55	45	35	30	25

255 (35) – M^+ $C_7H_{14}NO_3PS_2^+$ m/z
227 (25) – [M-28] loss of C_2H_4 to $C_5H_{10}NO_3PS_2^+$ m/z 226.9840
196 (55) – [M-59] loss of CH_2CHS to $(HSCN)(C_2H_5O)2PO^+$ $C_5H_{11}NO_3PS^+$ m/z 196.0197
168 (45) – [M-87] loss of CH_2CHS & C_2H_4 to $(HSCN)(C_2H_5O)(HO)PO^+$ $C_3H_7NO_3PS^+$ m/z 167.9884
140 (65) – [M-115] loss of CH_2CHS & $2C_2H_4$ to $(HSCN)(HO)_2PO^+$ $CH_3NO_3PS^+$ m/z 139.9571
92 (100) – [M-163] ring scission to $SCH_2CH_2S^+$ $C_2H_4S_2^+$ m/z 91.9754
60 (55) – [M-195] $CH_2CH_2S^+$ $C_2H_4S^+$ m/z 60.0034

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C947024&Units=SI&Mask=200#Mass-Spec

Phosmet $C_{11}H_{12}NO_4PS_2$ **M:317(5%)**

Theoretical molecular ion: m/z 316.9945 (100%), 317.9979 (12%), 318.9903 (4.5%)
Average MW: 317.31



Organophosphorus insecticide and acaricide. Used to control Lepidopterous larvae, aphids, suckers, spider mites and other pests. Approved for use in EU.

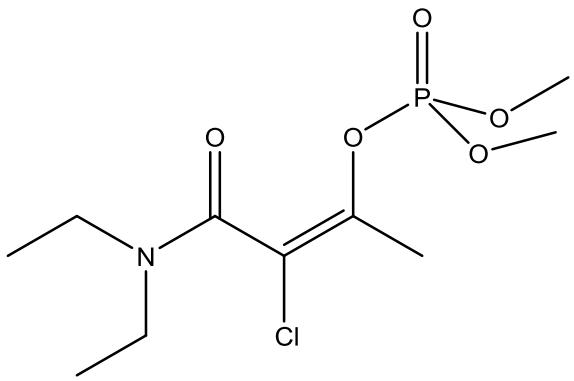
Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

m/z	160	77	93	76	161	317	104	133
%	100	15	15	15	10	5	5	5

317 (5) – M^+ $C_{11}H_{12}NO_3P^+$ m/z
160 (100) – [M-157] phthalimide moiety $C_6H_4{:}(CO)_2N.CH_2^+$ $C_9H_6NO_2^+$ m/z 160.0399
93 (15) – [M-224] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
77 (15) – [M-178] $C_6H_5^+$ m/z 77.0391
63 (5) – [M-254] PS^+ m/z 62.9458

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C732116&Mask=200#Mass-Spec

Phosphamidon **$C_{10}H_{19}ClNO_5P$** **M:299(0%)**
Theoretical molecular ion: m/z
Average MW: 299.69



Phosphamidon, (Z) –isomer

Organophosphorus insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

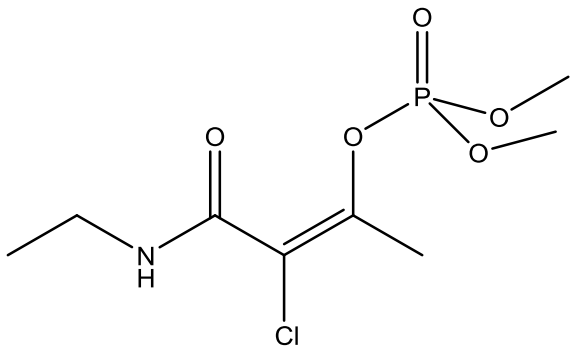
Technical phosphamidon contains 70% (Z) isomer and 30% (E) isomer. The isomers have rather similar mass spectra. They are easily resolved on GC, the (E)-isomer having the shorter retention time. Technical material may contain chloro- and dechloro- analogues (Carlstrom 1972).

m/z	127	72	264	138	109	67	193	158
%	100	60	25	25	20	15	10	10

299 (0) – M^+
264 (25) – [M-35] loss of Cl to $C_{10}H_{19}NO_5P^+$ m/z 264.1001
227,229 (6,2) – [M-72] $C_6H_8ClO_5P_+$ m/z 226.9876
193 (5) – [M-106] loss of Cl & C_4H_9N to $C_6H_{10}O_5P^+$ m/z 193.0266
138 (25) – [M-161] loss of Cl & $C_2H_7O_4P$ to $C_8H_{12}NO^+$ m/z 138.0919
127 (100) – [M-172] $(CH_3O)_2(HO)_2P^+$ $C_2H_8O_4P^+$ m/z 127.0160
109 (20) – [M-190] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
72 (60) – [M-227] $(C_2H_5)_2N^+$ $C_4H_{10}N^+$ m/z 72.0813

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C13171216&Mask=200

Phosphamidon, N-desethyl **$C_8H_{15}ClNO_5P$** **M:271,273(15,5%)**
Theoretical molecular ion: m/z 271.0376 (100%), 273.0347 (32%)
Average MW: 271.04



A metabolite of phosphamidon.

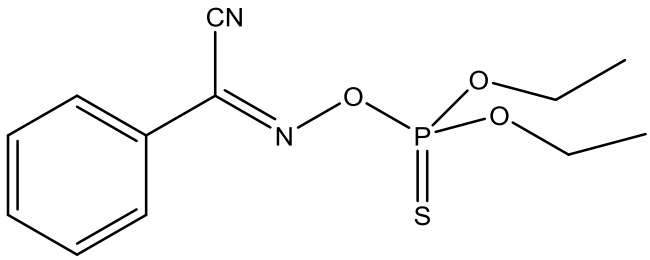
m/z	127	145	109	72	271	43	147	110
%	100	30	25	15	15	15	10	10

271,273 (15,5) – M^+
236 (4) – [M-35] loss of Cl to $C_8H_{15}NO_5P^+$ m/z 236.0688
226,228 (5, 2) – [M-45] loss of $CH_3CH_2NH_2$ to $C_6H_8NClO_5P^+$ m/z 225.9798 etc.
145 (30) – [M-126] $C_6H_8ClNO^+$ m/z 145.0294 etc.
127 (00) – [M-144] $(CH_3O)_2(HO)_2P^+$ $C_2H_8O_4P^+$ m/z 127.0160
72 (15) – [M-199] interesting - cannot be $(C_2H_5)_2N^+$ of phosphamidon as this is desethyl form, so probably due to CH_3CH_2NCO $C_3H_6NO^+$ m/z 72.0449

No NIST spectrum available.

Phoxim **$C_{12}H_{15}N_2O_3PS$** **M:298(10%)**

Theoretical molecular ion: m/z 298.0541 (100%), 299.0575 (13%), 300.0499 (4.5%)
Average MW: 298.30



Organophosphorus insecticide and acaricide. Used to control stored-product pests such as ants and some soil insects. Also used as a disinfectant. No longer approved for use in EU.

Acute oral LD50 for rat >2,000 mg/kg (moderate toxicity)

Usually poor GC peak shape/transmission. The mass spectra obtained for phoxim on different instruments may be surprisingly dissimilar. This may be due to different degrees of degradation. An abundant m/z103 signal appears to indicate significant conversion of phoxim to benzonitrile in the MS ion source. Such degradation effects are particularly likely to be observed at low source concentrations of phoxim.

m/z	103	109	135	76	77	81	298	50
%	100	50	40	30	30	30	10	10

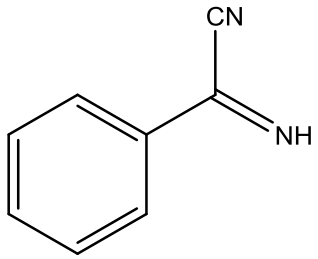
298 (10) – M^+ $C_{12}H_{15}N_2O_3PS^+$
169 (20) – [M-129] $(CH_3CH_2O)_2PSO^+$ $C_4H_{10}O_3PS^+$ m/z 169.0088
135 (40) – [M-163] $C_6H_5.C{=}NS^+$ $C_7H_5NS_2^+$ m/z 135.0143 [O/S swap]
109 (50) – [M-189] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
103 (100) – [M-195] benzonitrile $C_6H_5CN^+$ $C_7H_5N^+$ m/z 103.0422
77 (30) – [M-221] $C_6H_5^+$ m/z 77.0391

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C14816183&Units=SI&Mask=200#Mass-Spec which exhibits interesting differences. It has a base peak at m/z 109, and lower abundance m/z 103 (20%), an ion at m/z 168 (20%) rather than 169, as in this spectrum. The presence of the molecular ion indicates that this spectrum is not due to a lower MW degradation compound.

Phoxim related $C_8H_6N_2$ M:130(45%)

Benzimidoyl cyanide

Theoretical molecular ion: m/z 130.0531 (100%), 131.0565 (9%)
Average MW: 130.15



Phoxim may degrade on capillary GC to C_6H_5-C(CN)=NH, observed as a broad tailing GC peak at shorter RT than phoxim:

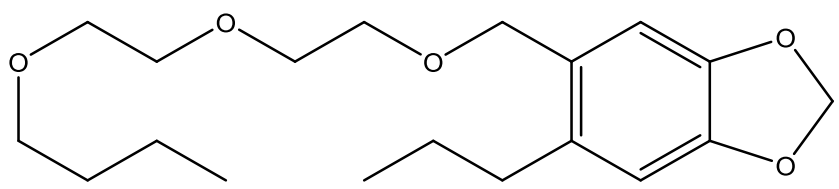
m/z	103	130	129	76	51	104	77	27
%	100	45	30	25	25	20	15	15

130 (45) – M^+
103 (100) – [M-27] loss of HCN to benzonitrile $C_6H_5CN^+$ $C_7H_5N^+$ m/z 103.0422

No NIST spectrum available.

Piperonyl butoxide $C_{19}H_{30}O_5$ M:338(5%)

Theoretical molecular ion: m/z 338.2093 (100%), 339.2127 (21%)
Average MW: 338.44



Synergist used with pyrethroid insecticides etc. to provide enhanced performance of the active ingredient. Used in the EU.

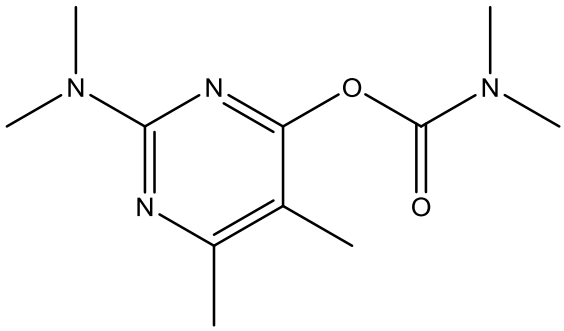
Acute oral LD50 for rat >7,000 mg/kg (low toxicity).

m/z	176	177	149	45	57	193	338	119
%	100	25	10	10	10	5	5	5

338 (5) – M^+
176 (100) – [M-162] $(OC_2H_4)(C_4H_9)(C_7H_4O_2)^+$ $C_{11}H_{12}O_2^+$ m/z 176.0834

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C51036&Mask=200#Mass-Spec

Pirimicarb **$C_{11}H_{18}N_4O_2$** **M:238(25%)**
Theoretical molecular ion: m/z 238.1430 (100%), 239.1463 (12%), 239.1400 (1.5%)
Average MW: 238.29



Carbamate insecticide. Approved for use in EU.

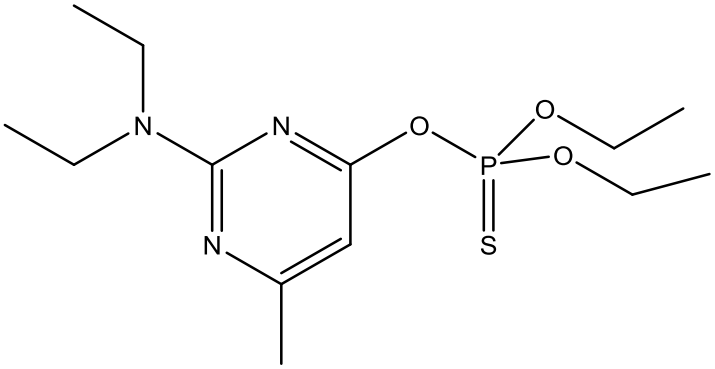
Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

m/z	166	72	238	167	123	138	152	110
%	100	90	25	10	10	10	10	5

238 (25) – M^+
166 (100) – [M-72] C8H12N3O+ m/z 166.0980
72 (90) – [M-166] dimethyl isocyanate $(CH_3)_2NCO^+$ $C_3H_6NO^+$ m/z 72.0870

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C23103982&Mask=200#Mass-Spec

Pirimiphos-ethyl **$C_{13}H_{24}N_3O3PS$** **M:333(100%)**
Theoretical molecular ion: m/z 333.1276 (100%), 334.1310 (14%)
Average MW: 333.39



Organophosphorus insecticide. No longer approved for use in EU.

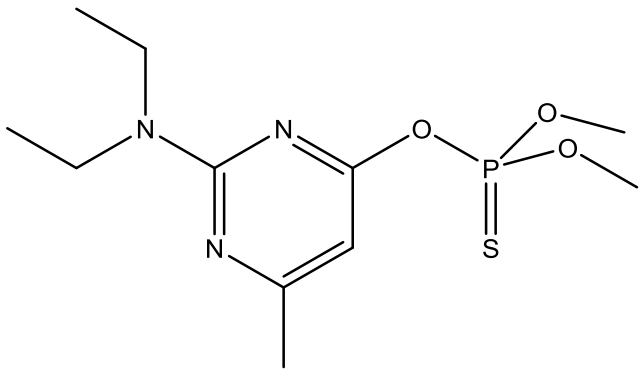
Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

m/z	333	318	304	168	180	152	166	109
%	100	95	80	45	40	40	35	25

333 (100) – M^+ $C_{13}H_{24}N_3O_3PS^+$ m/z
318 (95) – [M-15] loss of CH_3 to $C_{12}H_{21}N_3O_3PS^+$ m/z 318.1041
304 (80) – [M-29] loss of CH_3CH_2 to $C_{11}H_{19}N_3O_3PS^+$ m/z 304.0885
290 (30) – [M-43] loss of C_3H_7 to $C_{10}H_{17}N_3O_3PS^+$ m/z 290.0728
180 (30) – [M-153] loss of $(CH_3CH_2O)_2PS$ to $C_9H_{14}N_3O^+$ m/z 180.1137
168 (45) – [M-165] loss of $(CH_3CH_2O)_2PO$ & C_2H_4 to $C_7H_{10}N_3S^+$ m/z 168.0595
166 (35) – [M-167]
152 (40) – [M-181] loss of $(CH_3CH_2O)_2PS$ & C_2H_4 to $C_7H_{10}N_3O^+$ m/z 152.0824
125 (50) – [M-208] $(CH_3CH_2O)(HO)PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (25) – [M-224] $(CH_3CH_2O)(HO)PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (20) – [M-236] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
93 (30) – [M-240] $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C23505411&Mask=200#Mass-Spec
though some ions missing (m/z 151, 167, 281), probably because of poor MS resolution.

Pirimiphos-methyl **$C_{11}H_{20}N_3O_3PS$** **M:305(85%)**
Theoretical molecular ion: m/z 305.0963 (100%), 306.0997 (12%)
Average MW: 305.33



Organophosphorus insecticide and acaricide. Used as fumigant to control a wide range of insects and mites in stores, animal houses, domestic and industrial premises. Approved for use in EU.

Acute oral LD50 for rat approx. 1,000 mg/kg (moderate toxicity).

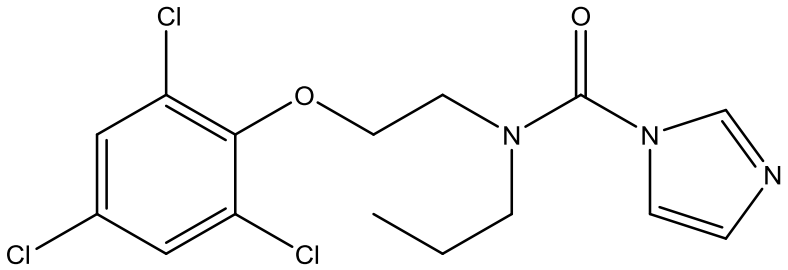
m/z	290	276	305	125	233	180	262	93
%	100	90	85	50	40	30	30	30

Assignments confirmed by accurate mass study (GCT Cardiff)
305 (85) – M^+ $C_{11}H_{20}N_3O_3PS^+$ m/z 305.0963
290 (100) – [M-15] loss of CH_3 to $C_{10}H_{17}N_3O_3PS^+$ m/z 290.0728
276 (90) – [M-29] loss of CH_3CH_2 to $C_9H_{15}N_3O_3PS^+$ m/z 276.0572
262 (30) – [M-43] loss C_3H_7 to $C_8H_{13}N_3O_3PS^+$ m/z 262.0415

233 (40) – [M-72] loss of $(C_2H_5)_2N$ to $C_7H_{10}N_2O_3PS^+$ m/z 233.0150
180 (30) – [M-125] loss of $(CH_3O)_2PS$ to $C_9H_{14}N_3O^+$ m/z 180.1137
141 (20) – [M-164] $C_2H_6O_2PS^+$ m/z 140.9775
125 (50) – [M-180] $(CH_3O)_2PS^+$ $C_2H_6O_2PS^+$ m/z 124.9826
93 (30) – [M-212] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C29232937&Mask=200#Mass-Spec

Prochloraz **$C_{15}H_{16}Cl_3N_3O_2$** **M:375,377,379(0,0,0%)**
Theoretical molecular ion: m/z 375.0308 (100%), 377.0279 (96%), 379.0249 (31%)
Average MW: 376.66



Conazole/amide fungicide. Sometimes sold as manganese complex. Approved for use in EU.

Acute oral LD50 for rat approx. 1,000 mg/kg (moderate toxicity).

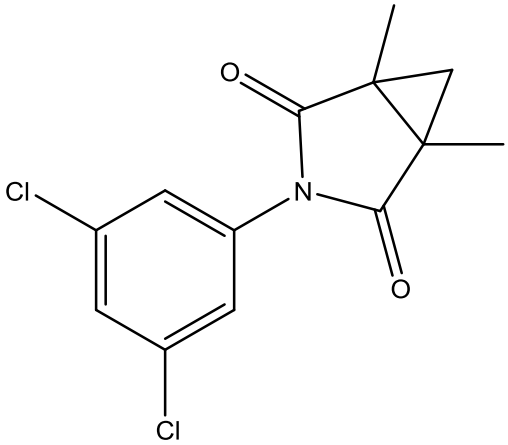
Rather long GC RT and sometimes poor GC transmission/peak shape.

m/z	43	70	180	308	310	266	268	312
%	100	80	55	20	20	15	15	10

375 (0) – M^+ absent
308,310,312 (20,20,10) – [M-67] loss of $(C_3H_3N_2)$ to $C_{12}H_{13}Cl_3NO_2^+$ m/z 308.0012 etc.
266,268,270 (15,15,5) – [M-109] loss of $(C_3H_3N_2CO)$ & CH2 to $C_{10}H_{11}Cl_3NO^+$ m/z 265.9906 etc.
180 (55) – [M-195] loss of $Cl_3C_6H_2O$ to $C_9H_{14}N_3O^+$ m/z 180.1137
70 (85) – [M-305] $CH_2CH_2NCO^+$ $C_3H_4NO^+$ m/z 70.0293
43 (100) – [M-332] $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C67747095&Mask=200#Mass-Spec

Procymidone **$C_{13}H_{11}Cl_2NO_2$** **M:283,285(35,25%)**
Theoretical molecular ion: m/z 283.0167 (100%), 285.0137 (64%), 287.0108 (10%)
Average MW: 284.14



Dicarboximide fungicide. Widely used in horticulture as a seed dressing, pre-harvest spray or post-harvest dip for the control of various diseases. No longer approved for use in EU.

Acute oral LD50 for rat > 5,000 mg/kg (low toxicity).

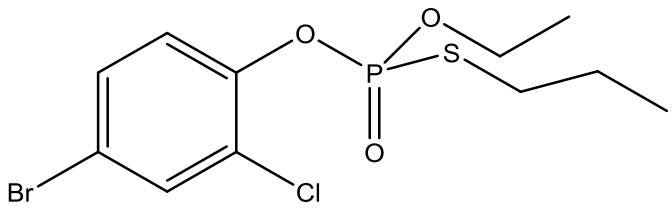
The toxic metabolite 3,5-dichloroaniline may be important (see iprodione degradation II).

m/z	96	283	67	68	41	53	285	39
%	100	35	35	35	25	25	25	15

283,285 (35,25) – M^+ $C_{14}H_{11}Cl_2NO_2^+$ m/z
96 (100) – [M-187] ring scission and loss of dichlorophenyl isocyanate to $C_6H_8O^+$ m/z 96.0575
68 (35) – [M-215] $CH_3(C_3H_2)CH_3^+$ $C_5H_8^+$ m/z 68.0626
67 (35) – [M-216] $CH_3(C_3H_2)CH_2^+$ $C_5H_7^+$ m/z 67.0548
53 (25) – [M-230] $CH_3(C_3H_2)^+$ $C_4H_5^+$ m/z 53.0391
39 (15) – [M-244] $(C_3H_3)^+$ $C_3H_3^+$ m/z 39.0235

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C32809168&Mask=200#Mass-Spec

Profenofos **$C_{11}H_{15}BrClO_3PS$** **M:372,374,376(25,30,10%)**
Theoretical molecular ion: m/z 371.9351 (100%), 373.9331 (97%), 375.9302 (31%)
Average MW: 373.63



Organophosphorus insecticide. No longer approved for use in EU.

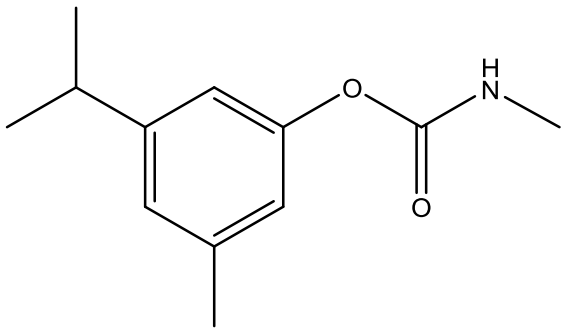
Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

m/z	139	43	97	208	339	337	206	125
%	100	90	85	70	55	55	45	45

372,374,376 (25,30,10) – M^+
337,339 (55,55) – [M-35] loss of Cl to $C_{11}H_{15}BrO_3PS^+$ m/z 336.9663 etc.
206,208,210 (50,70,15) – [M-166] $BrClC_6H_3OH^+$ $C_6H_4BrClO^+$ m/z 205.9134 etc.
139 (100) – [M-233] $(C_3H_7S)(HO)P{=}O^+$ $C_3H_8O_2PS^+$ m/z 138.9983
125 (45) – [M-247]] $(CH_3CH_2O)(HS)P{=}O^+$ $CH_6O_2PS^+$ m/z 124.9826 - not usual OP m/z 125!
97 (85) – [M-275] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9413
43 (90) – [M-329] $CH_3CH_2CH_2^+$ $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C41198087&Mask=200#Mass-Spec

Promecarb **$C_{12}H_{17}NO_2$** **M:207(1%)**
Theoretical molecular ion: m/z 207.1259 (100%), 208.1293 (13%)
Average MW: 207.27



Carbamate insecticide. No longer approved for use in EU.

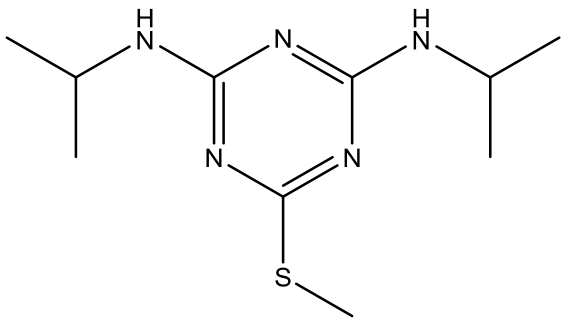
Acute oral LD50 for rat approx 30 mg/kg (high toxicity).

m/z	135	150	57	91	136	107	117	151
%	100	65	15	15	10	10	10	10

207 (1) – M^+
150 (65) – [M-57] loss of methyl isocyanate CH3NCO to phenol C10H14O+ m/z 150.2210
135 (100) – [M-72] loss of CH3NCO & CH3 to C9H11O+ m/z 135.0810

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2631370&Mask=200#Mass-Spec
N.B with incorrect empirical formula and MW – "$C_{12}H_{16}NO_2$, MW 206.26"

Prometryn **$C_{10}H_{19}N_5S$** **M:241(90%)**
Theoretical molecular ion: m/z 241.1361 (100%), 242.1395 (11%), 243.1319 (4.5%)
Average MW: 241.36



Methylthiotriazine herbicide. No longer approved for use in EU.

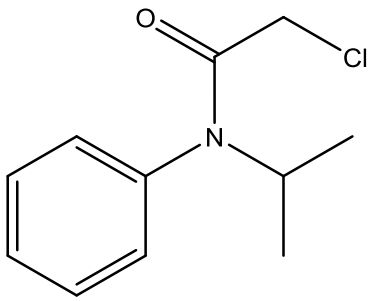
Acute oral LD50 for rat >2,000 (moderate toxicity).

m/z	58	241	184	226	43	106	68	69
%	100	90	65	60	55	45	40	35

241 (90) – M^+
226 (60) – [M-15] loss of CH_3 to $C_9H_{16}N_5S^+$ m/z 226.1126
184 (65) – [M-57] loss of $(CH_3)_2CNH$ to $C_7H_{12}N_4S^+$ m/z 184.2610
58 (100) – [M-183] $(CH_3)_2CHNH^+$ $C_3H_8N^+$ m/z 58.1040

Cf. similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C7287196&Mask=200#Mass-Spec

Propachlor **$C_{11}H_{14}ClNO$** **M:211,213(10,3%)**
Theoretical molecular ion: m/z 211.0764 (100%), 213.0734 (32%)
Average MW: 211.69



Chloroacetanilide herbicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity).

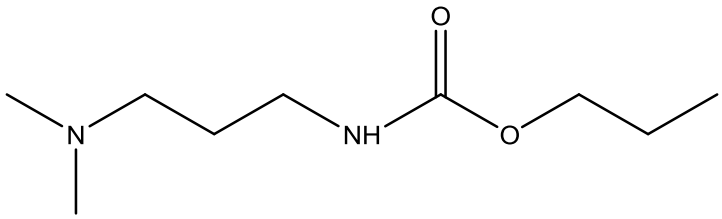
m/z	120	176	93	57	77	43	169	196
%	100	40	35	30	25	25	15	10

211,213 (10,3) – M^+
196,198 (10,3) – [M-15] loss of CH_3 to $C_{10}H_{11}ClNO^+$ m/z 196.0529 etc.
176 (40) – [M-35] loss of Cl to $C_{11}H_{14}NO^+$ m/z 176.1075
120 (100) – [M-91] $C_6H_5NCOH^+$ $C_7H_6NO^+$ m/z 120.0449
93 (35) – [M-118] aniline $C_6H_5NH_2^+$ $C_6H_7N^+$ m/z 93.0579

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1918167&Mask=200#Mass-Spec

Propamocarb **$C_9H_{20}N_2O_2$** **M:188(5%)**

Theoretical molecular ion: m/z 188.1525 (100%), 189.1558 (10%)
Average MW: 188.27



Carbamate fungicide. Used for specific control of *Phycomycetes* and effective against *Phytophthora spp*. and *Pythium spp*. Normally used as the hydrochloride salt. Approved for use in EU.

Acute oral LD50 for rat approx. 2,000 mg/kg (moderate toxicity).

Poor GC transmission/peak shape.

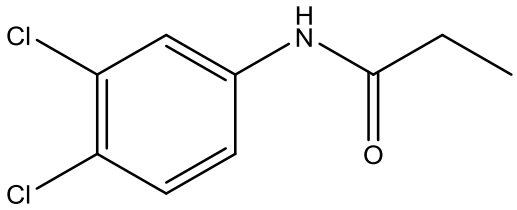
m/z	58	31	42	59	129	188	72	84
%	100	20	10	10	5	5	5	5

188 (5) – M^+
129 (5) – [M-58] loss of C_3H_7O to $C_6H_{13}N_2O^+$ m/z 129.1028
58 (100) – [M-130] $(CH_3)_2NCH_2^+$ $C_3H_8N^+$ m/z 58.0657

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C24579735&Mask=200#Mass-Spec

Propanil **$C_9H_9Cl_2NO$** **M:217,219,221(20,10,3%)**

Theoretical molecular ion: m/z 217.0061 (100%), 219.0032 (64%), 221.0002 (10%)
Average MW: 218.08



Anilide herbicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 1,000 mg/kg (moderate toxicity).

May exhibit poor GC transmission.

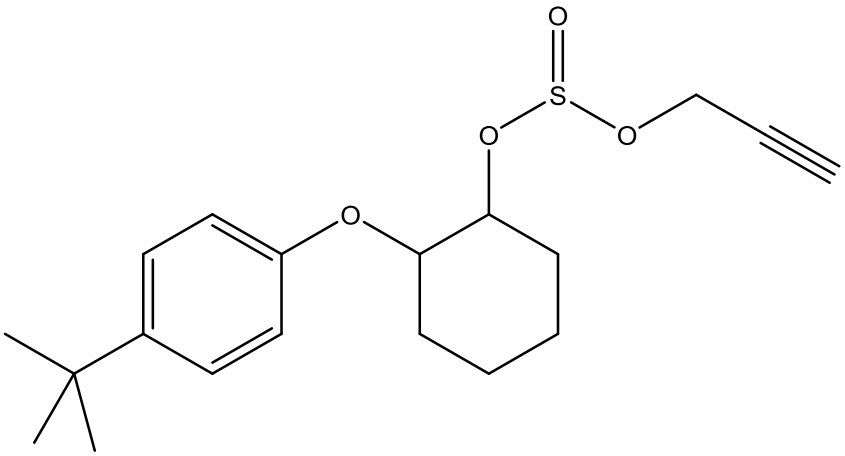
m/z	161	163	57	29	217	165	219	126
%	100	60	45	40	20	10	10	10

217,219 (20,10) – M^+
161,163 (100,60) – [M-56] dichloroaniline $C_6H_5Cl_2N^+$ m/z 160.9799 etc.
57 (45) – [M-160] $COCH_2CH_3^+$ $C_3H_5O^+$ m/z 57.0340

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C709988&Mask=200#Mass-Spec

Propargite $C_{19}H_{26}O_4S$ **M:350(15%)**

Theoretical molecular ion: m/z 350.1552 (100%), 351.1585 (21%), 352.1510 (4.5%)
Average MW: 350.47



Acaricide. Used for mite control on various field, fruit, vegetable and ornamental crops. No longer approved for use in EU.

Acute oral LD50 for rat approx. 2,500 mg/kg (low toxicity).

Sometimes poor GC transmission/peak shape.

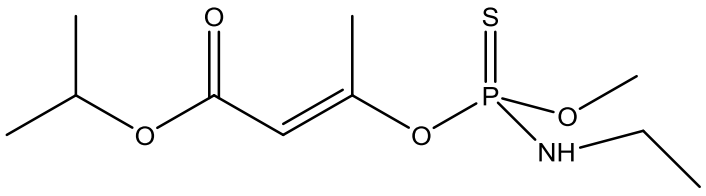
m/z	135	81	173	39	57	41	150	350
%	100	50	50	50	50	45	20	15

350 (15) – M^+
173 (50) – [M-177] scission of cyclohexane ring to $C_4H_6O.SO.OCH_2C{\equiv}CH$ $C_7H_9O_3S^+$ m/z 173.0272
135 (100) – [M-215] $(CH_3)_2C.C_6H_5.OH^+$ $C_9H_{11}O^+$ m/z 135.0910
81 (50) – [M-269] from cyclohexane moiety $C_6H_9^+$ m/z 81.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2312358&Mask=200#Mass-Spec

Propetamphos $C_{10}H_{20}NO_4PS$ **M:281(0%)**

Theoretical molecular ion: m/z 281.0851 (100%), 282.0884 (11%), 283.0809 (4.5%)
Average MW: 281.31



Organophosphorus phosphoramidothioate insecticide and acaricide. Used for household and public health control of cockroaches, flies, ants, ticks, moths, fleas and mosquitoes. Not approved for use in EU.

Acute oral LD50 for rat approx. 100 mg/kg (moderate toxicity).

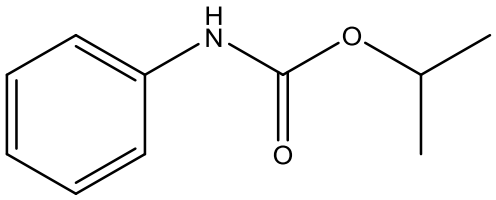
m/z	138	44	194	236	110	122	156	111
%	100	60	35	25	25	25	15	15

281 (0) – M^+ absent
236 (25) – [M-45] loss of $CH_3CH_2NH_2$ to $C_8H_{13}O_4PS^+$ m/z 236.0272
194 (35) – [M-187] loss of $(CH_3)_2CHO.CO$ to $C_6H_{13}NO_2PS^+$ m/z 194.0405
156 (15) – [M-125] $(CH_3O)(C_2H_5NH)P(SH)(OH)^+$ $C_3H_{11}NO_2PS^+$ m/z 156.0248
138 (100) – [M-143] $(CH_3O)(C_2H_5NH)P{=}S^+$ $C_3H_9NOPS^+$ m/z 138.0143
122 (25) – [M-143] $(CH_3O)(C_2H_5NH)P{=}O^+$ $C_3H_9NO_2P^+$ m/z 122.0371
110 (25) – [M-171] $(CH_3O)(NH_2)P{=}S^+$ CH_5NOPS^+ m/z 109.9830
106 (10) – [M-175] $(CH_3O)(C_2H_5NH)P^+$ $C_3H_9NOP^+$ m/z 106.0422
44 (60) – [M-237] $CH_3CH_2NH^+$ $C_2H_6N^+$ m/z 44.0770

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C31218834&Mask=200#Mass-Spec

Propham **$C_{10}H_{13}NO_2$** **M:179(50%)**

Theoretical molecular ion: m/z 179.0946 (100%), 180.0980 (11%)
Average MW: 179.22



Carbanilate herbicide. No longer approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

The data presented differ from those reported by Cairns (1983), in which the base peak is given as m/z 92.

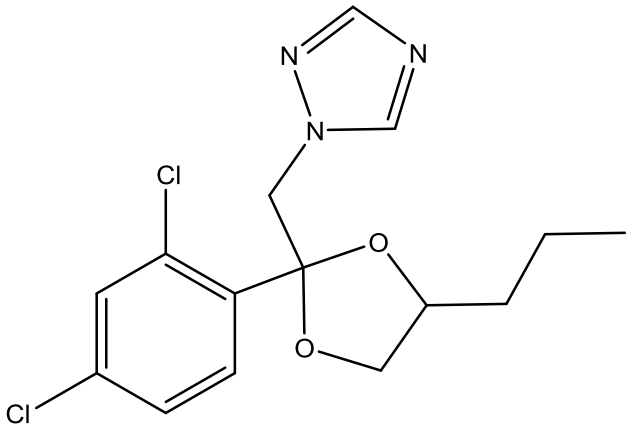
m/z	93	43	119	179	137	120	91	65
%	100	85	55	50	40	35	25	20

179 (50) – M^+
93 (100) – [M-186] aniline $C_6H_7N^+$ m/z 93.0579
43 (85) – [M-136] $(CH_3)_2CH^+$ $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C122429&Mask=200#Mass-Spec

Propiconazole **$C_{15}H_{17}Cl_2N_3O_2$** **M:341(0%)**

Theoretical molecular ion: m/z 341.0698 (100%), 343.0668 (64%), 345.0639 (10%)
Average MW: 342.22



Conazole fungicide. Broad activity against diseases caused by *Cochliobolus sativus*, *Erysiphe graminis* and *Leptosphaeria nodorum*. Approved for use in EU.

Acute oral LD50 for rat approx. 900 mg/kg (moderate toxicity).

Its diastereoisomers may be resolved on capillary GC (peak areas 1:3).

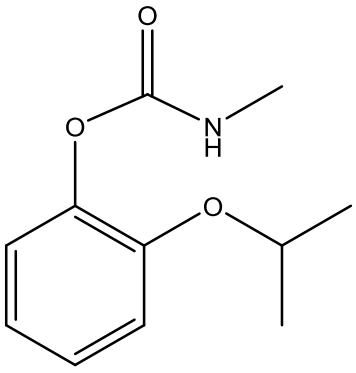
m/z	69	173	259	41	175	261	191	128
%	100	50	40	40	30	25	20	15

341 (0) – M+
259,261 (40,25) – [M-82] loss of $(C_2H_2N_3)CH_2$ to $C_{12}H_{13}Cl_2O_2^+$ m/z 259.0293
173,175 (50,30) – [M-168] scission of dioxolane to liberate $Cl_2C_6H_3CO^+$ $C_7H_3Cl_2O^+$ m/z 172.9561 etc.
69 (100) – [M-272] triazole moiety $C_2H_3N_3$+ m/z 69.0327

No NIST spectrum available, but very similar spectrum in Flamini (2010), page 300.

Propoxur **$C_{11}H_{15}NO_3$** **M:209(1%)**

Theoretical molecular ion: m/z
Average MW:



Carbamate insecticide and acaricide. No longer approved for use in EU.

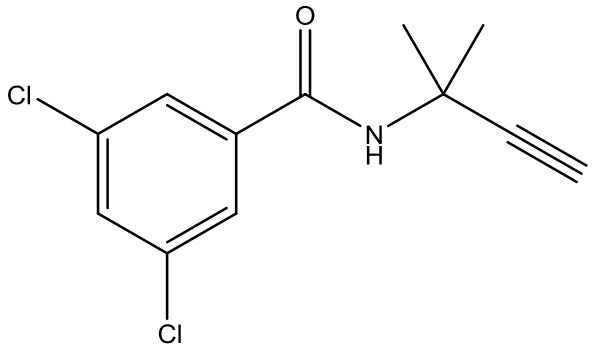
Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

m/z	110	57	41	39	52	56	152	80
%	100	50	35	25	20	20	15	10

209 (1) – M^+ weak or absent
152 (15) – [M-57] loss of CH_3NCO to $C_9H_{12}O_2^+$ m/z 152.0837
110 (100) – [M-99] loss of CH_3NCO & C_3H_6 to dihydroxybenzene $C_6H_6O_2^+$ m/z 110.0368

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C114261&Mask=200#Mass-Spec

Propyzamide **$C_{12}H_{11}Cl_2NO$** **M:255,257,259(25,15,3%)**
Theoretical molecular ion: m/z 255.0218 (100%), 257.0188 (64%), 259.0159 (10%)
Average MW: 256.13



Amide herbicide. Residual action for use in a wide range of crops to control annual and perennial grasses and some broad-leaved weeds. Approved for use in EU.

Acute oral LD50 for rat >2,500 mg/kg (low toxicity).

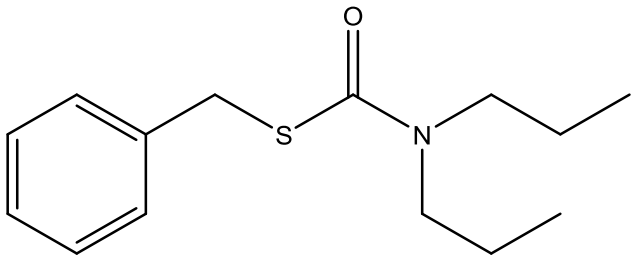
m/z	173	175	145	255	41	147	84	254
%	100	65	35	25	25	20	15	15

255,257,259 (25,15,3) – M^+
254,256,258,(15,25,15,15,3,3) – [M-1] curious appearance of molecular ion cluster due to facile deprotonation
240,242,244(10,5,1) – [M-15] loss of CH_3 to C11H8Cl2NO+ m/z 239.9983 etc.
173,175 (100,65) – [M-82] $Cl_2C_6H_4CO^+$ $C_7H_3Cl_2O^+$ m/z 172.9561 etc.
145,147 (35,20) – [M-110] $Cl_2C_6H_4^+$ $C_6H_3Cl_2^+$ m/z 144.9612 etc.

Cf. similar but weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C23950585&Mask=200#Mass-Spec

Prosulfocarb $C_{14}H_{21}NOS$ **M:251(15%)**

Theoretical molecular ion: m/z 251.1344 (100%), 252.1377 (15%), 253.1302 (4.5%)
Average MW: 251.39



Thiocarbamate herbicide. Used for post-emergence control of grass and broad-leaved weeds in a wide range of crops. Approved for use in EU.

Acute oral LD50 for rat approx. 1,800 mg/kg (moderate toxicity).

Sometimes poor GC transmission/peak shape.

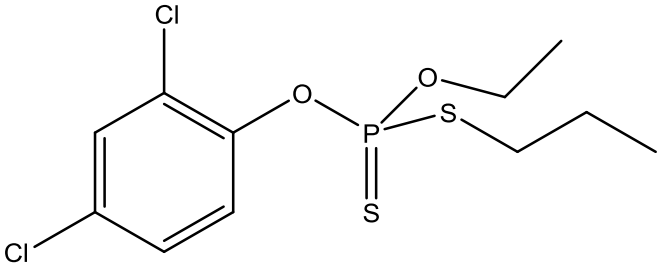
m/z	43	91	128	86	41	65	251	162
%	100	65	60	35	20	15	15	10

251 (15) – M^+
128 (60) – [M-123] $(C_3H_7)_2NCO^+$ $C_7H_{14}NO^+$ m/z 128.1075
91 (65) – [M-160] $C_6H_5CH_2^+$ tropylium ion $C_7H_7^+$ m/z 91.0548
43 (100) – [M-208] $C_3H_7^+$ m/z 43.0548

Cf. weak spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C52888809&Mask=200#Mass-Spec with less abundant m/z 43 ion (30%).

Prothiofos / Tokuthion $C_{11}H_{15}Cl_2O_2PS_2$ **M:344,346(1,1%)**

Theoretical molecular ion: m/z 343.9628 (100%), 345.9599 (64%), 347.9569 (10.2%)
Average MW: 345.23



Organophosphorus insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 900 mg/kg (moderate toxicity).

m/z	43	113	267	162	309	155	164	41
%	100	85	65	65	55	55	45	40

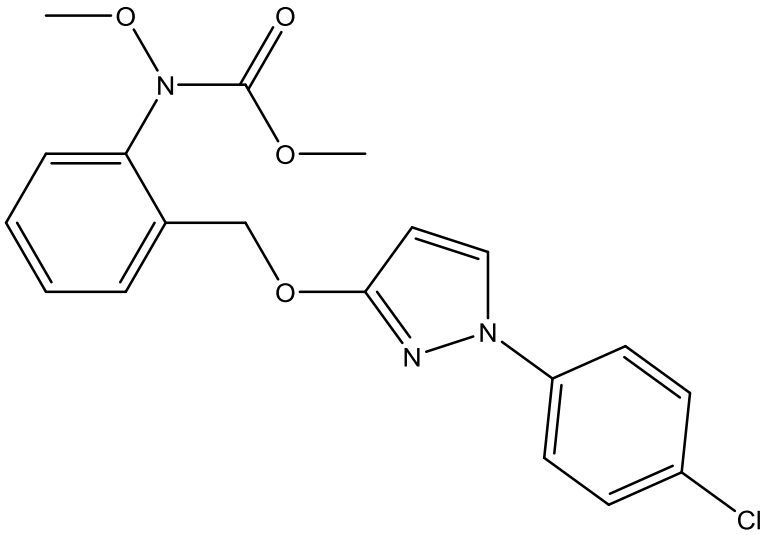
Assignments confirmed by accurate mass (Cardiff GCT)
344,346 (1,1) – M^+ weak $C_{11}H_{15}Cl_2O_2PS_2^+$
309,311 (55,20) – [M-35] loss of Cl to $C_{11}H_{15}ClO_2PS_2^+$ m/z 308.9940 etc.

302,304 (10,5) – [M-42] loss of C_3H_6 to $C_8H_9Cl_2O_2PS_2^+$ m/z 301.9159 etc.
281,283 (15,5) – [M-63] loss of Cl & C_2H_4 to $C_8H_9ClO_2PS_2^+$ m/z 280.9627 etc.
267,269 (65,20) – [M-77] loss of Cl & C_3H_6 to $C_8H_9ClO_2PS_2^+$ m/z 266.9470 etc.
255,257,259 (10,10,3) – [M-89] loss of C_2H_5 & C_3H_7 & OH to $C_6H_2Cl_2OPS_2^+$ m/z 254.8662 etc.
239,241,243 (45,30,10) – [M-105] interesting fragment. The NIST spectrum indicates presence of 2Cl atoms. Accurate mass indicates loss of $C_4H_{10}OP$ (or C_4H_9OS, C_8H_9, C_7H_5O), but difficult to see how this could be formed. Loss of $C_4H_{10}OP$ would give $C_7H_5Cl_2OS_2^+$ m/z 238.9159 etc.
183 (30) – [M-161] $(CH_3CH_2O)(CH_3CH_2CH_2S)P{=}S^+$ $C_5H_{12}OPS_2^+$ m/z 183.0067
162,164,166 (65,45,10) – [M-182] dichlorophenol $Cl_2C_6H_3OH^+$ $C_6H_4Cl_2O^+$ m/z 161.9639 etc.
155 (55) – [M-189] $(HO)(CH_3CH_2CH_2S)P{=}S^+$ $C_3H_8OPS_2^+$ m/z 154.9754
141 (30) – [M-203] $(CH_3CH_2O)(HS)P{=}S^+$ $C_2H_6OPS_2^+$ m/z 140.9598
133,135 (30,20) – [M-211] $C_5H_3Cl_2^+$ m/z 132.9612 etc.
113 (85) – [M-231] $(HO)(HS)PS^+$ $H_2OPS_2^+$ m/z 112.9285
98 (20) – [M-246] $C_5H_3Cl^+$ m/z 97.9923 etc.
73 (30) – [M-271] $C_3H_2Cl^+$ m/z 72.9835 etc.
63 (150) – [M-281] $C_5H_3^+$ m/z 63.0235
63 (20) – [M-281] PS^+ m/z 62.9458
43 (100) – [M-301] $CH_3CH_2CH_2^+$ $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C34643464&Mask=200#Mass-Spec
listed as "Phosphorodithioic acid, O-(2,4-dichlorophenyl) O-ethyl S-propyl ester"

Pyraclostrobin **$C_{19}H_{18}ClN_3O_4$** **M:387,389(0,0%)**

Theoretical molecular ion: m/z 387.0986 (100%), 389.0956 (32%)
Average MW: 387.82



Strobilurin fungicide. Protective and curative action. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

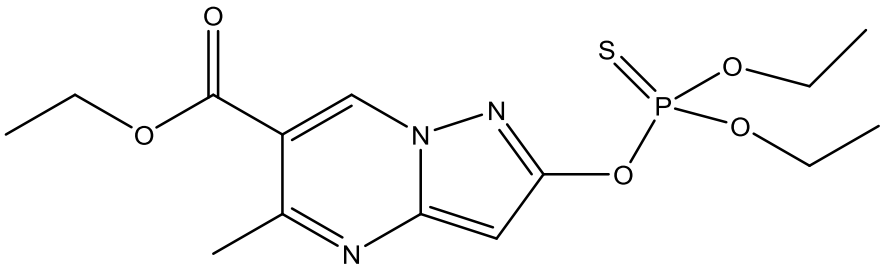
m/z	132	164	111	77	133	104	75	325
%	100	25	11	9	9	6	5	4

Assignments confirmed by accurate mass (Cardiff GCT)
387,389 (0,0) – M^+ absent
325,327 (4,1) – [M-62] loss of $2CH_3O$ to isocyanate $C_{17}H_{12}ClN_3O_2^+$ m/z 325.0618 etc.
164 (25) – [M-223] $(CH_3O)(CHO)N.C_6H_4.CH_2^+$ $C_9H_{10}NO_2^+$ m/z 164.0712
132 (100) – [M-255] $OCN.C_6H_4.CH_2^+$ $C_8H_6NO^+$ m/z 132.0449

111,113 (11,3) – [M-276] $C_6H_4Cl^+$ m/z 111.0002 etc.
104 (6) – [M-283] $C_7H_6N^+$ m/z 104.0494
77 (15) – [M-310] $C_6H_5^+$ m/z 77.0391

No NIST spectrum. Data from Restek website http://www.restek.com/compound/view/175013-18-0/Pyraclostrobin

Pyrazophos **$C_{14}H_{20}N_3O_5PS$** **M:373(30%)**
Theoretical molecular ion: m/z 373.0861 (100%), 374.0895 (15.1%), 375.0819 (4.5%)
Average MW: 373.36



Organophosphorus fungicide. Not approved for use in EU.

Acute oral LD50 for rat approx. 150 mg/kg (moderate toxicity).

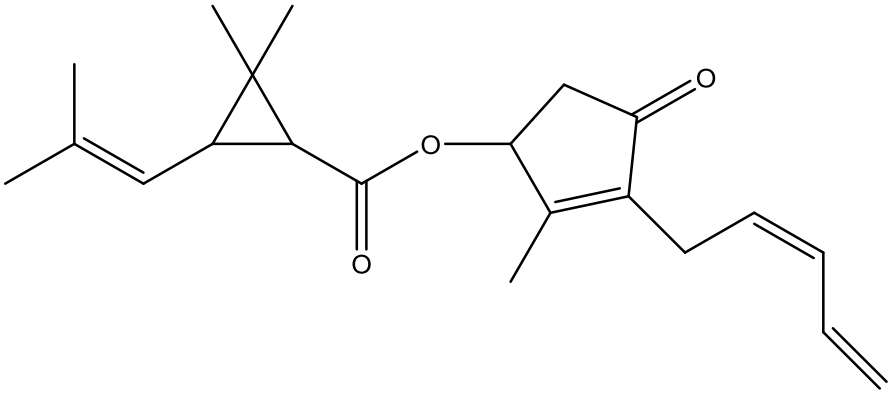
m/z	221	232	373	237	222	265	193	97
%	100	40	30	20	15	15	10	10

Assignments confirmed by accurate mass (Cardiff GCT)
373 (30) – M^+ $C_{14}H_{20}N_3O_5PS^+$ m/z 373.0861
345 (10) – [M-28] loss of C_2H_4 to $C_{12}H_{16}N_3O_5PS^+$ m/z 345.0548
328 (10) – [M-45] loss of CH_3CH_2O to $C_{12}H_{15}N_3O_4PS^+$ m/z 328.0521
300 (10) – [M-73] loss of C_4H_9O to $C_{10}H_{11}N_3O_4PS^+$ m/z 300.0208
265 (10) – [M-108] loss of $C_2H_5O_3P$ to $C_{12}H_{15}N_3O_2S^+$ m/z 265.0885
252 (10) – [M-121] loss of $C_4H_{10}O_2P$ to $C_{10}H_{10}N_3O_3S^+$ m/z 252.0443
237 (20) – [M-136] $CH_3CH_2OCO(C_7H_5N_3)SH^+$ $C_{10}H_{11}N_3O_2S^+$ m/z 237.0572
232 (40) – [M-141] loss of $C_2H_6O_3PS$ to $C_{12}H_{14}N_3O_2^+$ m/z 232.1086
221 (100) – [M-152] $CH_3CH_2OCO(C_7H_5N_3)OH^+$ $C_{10}H_{11}N_3O_3^+$ m/z 221.0800
204 (10) – [M-169] loss of $C_4H_{10}O_3PS$ to $C_{10}H_{10}N_3O_2^+$ m/z 204.0773
193 (10) – [M-180] $HOCO(C_7H_5N_3)OH^+$ $C_8H_7N_3O_3^+$ m/z 193.0487
176 (15) – [M-197] $CO(C_7H_5N_3)OH^+$ $C_8H_6N_3O_2^+$ m/z 176.0460
125 (5) – [M-248] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
97 (10) – [M-276] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
65 (5) – [M-308] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. nice spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C13457186&Mask=200#Mass-Spec

Pyrethrin I **$C_{21}H_{28}O_3$** **M:328(1%)**

Theoretical molecular ion: m/z 328.2038 (100%), 329.2072 (22.7%)
Average MW: 328.45



(Z) –(S)-pyrethrolone alcohol + (1R)-trans-chrysanthemic acid

A natural insecticide. See also cinerin I and II and jasmolin I and II.

See Pattenden (1973) for MS study of the pyrethrins and related compounds.

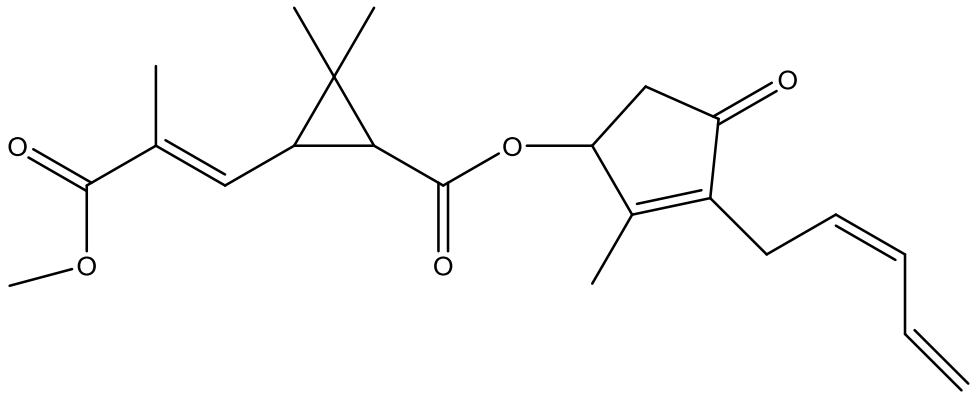
m/z	123	93	79	135	41	107	81	168
%	100	25	25	20	20	20	15	10

328 (1) – M^+
168 (10) – [M-160] $C_{10}H_{16}O_2^+$ m/z 168.1150
135 (20) – [M-193]
123 (100) – [M-205] $(CH_3)_2C{=}CH.C_3H_3(CH_3)_2^+$ $C_9H_{15}^+$ m/z 123.1174

No NIST spectrum available

Pyrethrin II **$C_{22}H_{28}O_5$** **M:372(1%)**

Theoretical molecular ion: m/z 372.1937 (100%), 373.1970 (23.8%)
Average MW: 372.19



(1R)-trans-pyrethric acid + (Z) –(S)-pyrethrolone alcohol

See cinerin I and II and jasmolin I and II (also natural pyrethrins).

m/z	133	160	161	107	166	91	105	41
%	100	85	80	80	75	70	55	45

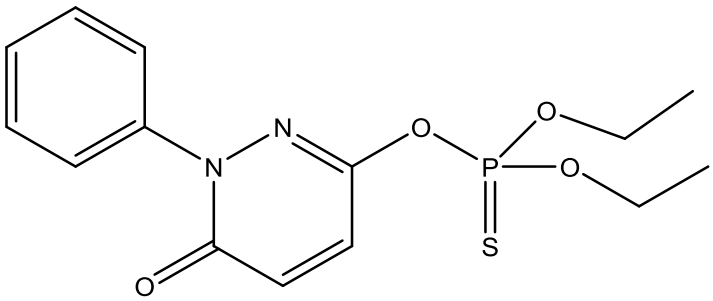
372 (1) – M^+
341 (2) – [M-31] $C_{21}H_{25}O_4^+$ m/z 341.1753
166 (75) – [M-206] $C_{10}H_{14}O_2^+$ m/z 166.0994
160 (85) – [M-212]
133 (100) – [M-239]

Pyrethrum, natural pyrethrins

Natural, botanical insecticide. An extract of *Chrysanthemum cinerariaefolium*. Six main esters:
Cinerin I – cinerolone chrysanthemate
Cinerin II – cinerolone pyrethrate
Jasmolin I – jasmolone chrysanthemate
Jasmolin II - jasmolone pyrethrate
Pyrethrin I - pyrethrolone chrysanthemate
Pyrethrin II – pyrethrolone pyrethrate

Pyridaphenthion $C_{14}H_{17}N_2O_4PS$ M:340(100%)

Theoretical molecular ion: m/z 340.0647 (100%), 341.0680 (15.1%), 342.0605 (4.5%)
Average MW: 340.34



Organophosphorus insecticide. Not approved for use in EU.

Acute oral LD50 for rat approx. 750 mg/kg (moderate toxicity).

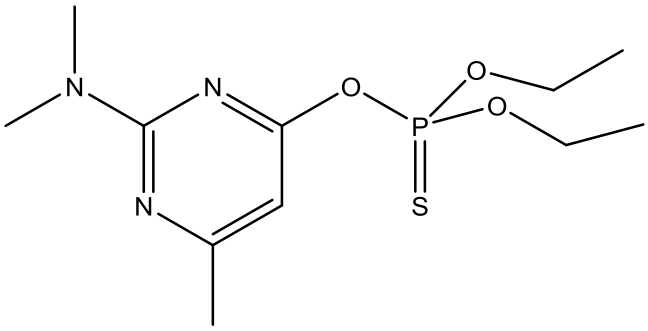
m/z	340	97	199	188	77	125	204	109
%	100	85	80	70	60	50	45	25

Assignments confirmed by accurate mass (Cardiff GCT)
340 (100) – M^+ $C_{14}H_{17}N_2O_4PS^+$ m/z 340.0572
204 (20) – [M-136] $C_6H_5(C_4H_2N_2O)SH^+$ $C_{10}H_8N_2OS^+$ m/z 204.0357 [O/S swap]
199 (80) – [M-141] loss of $C_2H_6O_3PS$ to $C_{12}H_{11}N_2O^+$ m/z 199.0871 - rearrangement & transfer of ethyl
188 (70) – [M-152] $C_6H_5(C_4H_2N_2O)OH^+$ $C_{10}H_8N_2O_2^+$ m/z 188.0586
125 (50) – [M-215] $(C_2H_5O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
109 (25) – [M-231] $(C_2H_5O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (85) – [M-243] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
82 (15) – [M-258] $C_4H_2O_2^+$ m/z 82.0055
77 (60) – [M-263] $C_6H_5^+$ m/z 77.0391
65 (20) – [M-275] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
54 (15) – [M-286] $C_3H_2O^+$ m/z 54.0106
51 (10) – [M-289] $C_4H_3^+$ m/z 51.0235

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C119120&Mask=200#Mass-Spec listed under "Phosphorothioic acid, O-(1,6-dihydro-6-oxo-1-phenyl-3-pyridazinyl) O,O-diethyl ester"

Pyrimitate **$C_{11}H_{20}N_3O_3PS$** **M:305(70%)**

Theoretical molecular ion: m/z 305.0963 (100%), 306.09965 (11.9%), 307.0921 (4.5%)
Average MW: 305.33



Organophosphorus insecticide and acaricide. Not approved for use in EU.

Acute oral LD50 for rat approx. 125 mg/kg (moderate toxicity).

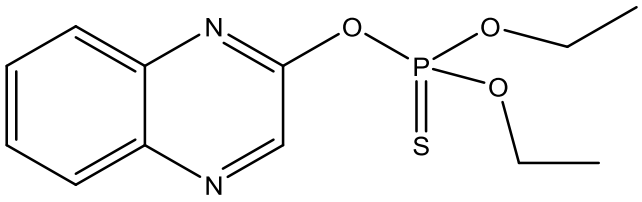
m/z	153	305	180	44	124	95	43	71
%	100	70	40	35	30	30	25	25

305 (70) – M^+ $C_{11}H_{20}N_3O_3PS^+$
180 (40) – [M-125] rearrangement to $(CH_3)_2N.C_4HN_2(CH_3)OCH_2CH_2^+$ $C_9H_{14}N_3O^+$ m/z 180.11369
153 (100) – [M-152] $(CH_3)_2N.C_4HN_2(CH_3)OH^+$ $C_7H_{11}N_3O^+$ m/z 153.0902
(and $(CH_3CH_2O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139 – but sulphur isotope too weak?)
124 (30) – [M-181] loss of CHO from phenol to $C_6H_{10}N_3^+$ m/z 124.0875
44 (35) – [M-261] $(CH_3)_2N^+$ $C_2H_6N^+$ m/z 44.0500

Cf. weak and noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C5221498&Units=SI&Mask=200#Mass-Spec which shares three most abundant ions, but other ions are lost in the background noise.

Quinalphos **$C_{12}H_{15}N_2O_3PS$** **M:298(25%)**

Theoretical molecular ion: m/z 298.0541 (100%), 299.05745 (13.0%), 300.0499 (4.5%)
Average MW: 298.30



Organophosphorus insecticide. Used against a range of insect pests including caterpillars, aphids, mealy bugs and mites. Not approved for use in EU.

Acute oral LD50 for rat approx. 70 mg/kg (high toxicity).

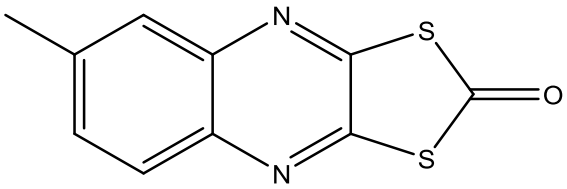
m/z	146	157	156	118	97	129	298	158
%	100	65	50	40	30	25	25	25

Assignments confirmed by accurate mass data (Cardiff GCT)
298 (25) – M^+ 298.0541
270 (10) – [M-28] loss of C_2H_4 to $C_{10}H_{11}N_2O_3PS^+$ m/z 270.0228
241 (10) – [M-57] loss of C_2H_4 & C_2H_5 to $C_8H_6N_2O_3PS^+$ m/z 240.9770
225 (5) – [M-73] loss of C_2H_4 & C_2H_5O to $C_8H_6N_2O_2PS^+$ m/z 224.9888
193 (5) – [M-105] loss of C_2H_4 & C_2H_5O & S to $C_8H_6N_2O_2P^+$ m/z 193.0164

173 (10) – [M-125] loss of $C_2H_6O_2PS$ to $C_{10}H_9N_2O^+$ m/z 173.07149 [interesting rearrangement/loss]
162 (20) – [M-136] quinoxaline thiol $(C_8H_5N_2)SH$ $C_8H_6N_2S^+$ m/z 162.0252
157 (65) – [M-141] loss of $C_2H_6O_3PS$ to $C_{10}H_9N_2^+$ m/z 157.0766 [interesting rearrangement/loss]
146 (100) – [M-152] quinoxalinol $(C_8H_5N_2)OH$ $C_8H_6N_2O^+$ m/z 146.0480
129 (25) – [M-169] quinoxaline core $C_8H_5N_2^+$ m/z 129.0453
118 (40) – [M-180] loss of CO from m/z 146 to $C_7H_6N_2^+$ m/z 118.05310
102 (25) – [M-196] $C_7H_4N^+$ m/z 102.0344
97 (30) – [M-201] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
90 (30) – [M-208] $C_6H_4N^+$ m/z 90.0344

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C13593038&Mask=200

Quinomethionate / Chinomethionat $C_{10}H_6N_2OS_2$ M:234(95%)
Theoretical molecular ion: m/z 233.99215 (100%), 234.9955 (10.8%), 235.98795 (9.0%)
Average MW: 234.29



Quinoxaline acaricide and fungicide. used to control powdery mildew and spider mite. Not approved for use in EU.

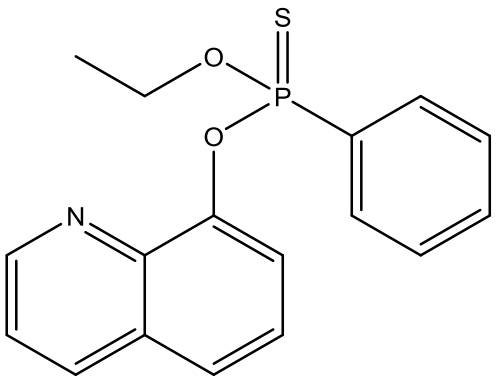
Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

m/z	206	234	116	174	173	148	89	103
%	100	95	60	45	30	30	20	10

234 (95) – M^+
206 (100) – [M-28] loss of CO to give $C_9H_6N_2S_2^+$ m/z 05.9972
174 (45) – [M-60] loss of COS to give $C_9H_6N_2S^+$ m/z 174.0252
116 (60) – [M-118] loss of C_2NOS_2 to $C_8H_6N^+$ m/z 116.0500

http://webbook.nist.gov/cgi/cbook.cgi?ID=C2439012&Mask=200#Mass-Spec (N.B. incorrect formula & MW)

Quintiofos $C_{17}H_{16}NO_2PS$ M:329(20%)
Theoretical molecular ion: m/z 329.0639 (100%), 330.0673 (18.4%), 331.0597 (4.5%)
Average MW: 329.3538



Organophosphorus veterinary insecticide. Used for control of a range of crop and livestock pests. Not approved for use in EU.

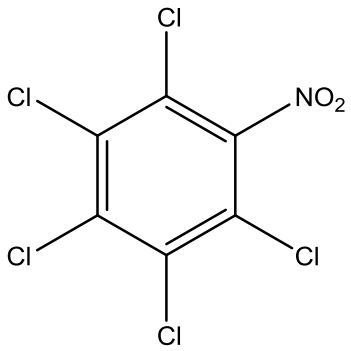
Acute oral LD50 for rat approx. 150 mg/kg (moderate toxicity).

m/z	237	157	145	141	172	252	156	236
%	100	80	70	60	60	60	40	30

329 (20) – M^+
252 (60) – [M-77] loss of C_5H_3N to give $C_{12}H_{13}O_2PS_2^+$ m/z 252.0374
237 (100) – [M-92] loss of CH_3 & C_6H_5 to give $C_{10}H_8NO_2PS^+$ m/z 237.0013
and/or loss of CH_3 & C_5H_3N ?
157 (80) – [M-172]
145 (70) – [M-184] $C_9H_7NO^+$ m/z 145.058

No NIST spectrum available.

Quintozene **$C_6Cl_5NO_2$** **M:293,295,297,299(50,90,45,15%)**
Theoretical molecular ion: m/z 292.8372 (63%), 294.8342 (100%), 296.8313 (65%), 298.8283 (20%)
Average MW: 295.32



Fungicide. No longer approved for use in EU.

Acute oral LD50 for rat >1,500 mg/kg (moderate toxicity).

KI (OV-17) = 20.4

m/z	237	295	30	214	249	212	235	251
%	100	90	90	85	80	60	55	50

293,295,297,299 (50,90,45,15) – M^+
263,265,267 (25,35,25) – [M-30] loss of NO from nitro group to $C_6Cl_5O^+$ m/z 262.8392 etc.
247,249,251 (50,90,50) – [M-46] loss of NO_2 to $C_6Cl_5^+$ m/z 246.8443 etc.
235,237,239 (55,100,55) – [M-58] loss of CO+NO to $C_5Cl_5^+$ m/z 234.8443 etc.
212,214,216 (60,85,40) – [M-81] loss of NO_2+Cl to $C_6Cl_4^+$ m/z 211.8754
30 (90) – [M-263] NO^+ m/z 29.9980

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C82688&Mask=200#Mass-Spec

Quintozene related i), pentachloroaniline $C_6H_2Cl_5N$ M:263,265,267,269(65,100,65,20%)
Theoretical molecular ion: m/z 262.8630 (63%), 264.8600 (100%), 266.8571 (64%), 268.8541 (20%)
Average MW: 265.35

Pentachloroaniline, C_6Cl_5-NH_2
Reductive metabolite of quintozene. May be produced in GC injector. Included in quintozene MRLs. KI (OV-17) = 21.4, (SE-30) =17.7

m/z	265	263	267	269	194	192	133	96
%	100	65	65	20	15	15	15	10

Cf. similar but noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C527208&Mask=200#Mass-Spec - inadequate MS resolution, as ^{13}C ions not exhibited in M^+.

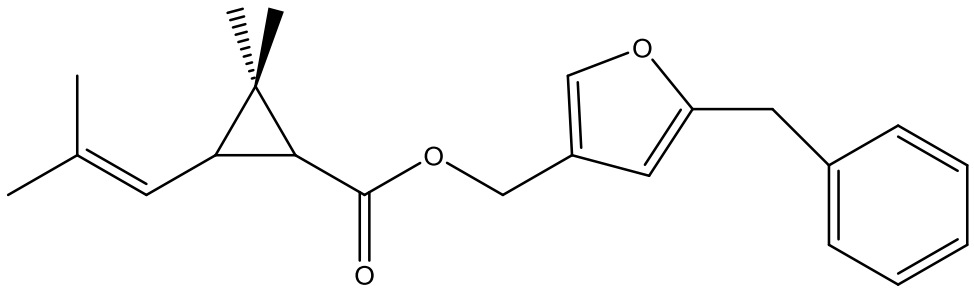
Quintozene related ii), pentachlorothioanisole $C_7H_3Cl_5S$ M:294,296,298,300(60,100,65,20%)
Theoretical molecular ion: m/z 293.8398 (63%), 295.8369 (100%), 297.8339 (64%), 299.8310 (20%)
Average MW: 296.41

Pentachlorothioanisole, C_6Cl_5-SCH_3
A metabolite of quintozene. Included in quintozene MRLs.
KI (OV-17) = 22.2

m/z	296	298	294	246	244	263	45	248
%	100	65	60	55	40	40	35	30

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1825190&Units=SI&Mask=200#Mass-Spec

Resmethrin **$C_{22}H_{26}O_3$** **M:338(5%)**
Theoretical molecular ion: m/z
Average MW: 338.44



Synthetic pyrethroid. No longer approved for use in EU.

Acute oral LD50 for rat > 2,500 mg/kg (low toxicity).

May be resolved into two peaks on capillary GC (*ca.* 1:3).

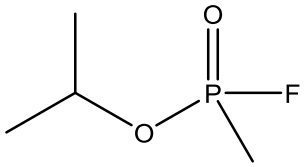
m/z	123	171	143	128	91	81	43	172
%	100	50	35	35	30	30	30	15

338 (5) – M^+
171 (50) – [M-167] $C_6H_5.CH_2.C_4H_2O.CH_2^+$ $C_{12}H_{11}O^+$ m/z 171.0810
123 (100) – [M-215] $(CH_3)_2C{=}CH.C_3H_2(CH_3)_2^+$ $C_9H_{15}^+$ m/z 123.1174

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C10453868&Units=SI&Mask=200#Mass-Spec

Sarin / GB - nerve agent **$C_4H_{10}FO_2P$** **M:140(0%)**

Theoretical molecular ion: m/z 140.0402 (100%), 141.0436 (4%)
Average MW: 140.09



Sarin, O-isopropyl methylphosphonofluoridate

Organophosphorus chemical warfare agent, originally developed as an insecticide in Germany in 1938.

Acute oral LD50 for rat approx. **0.1 mg/kg** (high toxicity).

Superseded organophosphorus insecticide/acaricide, named for its discoverer, Gerhard Schrader, who also synthesised the related chemical weapon nerve agents **sarin** and **tabun**. Schradan is extremely toxic (human LD_{50} estimated at 5-50mg/kg, so only a few drops may be enough to kill an adult).

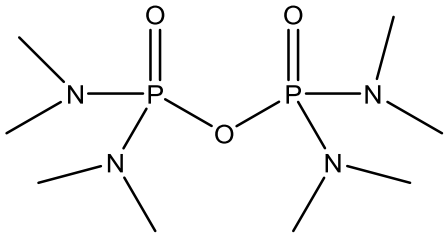
m/z	99	125	81	43	41	39	-	-
%	100	35	10	10	10	5	-	-

140 (0) – M^+ absent
125 (35) – [M-15] loss of CH_3 to $C_3H_7FO_2P^+$ m/z 125.0168 (NOT the typical OP ion!)
99 (100) – [M-41] loss of C_3H_5 to $CH_3(HO)_2FP^+$ $CH_5FO_2P^+$ m/z 99.0011
81 (10) – [M-59] loss of C_3H_5 & H_2O to give CH_3FOP+ m/z 80.9906

Data from NIST spectrum http://webbook.nist.gov/cgi/cbook.cgi?ID=C107448&Mask=200#Mass-Spec

Schradan **$C_8H_{24}N_4O_3P_2$** **M:286(20%)**

Theoretical molecular ion: m/z 286.1324 (100%), 287.1357 (9%)
Average MW: 286.29



Schradan, "octamethylpyrophosphoramide, OMPA"

Organophosphorus insecticide and acaricide. Largely obsolete. Used on potatoes and cotton.

Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

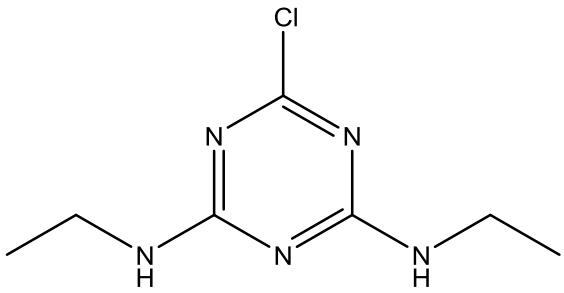
Superseded organophosphorus insecticide/acaricide, named for its discoverer, Gerhard Schrader, who also synthesised the related chemical weapon nerve agents **sarin** and **tabun**. Schradan is extremely toxic (human LD_{50} estimated at 5-50mg/kg, so only a few drops may be enough to kill an adult).

m/z	44	135	153	92	199	243	286	200
%	100	65	45	45	40	20	20	20

286 (20) – M^+
243 (20) – [M-43] loss of CH_2NCH_3 to $C_6H_{19}N_3O_3P_2^+$ m/z 243.0902
199 (40) – [M-87] loss of CH_2NCH_3 & $(CH_3)_2N$ to $C_4H_{13}N_2O_3P_2^+$ m/z 199.0401
153 (45) – [M-133] $[(CH_3)_2N]_2(HO)_2P^+$ $C_4H_{14}N_2O_2P^+$ m/z 153.0793
135 (65) – [M-153] $[(CH_3)_2N]_2PO^+$ $C_4H_{12}N_2OP^+$ m/z 135.0687
92 (45) – [M-151] $(CH_3)_2N(HO)P^+$ $C_2H_7NOP^+$ m/z 92.0265
44 (100) – [M-242] $(CH_3)_2N^+$ $C_2H_6N^+$ m/z 44.0500

Cf. Similar but noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C152169&Mask=200
(filed as "Diphosphoramide, octamethyl-")

Simazine **$C_7H_{12}ClN_5$** **M:201,203(90,30%)**
Theoretical molecular ion: m/z 201.0781 (100%), 203.0752 (32%)
Average MW: 201.66



Chlorotriazine herbicide. No longer approved for use in EU.

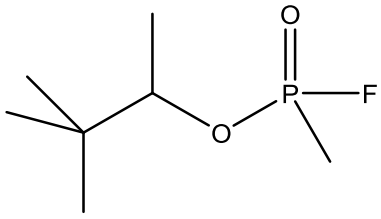
Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

m/z	44	201	186	173	43	68	203	158
%	100	90	55	45	35	30	30	25

201,203 (90,30) – M^+
186,188 (55,20) – [M-15] loss of CH_3 to $C_6H_9ClN_5^+$ m/z 186.05465 etc.
173,175 (45,15) – [M-28] loss of C_2H_4 to $C_5H_8ClN_5^+$ m/z 173.0468 etc.
68 (30) – [M-142] $C_2H_2N_3^+$ m/z 68.0249
44 (100) – [M-157] $CH_3CH_2NH^+$ $C_2H_6N^+$ m/z 44.0500

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C122349&Mask=200#Mass-Spec

Soman / GD nerve agent **$C_7H_{16}FO_2P$** **M:182(0%)**
Theoretical molecular ion: m/z 182.0872 (100%), 183.0906 (8%)
Average MW: 182.17



Soman, O-pinacolyl methylphosphonofluoridate

Organophosphorus chemical warfare agent, originally developed in 1944 by Richard Kuhn as a more toxic variant of sarin and tabun.

Acute oral LD50 for rat approx. **0.1 mg/kg** (high toxicity).

Extremely toxic (human LD_{50} estimated at 5-50mg/kg, so only a few drops may be enough to kill an adult).

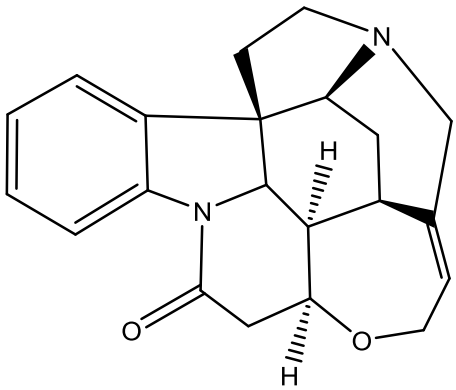
m/z	126	99	82	69	41	57	43	83
%	100	85	55	50	35	20	15	15

182 (0) – M^+ absent
126 (35) – [M-56] loss of C_4H_8 to $C_3H_8FO_2P^+$ m/z 126.0246
99 (100) – [M-83] loss of C_6H_{11} to $CH_3(HO)_2FP^+$ $CH_5FO_2P^+$ m/z 99.0011
82 (10) – [M-100] loss of C_6H_{10} & H_2O to give to $CH_3(HO)FP^+$ CH_4FOP^+ m/z 81.9984

Data from NIST spectrum http://webbook.nist.gov/cgi/cbook.cgi?ID=C96640&Units=SI&Mask=200#Mass-Spec

Strychnine **$C_{21}H_{22}N_2O_2$** **M:334(100%)**

Theoretical molecular ion: m/z 334.1681 (100%), 335.1715 (23%)
Average MW: 334.41



Rodenticide. No longer approved for use in EU.

Highly toxic natural plant alkaloid derived from *Strychnos nux-vomica*. 30-120 mg is enough to kill a person. Acute oral LD50 for rat approx. 0.2 mg/kg (high toxicity).

Long GC RT and poor transmission.

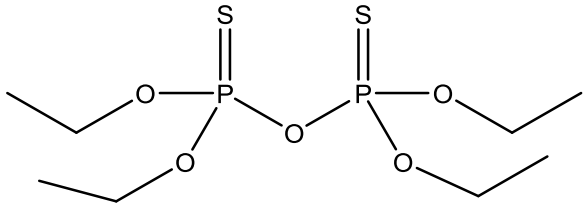
m/z	334	120	162	107	55	124	335	143
%	100	20	20	20	20	20	20	20

334 (100) – M^+
120 (20) – [M-214] $C_6H_5NCO.H^+$ $C_7H_6NO^+$ m/z 120.0449

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C57249&Mask=200#Mass-Spec

Sulfotep **$C_8H_{20}O_5P_2S_2$** **M:322(100%)**

Theoretical molecular ion: m/z 322.0227 (100%), 323.0261 (9%), 324.0185 (9%)
Average MW: 322.32



Organophosphorus insecticide and acaricide. Used as a fumigant to control aphids, thrips, spider mites and other insects in glasshouses and other situations. No longer approved for use in EU.

Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

m/z	322	202	121	93	65	174	97	238
%	100	55	55	50	45	40	40	35

Assignments confirmed by accurate mass study (Cardiff GCT).
322 (100) – M^+ $C_8H_{20}O_5P_2S_2^+$ m/z 322.0227
294 (15) – [M-28] loss of C_2H_4 to $C_6H_{16}O_5P_2S_2^+$ m/z 293.9914
266 (30) – [M-56] loss of $2C_2H_4$ to $C_4H_{12}O_5P_2S_2^+$ m/z 265.9601
245 (25) – [M-77] loss of C_2H_5OS to $C_6H_{15}O_4P_2S^+$ m/z 245.0166
238 (30) – [M-84] loss of $3C_2H_4$ to $C_2H_8O_5P_2S_2^+$ m/z 237.9225
221 (10) – [M-101] loss of $C_6H_{13}O$ to $C_2H_7O_4P_2S_2^+$ m/z 220.9261
217 (25) – [M-105] loss of C_4H_9OS to $C_4H_{11}O_4P_2S^+$ m/z 216.9853
209 (35) – [M-113] loss of C_8H_{17} to $H_3O_5P_2S_2^+$ m/z 208.8897
202 (55) – [M-120] loss of $C_4H_9O_2P$ to $C_4H_{11}O_3PS_2^+$ m/z 201.9887
193 (25) – [M-129] loss of $C_8H_{17}O$ to $H_3O_4P_2S_2^+$ m/z 192.8948
174 (25) – [M-148] loss of $C_6H_{13}O_2P$ to $C_2H_7O_3PS_2^+$ m/z 173.9574
153 (15) – [M-169] loss of $C_4H_{10}O_3PS$ to $C_4H_{10}O_2PS^+$ m/z 153.0139
145 (15) – [M-177] loss of $C_8H_{17}S_2$ to $H_3O_5P_2^+$ m/z 144.9456
125 (10) – [M-197] $(C_2H_5O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121 (55) – [M-201] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
97 (40) – [M-225] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
93 (50) – [M-229] $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105
81 (10) – [M-240] $H_2O_3P^+$ m/z 80.9742
65 (45) – [M-257] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3689245&Mask=200#Mass-Spec which exhibits similar dominant ions, but with different relative intensities (m/z 322, 29, 97, 202, 65, 27 etc. by abundance).

Sulphur **S_8** **M:256,258, 260 (95,35, 6%)**

Theoretical molecular ion: m/z 255.7766 (100%), 257.7724 (35.4%), 259.7682 (5.5%)
Average MW: 256.52

Fungicide and acaricide. Approved for use in EU.

Acute oral LD50 for rat >2,000 mg/kg (moderate toxicity).

Difficult to quantify because of different solubilities of various allotropes.

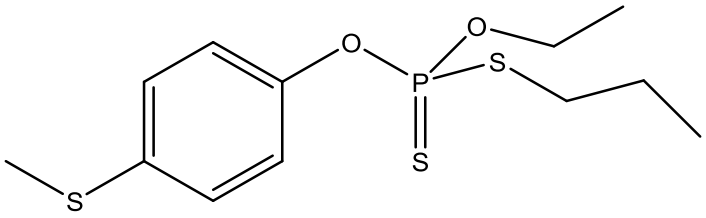
m/z	64	256	160	128	192	258	96	162
%	100	95	75	70	40	35	25	20

256,258 (95,35) – M^+ N.B. Easily mistaken for a chlorinated isotope cluster.

64 (100) – [M-192] S_2^+ m/z 63.9441 etc.
160 (75) – [M-96] S_5^+ m/z 159.8604 etc.

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C10544500&Units=SI&Mask=200#Mass-Spec
listed under “Cyclic octaatomic sulfur"

Sulprofos / Bolstar **$C_{12}H_{19}O_2PS_3$** **M:322(100%)**
Theoretical molecular ion: m/z 322.0285 (100%), 323.0318 (13.0%), 324.0243 (13.6%)
Average MW: 322.45



Organophosphorus insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 200 mg/kg (moderate toxicity).

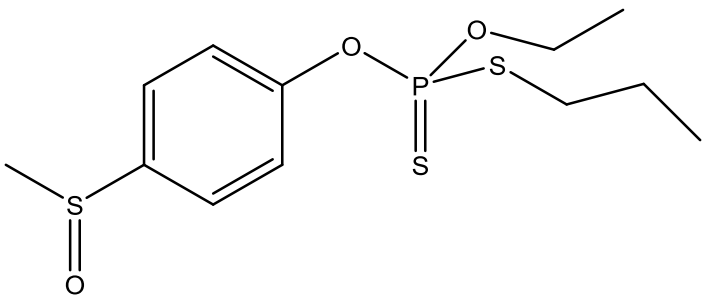
N.B. Several oxidative metabolites (below).

m/z	322	156	140	139	113	43	125	280
%	100	80	60	55	30	25	20	15

322 (100) – M^+
280 (15) – [M-42] loss of propene C_3H_6 to $C_9H_{13}O_2PS_3^+$ m/z 279.9815
156 (80) – [M-166] $CH_3SC_6H_4SH^+$ $C_7H_8S_2^+$ m/z 156.0067 [O/S swap]
140 (60) – [M-182] $CH_3SC_6H_4OH^+$ $C_7H_8OS^+$ m/z 140.0296
139 (55) – [M-183] $CH_3SC_6H_4O^+$ $C_7H_7OS^+$ m/z 139.0218
125 (20) – [M-197] $(CH_3CH_2O)(SH)P{=}O^+$ $C_2H_6O_2PS^+$ m/z 124.9826
113 (30) – [M-209] $(HO)(HS)P{=}S^+$ $H_2OPS_2^+$ m/z 112.9285
97 (15) – [M-225] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
63 (10) – [M-259] PS^+ m/z 62.9458

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C35400432&Mask=200#Mass-Spec

Sulprofos sulphoxide **$C_{12}H_{19}O_3PS_3$** **M:338(40%)**
Theoretical molecular ion: m/z 338.0234 (100.0%), 339.02675 (13.0%), 340.0192 (13.6%)
Average MW: 338.43



Oxidative metabolite of sulprofos.

m/z	296	141	43	281	139	156	113	140

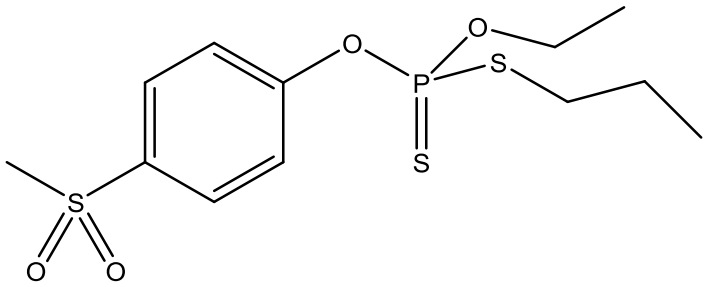
%	100	95	85	80	75	75	70	65

338 (0) – M^+ absent
296 (100) – [M-42] loss of propene C_3H_6 to $C_9H_{13}O_3PS_3^+$ m/z 295.9764
281 (80) – [M-57] loss of C_3H_6 & CH_3 from sulphoxide moiety, to $C_8H_{10}O_3PS_3^+$ m/z 280.9530
156 (75) – [M-182] $CH_3SOC_6H_4OH^+$ $C_7H_8O_2S^+$ m/z 156.0245
141 (95) – [M-197] $(CH_3CH_2O)(SH)P{=}S^+$ $C_2H_6OPS_2^+$ m/z 140.9598

No NIST spectrum available

Sulprofos sulphone **$C_{12}H_{19}O_4PS_3$** **M:354(15%)**

Theoretical molecular ion: m/z 354.0183 (100%), 355.0217 (13.0%), 356.0141 (13.6%)
Average MW: 354.43



Oxidative metabolite of sulprofos.

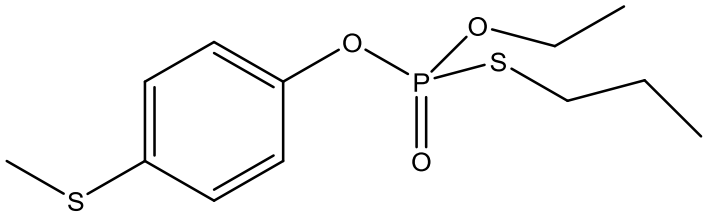
m/z	188	312	43	113	172	141	125	155
%	100	70	40	30	30	20	15	15

354 (15) – M^+
312 (70) – [M-42] loss of propene C_3H_6 to $C_9H_{13}O_4PS_3^+$ m/z 312.3528
188 (100) – [M-166] $CH_3SO_2C_6H_4SH^+$ $C_7H_8O_2S_2^+$ m/z 187.9966 [O/S swap]
172 (30) – [M-182] $CH_3SO_2C_6H_4OH^+$ $C_7H_8O_3S^+$ m/z 172.0194
141 (95) – [M-213] $(CH_3CH_2O)(SH)P{=}S^+$ $C_2H_6OPS_2^+$ m/z 140.9598
113 (30) – [M-241] $(HO)(HS)P{=}S^+$ $H_2OPS_2^+$ m/z 112.9285

No NIST spectrum available

Sulprofos oxon **$C_{12}H_{19}O_3PS_2$** **M:306(90%)**

Theoretical molecular ion: m/z 306.0513 (100%), 307.0547 (13.0%), 308.0471 (9.0%)
Average MW: 306.37



Oxidative metabolite of sulprofos.

m/z	140	306	139	43	125	156	307	97
%	100	90	35	20	20	15	15	15

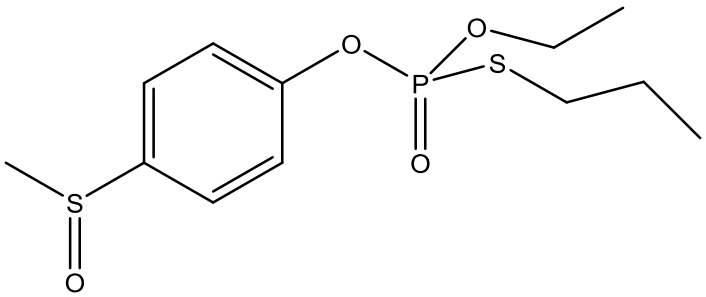
306 (90) – M^+
156 (15) – [M-150] $CH_3SC_6H_4SH^+$ $C_7H_8S_2^+$ m/z 156.0067 [O/S swap]
140 (100) – [M-166] $CH_3SC_6H_4OH^+$ $C_7H_8OS^+$ m/z 140.0296

139 (35) – [M-167] $CH_3SC_6H_4O^+$ $C_7H_7OS^+$ m/z 139.0218

No NIST spectrum available.

Sulprofos oxon sulphoxide **$C_{12}H_{19}O_4PS_2$** **M:322(20%)**

Theoretical molecular ion: m/z 322.0462 (100%), 323.04960 (13.0%), 324.0420 (9.0%)
Average MW: 322.37



Oxidative metabolite of sulprofos.

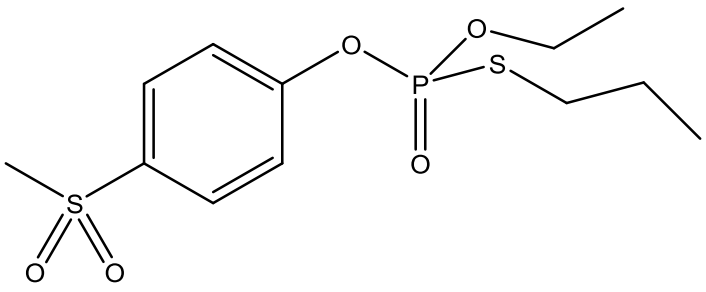
m/z	307	139	167	43	97	141	125	140
%	100	75	50	40	35	30	30	20

322 (0) – M+
307 (100) – [M-15] loss of CH3 from sulphoxide moiety $C_{11}H_{16}O_4PS_2^+$ m/z 307.0228
167 (50) – [M-155] $(C_2H_5O)(C_3H_7S)P{=}O^+$ $C_5H_{12}O_2PS^+$ m/z 167.0296
139 (75) – [M-183] $CH_3SC_6H_4O^+$ $C_7H_7OS^+$ m/z 139.0296
141 (30) – [M-185] $(C_2H_5O)(HS)PO_2^+$ $C_2H_6O_3PS^+$ m/z 140.9775

No NIST spectrum available.

Sulprofos oxon sulphone **$C_{12}H_{19}O_5PS_2$** **M:338(15%)**

Theoretical molecular ion: m/z 338.04115 (100%), 339.0445 (13.0%), 340.0370 (9.0%)
Average MW: 338.37



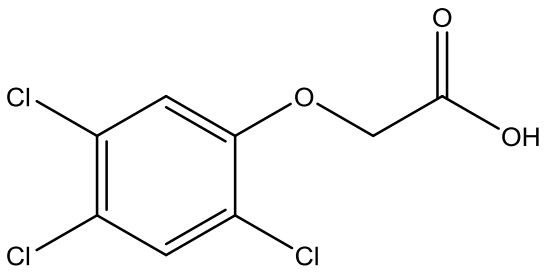
Oxidative metabolite of sulprofos.

m/z	172	196	43	139	296	188	97	157
%	100	60	55	50	35	35	35	30

338 (15) – M+
196 (60) – [M-142]
188 (100) – [M-150] $CH_3SO_2C_6H_4SH^+$ $C_7H_8O_2S_2^+$ m/z 187.9966 [O/S swap]
172 (100) – [M-166] $CH_3SO_2C_6H_4OH^+$ $C_7H_8O_3S^+$ m/z 172.0194

No NIST spectrum available.

2,4,5-T, acid **$C_8H_5Cl_3O_3$** **M:254,256,258(55,55,20%)**
Theoretical molecular ion: m/z 253.9304 (100%), 255.9275 (96%), 257.9245 (31%)
Average MW: 255.48



2,4,5-trichlorophenoxyacetic acid

Herbicide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity).

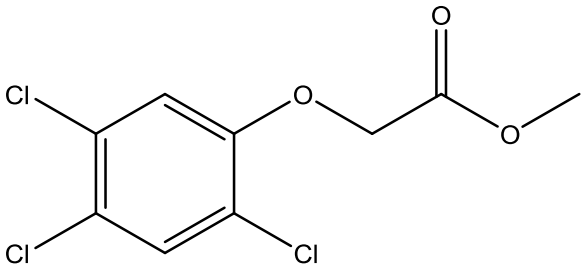
Poor transmission on GC unless derivatised.

m/z	196	198	254	256	200	209	211	167
%	100	95	55	55	30	20	20	20

254,256,258 (55,55,20) – M^+
196,198,200 (100,95,30) – [M-58] loss of CHCOOH to phenol $Cl_3C_6H_2OH^+$ $C_6H_3Cl_3O^+$ m/z 195.9250 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C93765&Mask=200#Mass-Spec

2,4,5-T methyl **$C_9H_7Cl_3O_3$** **M:268,270,272(65,65,20%)**
Theoretical molecular ion: m/z 267.9461 (100%), 269.9431 (96%), 271.9402 (31%)
Average MW: 269.50

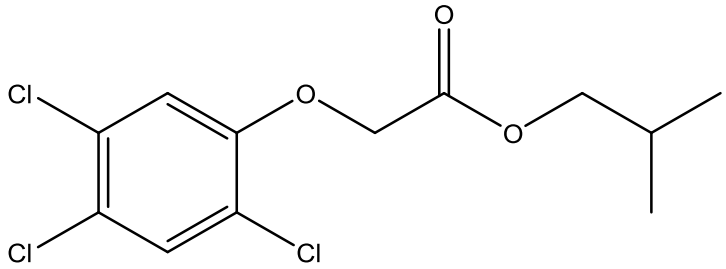


m/z	233	73	45	235	268	270	209	211
%	100	85	80	70	65	65	60	50

268,270,272 (65,65,20) – M^+
233,235 (100,70) – [M-35] loss of Cl to $C_9H_7Cl_2O_3^+$ m/z 232.9772 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1928376&Mask=200#Mass-Spec

2,4,5-T i-butyl **$C_{12}H_{13}Cl_3O_3$** **M:310,312,314(10,10,3%)**
Theoretical molecular ion: m/z 309.9930 (100%), 311.9901 (96%), 313.9871 (31%)
Average MW: 311.58



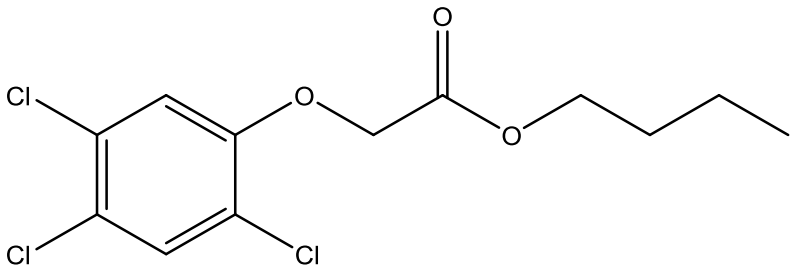
KI (SE-30) = 18.8

m/z	57	41	29	310	312	196	198	211
%	100	35	30	10	10	10	10	10

310,312,314 (10,10,3) – M^+
254,256 (8,8,2) – [M-56] loss of C_4H_8 to $C_8H_5Cl_3O_3^+$ m/z 253.9304 etc.
219,221 (6,4) – [M-91] loss of C_4H_8 & Cl to $C_8H_5Cl_2O_3^+$ m/z 218.9616 etc.

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C4938721&Mask=200#Mass-Spec

2,4,5-T n-butyl **$C_{12}H_{13}Cl_3O_3$** **M:310,312,314(15,15,5%)**
Theoretical molecular ion: m/z 309.9930 (100%), 311.9901 (96%), 313.9871 (31%)
Average MW: 311.58

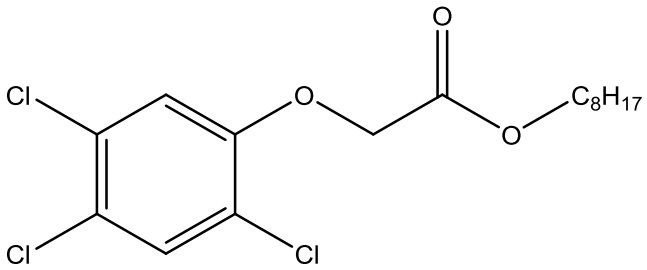


KI (SE-30) = 19.8 (longer RT than 2,4,5-T i-butyl)

m/z	57	29	41	310	312	219	196	211
%	100	40	40	15	15	15	10	10

310,312,314 (15,15,5) – M^+
254,256 (8,8,2) – [M-56] loss of C_4H_8 to $C_8H_5Cl_3O_3^+$ m/z 253.9304 etc.
219,221 (15,10) – [M-91] loss of C_4H_8 & Cl to $C_8H_5Cl_2O_3^+$ m/z 218.9616 etc.

2,4,5-T i-octyl **$C_{16}H_{21}Cl_3O_3$** **M:366,368,370(12,12,4%)**
Theoretical molecular ion: m/z 366.0556 (100%), 368.0527 (64%), 368.0527 (32%)
Average MW: 367.69

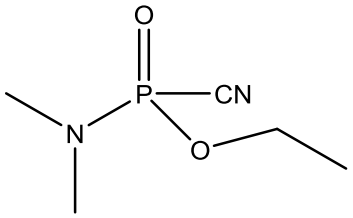


m/z	57	43	71	41	70	256	254	55
%	100	70	50	40	40	25	25	25

366,368,370 (12,12,4) - M^+
254,256,258 (23,23,8) – [M-112] loss of C_8H_{16} to acid $C_8H_5Cl_3O_3^+$ m/z 253.9304 etc.

No NIST spectrum available.

Tabun - nerve agent **$C_5H_{11}N_2O_2P$** **M:162(30%)**
Theoretical molecular ion: m/z 162.0558 (100%)
Average MW: 162.13



Tabun, O-ethyl N,N-dimethyl phosphoramidocyanidate

Organophosphorus chemical warfare agent, originally developed as an insecticide in Germany in 1938.

Acute oral LD50 for rat approx. **0.2 mg/kg** (very high toxicity).

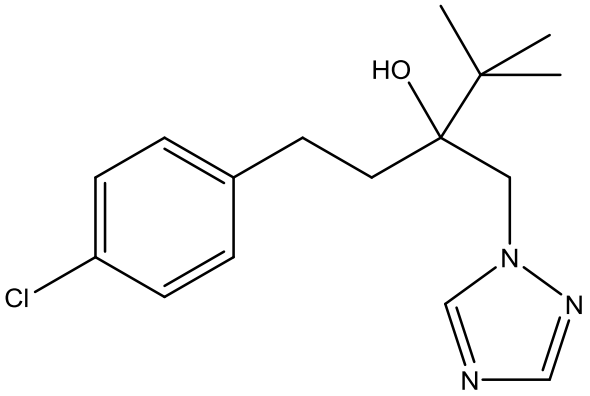
m/z	43	70	44	133	162	106	117	147
%	100	85	55	45	30	20	15	10

162 (30) – M^+
147 (5) – [M-15] loss of CH_3 to $C_4H_8N_2O_2P^+$ m/z 147.0323
133 (45) – [M-29] loss of CH_3CH_2 to $C_3H_6N_2O_2P^+$ m/z 133.0167
117 (15) – [M-45] loss of CH_3CH_2O to $C_3H_6N_2OP^+$ m/z 117.0218
106 (20) – [M-56] loss of CH_3CH_2 & HCN to $(CH_3)CH_2N.PO_2^+$ $C_2H_5NO_2P^+$ m/z 106.0058
70 (85) – [M-59] dimethyl cyanamide, $N{\equiv}C\text{-}N(CH_3)_2$ $C_3H_6N_2^+$ m/z 70.0531
43 (100) – [M-119] $(CH_3)NCH_2^+$ $C_2H_5N^+$ m/z 43.0422

Data from NIST spectrum http://webbook.nist.gov/cgi/cbook.cgi?ID=C77816&Mask=200

TDE (DDD), see DDT metabolites and degradation products

Tebuconazole **$C_{16}H_{22}ClN_3O$** **M:307,309(5,2%)**
Theoretical molecular ion: m/z 307.1451 (100%), 309.1422 (32%)
Average MW: 307.82



Conazole fungicide. Used to control smut and bunt diseases in cereals and other field crops. Approved for use in EU.

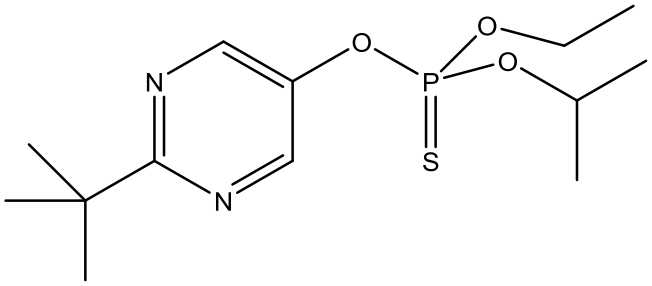
Acute oral LD50 for rat approx. 1,700 mg/kg (moderate toxicity).

m/z	125	70	250	83	57	127	252	163
%	100	80	70	60	45	30	25	20

307,309 (5,2) – M^+ $C_{16}H_{22}ClN_3O^+$
289,291 (5,2) – [M-18] loss of H_2O to $C_{16}H_{20}ClN_3^+$ m/z 289.1346 etc.
250,252 (70,25) – [M-57] loss of $(CH_3)_3C$ to $C_{12}H_{13}ClN_3O^+$ m/z 250.0747 etc.
125,127 (100,30) – [M-182] $ClC_6H_4CH_2^+$ $C_7H_6Cl^+$ m/z 125.0158 etc.
83 (60) – [M-224] $(C_2H_2N_3)CH_2/H^+$ m/z 83.04835
70 (80) – [M-237] $(C_2H_2N_3)H_2^+$ m/z 70.0405
57 (45) – [M-250] $(CH_3)_3C^+$ $C_4H_9^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C107534963&Mask=200#Mass-Spec

Tebupirimfos / Phostebupirim **$C_{13}H_{23}N_2O_3PS$** **M:318(100%)**
Theoretical molecular ion: m/z 318.1167 (100%)
Average MW: 318.37



Pyrimidine organophosphorus insecticide. Used to control a range of soil insects including maggots, rootworms, wireworms and cutworms on corn. Not approved for use in EU.

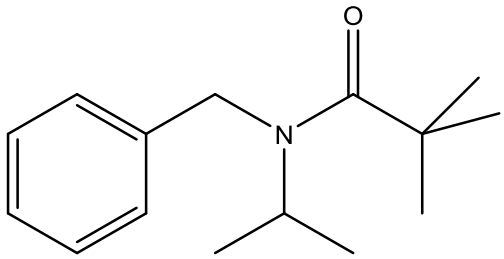
Acute oral LD50 for rat approx. 1.3 mg/kg (high toxicity).

m/z	318	261	234	276	152	137	303	110
%	100	60	55	40	35	20	20	15

318 (100) – M^+ $C_{13}H_{23}N_2O_3PS^+$
303 (20) – [M-15] loss of CH_3 to $C_{12}H_{20}N_2O_3PS^+$ m/z 303.0932
276 (40) –[M-42] loss of C_3H_6 to $C_{10}H_{17}N_2O_3PS^+$ m/z 276.0698
261 (60) – [M-57] loss of $(CH_3)_3C$ to $C_9H_{14}N_2O_3PS^+$ m/z 261.0463
234 (55) – [M-84] loss of $(CH_3)_3C$ & HCN to $C_8H_{13}NO_3PS^+$ m/z 234
152 (35) – [M-166] $(CH_3)_3C.C_4H_2N_2.OH^+$ $C_8H_{12}N_2O^+$ m/z 152.0950
137 (20) – [M-181] $(CH_3)_2C.C_4H_2N_2.OH^+$ $C_7H_9N_2O^+$ m/z 137.0715
110 (15) – [M-208] $(CH_3)_2C.C_3HN.OH^+$ $C_6H_8NO^+$ m/z 110.0606

No NIST spectrum. Data from Kuklenyik dissertation (2009).

Tebutam **$C_{15}H_{23}NO$** **M:233(5%)**
Theoretical molecular ion: m/z 233.1780 (100%), 234.1813 (16%)
Average MW: 233.36



Herbicide. Not approved for use in EU.

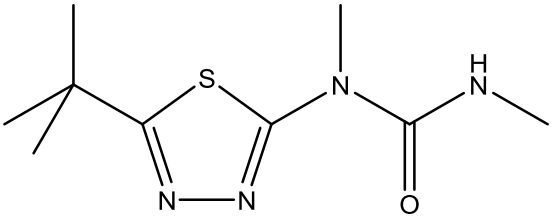
Acute oral LD50 for rat approx. 6,000 mg/kg (low toxicity).

m/z	91	57	190	106	92	134	142	233
%	100	60	25	10	5	5	5	5

233 (5) – M^+ $C_{15}H_{23}NO^+$
190 (25) – [M-43] loss of $(CH_3)_2CH$ to $C_{12}H_{16}NO^+$ m/z 190.1232
91 (100) – [M-142] tropylium ion $C_6H_5CH_2^+$ $C_7H_7^+$ m/z 91.0548
57 (60) – [M-176] $(CH_3)_3C^+$ $C_4H_9^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C35256850&Mask=200#Mass-Spec

Tebuthiuron **$C_9H_{16}N_4OS$** **M:228(2%)**
Theoretical molecular ion: m/z 228.1045 (100%), 229.1078 (9.7%), 230.1003 (4.5%)
Average MW: 228.31



Herbicide. Not approved for use in EU.

Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity)

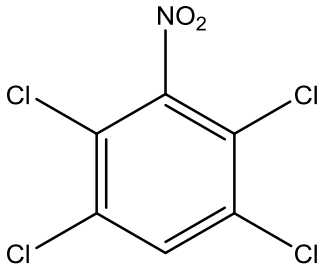
Poor GC transmission.

m/z	171	156	98	57	41	74	88	172
%	100	65	65	55	20	10	10	10

228 (2) – M^+
171 (100) – [M-57] loss of methyl isocyanate CH_3NCO to $C_7H_{13}N_3S^+$ m/z 171.0830
156 (65) – [M-72] loss $CH_3NCO+CH_3$ to $C_6H_{10}N_3S^+$ m/z 156.0595
98 (65) – [M-120] loss of $SCN.N(CH_3)CONHCH_3$ to $(CH_3)_3C.CN_2H^+$ $C_5H_{10}N_2^+$ m/z 98.0844

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C34014181&Mask=200#Mass-Spec which has base peak at m/z 156 and lacks molecular ion at m/z 218. This spectrum is probably not due to tebuthiuron but its degradation product, formed by loss of methyl isocyanate, $(CH_3)_3C.(C_2N_2S).NHCH_3$ ($C_7H_{13}N_3S$, mw 171).

Tecnazene **$C_6HCl_4NO_2$** **M:259,261,263(60,80,35%)**
Theoretical molecular ion: m/z 258.8761 (78%), 260.8732 (100%), 262.8702 (48%), 264.8673 (10%)
Average MW: 260.89

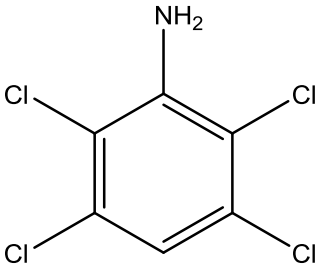


m/z	203	215	261	201	30	259	213	205
%	100	85	80	70	70	60	55	45

259,261,263 (60,80,35) – M^+ $C_6HCl_4NO_2^+$
213,215,217 (55,85,40) – [M-46] loss of NO_2 to $C_6HCl_4^+$ m/z 212.8832 etc
201,2013,205 (70,100,45) – [M-58] loss of NO+CO to $C_5HCl_4^+$ m/z 200.8832 etc.
178,180,182 (40,40,10) – [M-81] loss of NO2+Cl to $C_6HCl_3^+$ m/z 177.9144 etc.
143,145 (40,30) – [M-116] loss of NO2+2Cl to $C_6HCl_2^+$ m/z 142.9455 etc.
30 (70) – [M-229] NO^+ m/z 29.9980

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C117180&Mask=200#Mass-Spec
listed as "Benzene, 1,2,4,5-tetrachloro-3-nitro-"

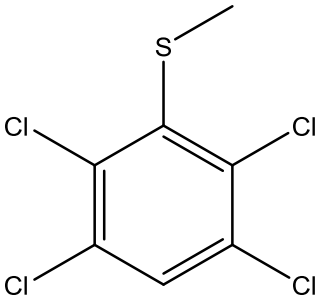
Tecnazene related i) **$C_6H_3Cl_4N$** **M:229,231,233(80,100,45%)**
2,3,5,6-tetrachloroaniline
Theoretical molecular ion: m/z 228.9020 (78%), 230.8990 (100%), 232.8961 (48%), 234.8931 (10%)
Average MW: 230.90



Reductive metabolite of tecnazene which may be produced in "active" GC systems.

m/z	231	229	233	158	160	235	169	196
%	100	80	45	20	15	10	10	10

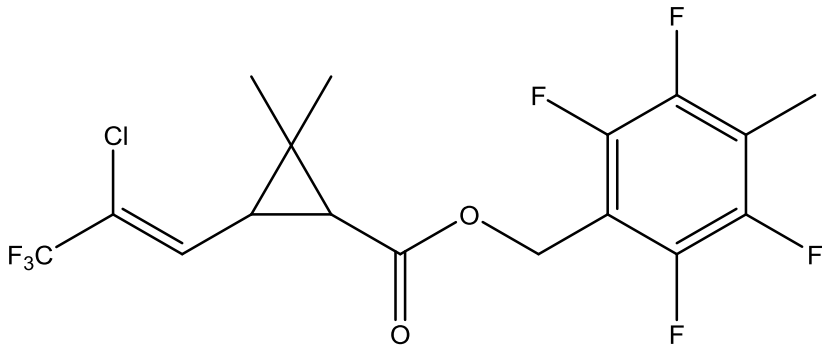
Tecnazene related ii) **$C_7H_4Cl_4S$** **M:260,262,264(75,100,50%)**
2,3,5,6-tetrachlorothioanisole
Theoretical molecular ion: m/z 259.8788 (78%), 261.8758 (100%), 263.8729 (48%), 265.8699 (10%)
Average MW: 261.97



Metabolite of tecnazene:

m/z	262	260	264	227	229	45	210	212
%	100	75	50	40	40	40	35	35

Tefluthrin **$C_{17}H_{14}ClF_7O_2$** **M:418,420(0,0%)**
Theoretical molecular ion: m/z 418.0571 (100%), 420.0541 (32%)
Average MW: 418.74



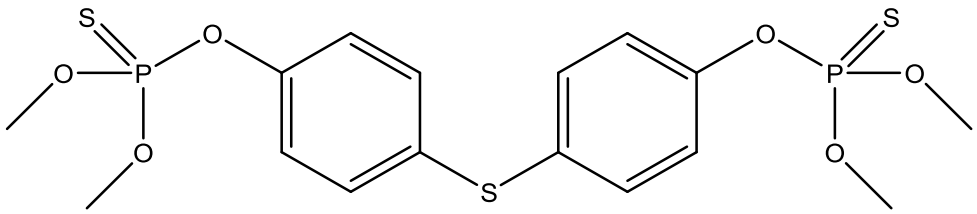
m/z	177	197	141	127	178	199	91	225	
	%	100	80	60	55	55	55	45	30

418 (0) – M^+
225 (30) – [M-193]

197 (80) – [M-221] $CF_3(Cl)C=CH[C_3H_2(CH_3)_2]^+$ $C_8H_9ClF_3^+$ m/z 197.0345 etc.
177 (100) – [M-241] $CH_3C_6F_4CH_2^+$ $C_8H_5F_4^+$ m/z 177.0327
141 (60) – [M-277] $CF_3(Cl)C=CCH^+$ $C_4HClF_3^+$ m/z 140.9719 etc.

No NIST spectrum available

Temephos / "Abate **$C_{16}H_{20}O_6P_2S_3$** **M:466(100%)**
Theoretical molecular ion: m/z 465.9897 (100%), 466.9931 (17%), 467.9855 (14%),
Average MW: 466.46



Organophosphorus insecticide. Used in public health programmes to control mosquitoes, midges, and black fly larvae often in aquatic situations.

Acute oral LD50 for rat approx 4,000 mg/kg (low toxicity).

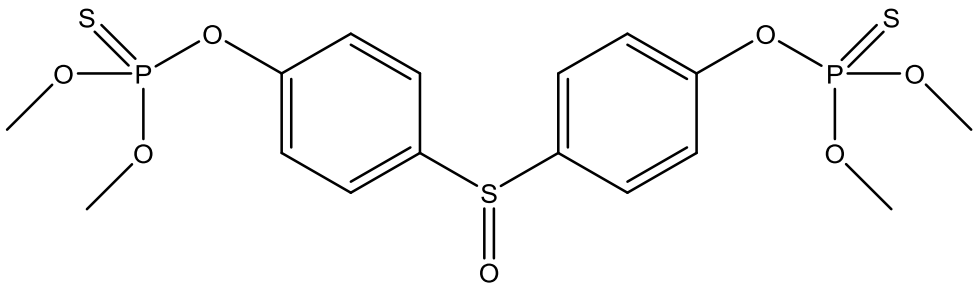
N.B. Several oxidative metabolites. Not amenable to GC.

m/z	466	93	203	125	467	468	357	155
%	100	20	20	20	20	20	5	5

466 (100) – M^+
203 (20) – [M-263] $C_6H_4OPS(OCH_3)(OH)^+$ $C_7H_8O_3PS^+$ m/z 202.9932
125 (20) – [M-341] $(CH_3O)_2PS^+$ $C_2H_6O_2P^+$ m/z 124.9826
109 (5) – [M-357] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (20) – [M-373] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C3383968&Mask=200

Temephos sulphoxide **$C_{16}H_{20}O_7P_2S_3$** **M:482(15%)**
Theoretical molecular ion: m/z 481.9846 (100%), 482.9880 (17%), 483.9804 (14%),
Average MW: 482.46



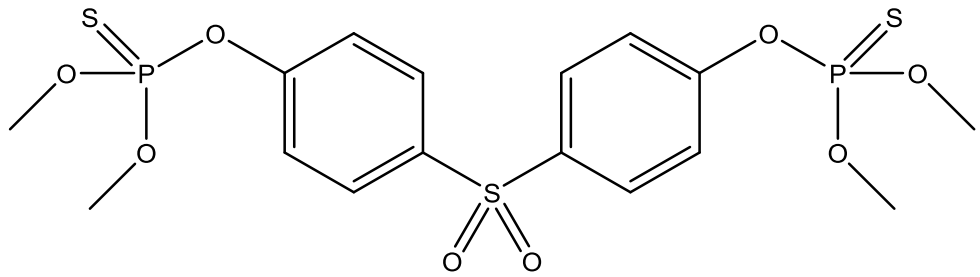
Not amenable to GC.

m/z	125	434	109	93	233	435	482	466
%	100	65	25	25	15	15	15	10

482 (15) – M^+
466 (10) – [M-16] loss of O (ion source reduction?) to give temephos M^+
434 – [M-48] loss of SO to give $C_{16}H_{20}O_6P_2S_2^+$ m/z 434.0177
233 (15) – [M-249] $SOC_6H_4OPS(OCH_3)^+$ $C_7H_7O_3PS_2^+$ m/z 233.9574
125 (100) – [M-357] $(CH_3O)_2PS^+$ $C_2H_6O_2P^+$ m/z 124.9826
109 (25) – [M-373] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (25) – [M-389] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105

Temephos sulphone **$C_{16}H_{20}O_8P_2S_3$** **M:498(50%)**

Theoretical molecular ion: m/z 497.9796 (100%), 498.9829 (17%), 499.97535 (14%)
Average MW: 498.98



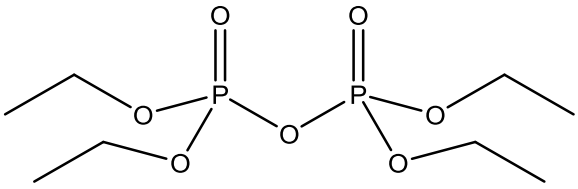
Not amenable to GC.

m/z	203	125	498	109	93	388	265	499
%	100	65	50	50	40	15	15	10

498 (50) – M+
203 (100) – [M-295] $C_6H_4OPS(OCH_3)(OH)^+$ $C_7H_8O_3PS^+$ m/z 202.9932
388 (15) – [M-110] loss of $(CH_3O)_2(HO)PO$ to give $C_{14}H_{13}O_5S_2^+$ m/z 387.9663
125 (65) – [M-373] $(CH_3O)_2PS^+$ $C_2H_6O_2P^+$ m/z 124.9826
109 (50) – [M-389] $(CH_3O)_2PO^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (40) – [M-405] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105

TEPP (tetraethyl pyrophosphate) **$C_8H_{20}O_7P_2$** **M:290(10%)**

Theoretical molecular ion: m/z 290.0684 (100%), 291.0718 (8.7%)
Average MW: 290.19



Organophosphorus insecticide and acaricide. Used to control aphids, mites, spiders, mealybugs and many other insects. No longer approved for use in EU.

Acute oral LD50 for rat approx. 1 mg/kg (high toxicity).

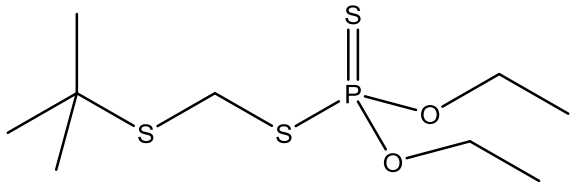
m/z	263	161	235	179	207	162	99	81
%	100	85	80	75	65	55	40	40

290 (10) – M^+
263 (100) – [M-27] loss of C_2H_3 to give $C_6H_{17}O_7P_2^+$ m/z 263.0450
235 (80) – [M-55] loss of C_2H_3+C_2H_4 to give $C_4H_{13}O_7P_2^+$ m/z 235.0137
207 (65) – [M-83] loss of C_2H_3+2C_2H_4 to give $C_2H_9O_7P_2^+$ m/z 206.9824
179 (75) – [M-111] loss of C_2H_3+3C_2H_4 to give $(HO)_2PO.O.P(OH)_3$ $H_5O_7P_2^+$ m/z 178.9511
161 (100) – [M-129] $(HO)_2PO.O.P(OH)_2$ $H_3O_6P_2^+$ m/z 160.9405
99 (40) – [M-191] $((HO)_4P^+$ $H_4O_4P^+$ m/z 98.9847
81 (40) – [M-209] $(HO)_2P{=}O^+$ $H_2O_2P^+$ m/z 80.9742

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C107493&Mask=200

Terbufos **$C_9H_{21}O_2PS_3$** **M:288(5%)**

Theoretical molecular ion: m/z 288.0441 (100%), 290.0399 (13.6%), 289.0475 (9.7%)
Average MW: 288.42



Organophosphorus insecticide and nematicide used to control wireworm, maggots, rootworm larvae and other pests. No longer approved for use in EU.

Acute oral LD50 for rat approx 1 mg/kg (high toxicity).

N.B. See oxidative metabolites below, all of which are included in MRLs.

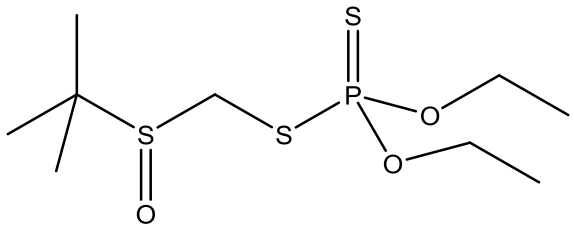
m/z	57	231	29	103	153	41	65	186
%	100	40	25	20	15	15	15	10

288 (5) – M^+
231 (40) – [M-57] loss of C_4H_9 to give $C_5H_{12}O_2PS_3^+$ m/z 230.9737
186 (10) – [M-102] loss of $(CH_3)_3CSCH$ to give $(CH_3CH_2O)_2PS.SH^+$ $C_4H_{11}O_2PS_2^+$ m/z 185.9938
153 (15) – [M-135] $(CH_3CH_2O)_2PS^+$ $C_4H_{10}O_2PS_2^+$ m/z 153.0139
142 (10) – [M-146] $(HO)_2PS.SCH^+$ $CH_4O_2PS_2^+$ m/z 141.9312
129 (10) – [M-159] $(HO)_2PS_2^+$ $H_2O_2PS_2^+$ m/z 128.9234
125 (10) – [M-163] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121(10) – [M-167] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
103 (20) – [M-185] $(CH_3)_3CSCH_2^+$ $C_5H_{11}S^+$ m/z 103.0582
97 (10) – [M-191] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
65 (15) – [M-223] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
57 (100) – [M-231] $(CH_3)_3C^+$ $C_4H_9^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C13071799&Mask=200#Mass-Spec

Terbufos sulphoxide $C_9H_{21}O_3PS_3$ **M:304(0%)**

Theoretical molecular ion: m/z 304.0390 (100%), 306.0348 (14%), 305.0424 (9.7%),
Average MW: 304.42

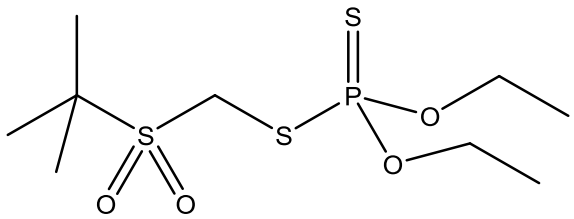


Not amenable to GC.

m/z	57	97	153	29	125	41	199	186
%	100	85	55	50	50	40	35	30

Terbufos sulphone $C_9H_{21}O_4PS_3$ **M:320(5%)**

Theoretical molecular ion: m/z 320.0340 (100%), 322.0298 (14%), 321.03731 (9.7%)
Average MW: 320.42

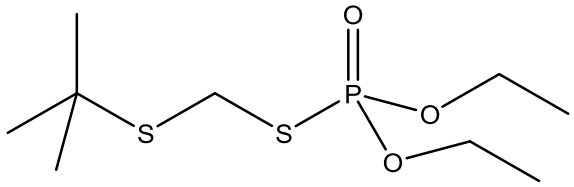


m/z	153	199	57	125	97	264	200	172
%	100	60	55	55	35	35	25	25

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C56070167&Mask=200#Mass-Spec

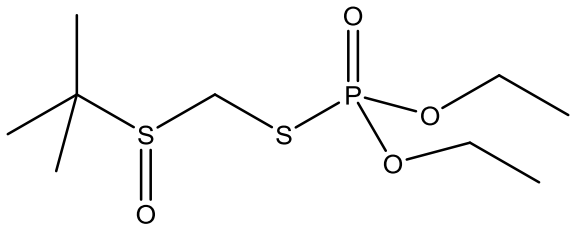
Terbufos oxon $C_9H_{21}O_3PS_2$ **M:272(30%)**

Theoretical molecular ion: m/z
Average MW:



m/z	171	57	215	170	272	143	115	126
%	100	65	60	55	30	30	20	15

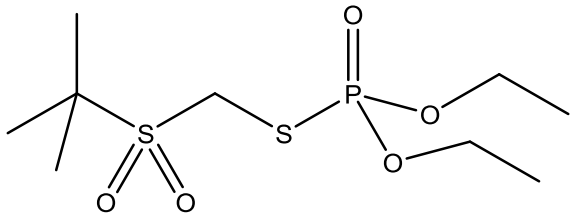
Terbufos oxon sulphoxide **$C_9H_{21}O_4PS_2$** **M:288(0%)**
Theoretical molecular ion: m/z 288.0619 (100%), 289.0652 (9.7%), 290.0577 (9.0%),
Average MW: 288.36



Not amenable to GC.

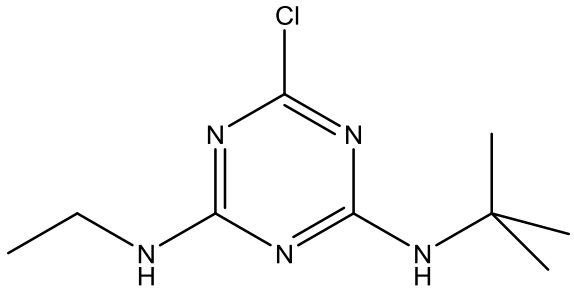
m/z	170	232	109	183	57	139	41	137
%	100	45	35	25	20	15	15	15

Terbufos oxon sulphone **$C_9H_{21}O_5PS_2$** **M:304(0%)**
Theoretical molecular ion: m/z 304.0568 (100%), 305.060 (9.7%), 306.0526 (9.0%)
Average MW: 304.36



m/z	156	183	184	109	140	57	75	155
%	100	85	85	85	85	80	45	35

Terbuthylazine **$C_9H_{16}ClN_5$** **M:229,231(30,10%)**
Theoretical molecular ion: m/z 229.1094 (100%), 231.1065 (32%)
Average MW: 229.71



Chlorotriazine herbicide. Used to control grass and broad-leaved weeds in a variety of situations, including forestry, and for control slime-forming algae, fungi, and bacteria in non-agricultural situations. Approved for use in EU.

Acute oral LD50 for rat >1,000 mg/kg (moderate toxicity).

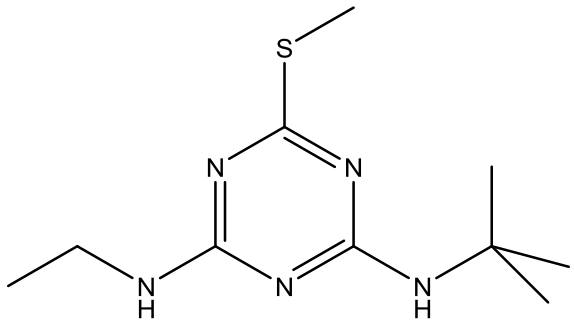
m/z	214	173	216	229	68	43	175	132
%	100	40	35	30	15	15	15	15

229,231 (30,10) – M^+ $C_9H_{16}ClN_5^+$ m/z 229.1094
214,216 (100,35) – [M-15] loss of CH_3 to $C_8H_{13}ClN_5^+$ m/z 214.0860 etc.
173,175 (40,15) – [M-56] loss of butene C_4H_8 to $C_5H_8ClN_5^+$ m/z 173.0468
132 (15) – [M-97] $C_2H_5N.CNC(Cl)NH^+$ $C_4H_7ClN_3^+$ m/z 132.0329 etc.
68 (15) – [M-161] e.g. $C_2H_2N_3^+$ m/z 68.0249 or $C_3H_4N_2^+$ m/z 68.0375? (compare other triazines)

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C5915413&Mask=200#Mass-Spec

Terbutryn **$C_{10}H_{18}N_5S$** **M:241(80%)**

Theoretical molecular ion: m/z 241.1361 (100%), 242.1395 (11%), 243.1319 (4.5%)
Average MW: 241.36



Methylthiotriazine herbicide and algicide. No longer approved for use in EU.

Acute oral LD50 for rat >2,500 (low toxicity).

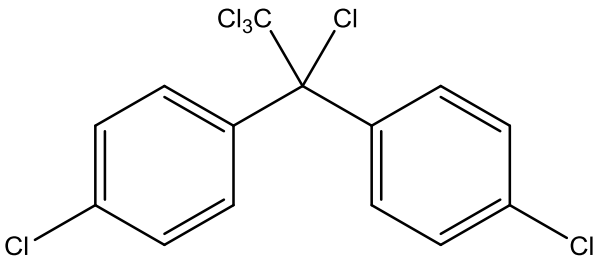
m/z	226	185	241	170	106	157	71	43
%	100	90	80	50	25	20	15	15

241 (80) – M^+
226 (100) – [M-15] loss of CH3 to C9H16N5S+ m/z 226.1126
185 (90) – [M-56] loss of butene C4H8 to C6H11N5S+ m/z 185.0735
170 (50) – [M-71] loss of CH3 & C4H8 to C5H8N5S+ m/z 170.0500

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C886500&Mask=200#Mass-Spec

"Tetrachloro-DDT" **$C_{14}H_8Cl_6$** **M:386,388,390(0,0,0%)**

Theoretical molecular ion: m/z 385.8757 (52%), 387.8728 (100%), 389.8698 (64%), 391.8669 (17%)
Average MW: 388.92



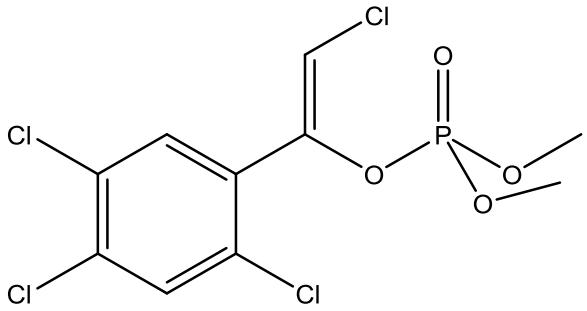
Trivial (and misleading, as hexachloro compound!) name for a formulation contaminant of dicofol.

m/z	269	271	246	248	273	318	176	316
%	100	95	65	45	40	35	35	30

386,388,390 (0,0,0) – M^+ absent
316,318,320 (30,35,15) – [M-70] loss of 2Cl to "DDE" $C_{14}H_8Cl_4^+$ m/z 315.9689 etc.
269,271,273 (100,95,40) – [M-117] loss of CCl_3 to $C_{13}H_8Cl_3^+$ m/z 268.9792 etc.
246,248 (65,45) – [M-140] loss of 4Cl to $C_{14}H_8Cl_2^+$ m/z 246.0003 etc.
176 (30) – [M-210] $C_{14}H_8^+$ m/z 146.0626

No NIST spectrum available.

Tetrachlorvinphos / Stirofos **$C_{10}H_9Cl_4O_4P$** **M:364,366,368(0.5,1,0.5%)**
Theoretical molecular ion: m/z 363.8993 (78%), 365.8963 (100%), 367.8934 (48%)
Average MW: 365.95



Organophosphorus insecticide and acaricide. No longer approved for use in EU.

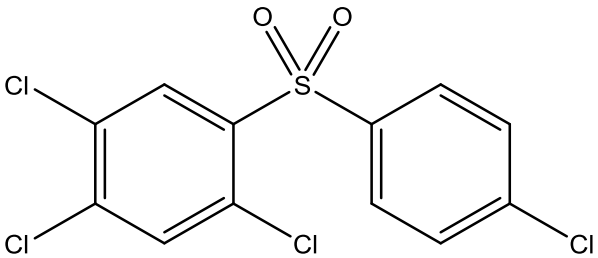
Acute oral LD50 for rat >4,000 (low toxicity).

m/z	109	329	331	333	79	240	204	93
%	100	65	65	20	15	10	10	5

364,366,368 (0.5,1,0.5) – M^+
329,331,333 (65,65,20) – [M-35] loss of Cl to $C_{10}H_9Cl_3O_4P$+ m/z 328.9304
238,240,242 (10,10,5) – [M-126] loss of $(CH_3O)_2PO_2H$ to $C_8H_2Cl_4^+$ m/z 237.8911 etc.
109 (100) – [M-255] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (5) – [M-271] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (15) – [M-285] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C22248799&Mask=200#Mass-Spec

Tetradifon **$C_{12}H_6Cl_4O_2S$** **M:354,356,358(25,35,20%)**
Theoretical molecular ion: m/z 353.8843 (78%), 355.8813 (100%), 357.8784 (48%), 359.8754 (10%)
Average MW: 356.04



Acaricide. Used on horticultural crops to control a wide range of phytophagous mites. No longer approved for use in EU.

Acute oral LD50 for rat >14,700 mg/kg (low toxicity).

This spectrum exhibits an interesting MS fragmentation of the bridged aromatic sulphone:

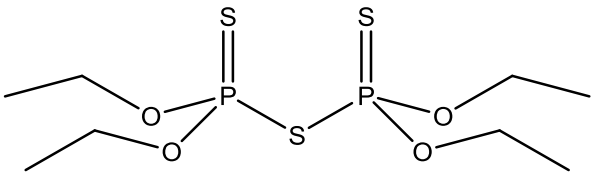
$$Ar\text{-}SO_2\text{-}Ar' \rightarrow ArO^+ \; ArSO^+ \text{ and } ArSO_2^+$$

m/z	159	111	75	227	229	356	161	127
%	100	80	55	50	50	35	35	30

354,356,358 (25,35,20) – M^+
227,229 (50,50) – [M-127] loss of ClC_6H_4O to $C_6H_2Cl_3OS^+$ m/z 226.8892 etc.
195,197 (2,2) – [M-159] loss of ClC_6H_4OS to $C_6H_2Cl_3O^+$ m/z 194.9171 etc.
179,181 (5,5) – [M-175] loss of $ClC_6H_4O_2S$ to $C_6H_2Cl_3^+$ m/z 178.9222 etc.
175, 177 (20,10) – [M-179] loss of $C_6H_2Cl_3$ to $C_6H_4ClO_2S^+$ m/z 174.9621 etc.
159,161 (100,35) – [M-195] loss of $Cl_3C_6H_2O$ to $C_6H_4ClOS^+$ m/z 158.9671 etc.
127,129 (30,10) – [M-243] $C_6H_4ClO^+$ m/z 126.9951 etc.
111,113 (80,25) – [M-243] $C_6H_4Cl^+$ m/z 111.0002 etc.
75 (55) – [M-279] $C_6H_3^+$ m/z 75.0235

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C116290&Mask=200#Mass-Spec

Tetraethyl pyrophosphorotrithioate $C_8H_{20}O_4P_2S_3$ M:338(45%)
Theoretical molecular ion: m/z 337.9999 (100%), 338.9993 (2.4%), 339.9957 (14%)
Average MW: 338.37



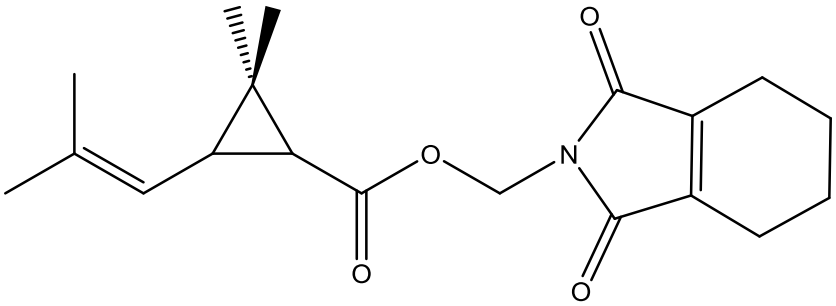
A formulation contaminant of phorate etc.

m/z	97	121	65	93	125	29	338	153
%	100	90	80	65	50	50	45	35

338 (45) – M^+
153 (35) – [M-185] $(C_2H_5O)_2P{=}S^+$ $C_4H_{10}O_2PS^+$ m/z 153.0139
125 (50) – [M-185] $(C_2H_5O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
121 (90) – [M-217] $(C_2H_5O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
97 (100) – [M-241] $(HO)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
93 (65) – [M-245] $(C_2H_5O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105
65 (80) – [M-273] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

No NIST spectrum available.

Tetramethrin $C_{19}H_{25}NO_4$ **M:331(0.5%)**
Theoretical molecular ion: m/z 331.1784 (100%), 332.1817 (21%)
Average MW: 331.41



Tetramethrin (N.B. structure in Wikipedia incorrect)

Synthetic pyrethroid insecticide. Used to control public health pests such as flies, cockroaches, mosquitoes. No longer approved for use in EU.

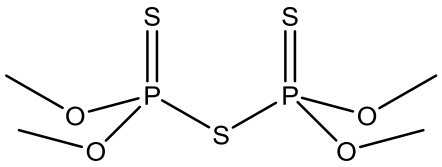
Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

m/z	164	123	81	165	107	79	43	41
%	100	40	15	10	10	10	10	10

331 (0.5) – M^+ weak
164 (100) – [M-167] $CH_2N(CO)_2.C_6H_8^+$ $C_9H_{10}NO_2^+$ m/z 154.0712
123 (40) – [M-208] $(CH_3)_2C{=}CH.C_3H_2(CH_3)_2^+$ $C_9H_{15}^+$ m/z 123.1174

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C7696120&Mask=200#Mass-Spec

Tetramethyl pyrophosphorotrithioate $C_4H_{12}O_4P_2S_3$ **M:282(20%)**
Theoretical molecular ion: m/z 281.9373 (100%), 283.9331 (13.6%)
Average MW: 282.26



Organophosphorus pesticide formulation contaminant of e.g. malathion.

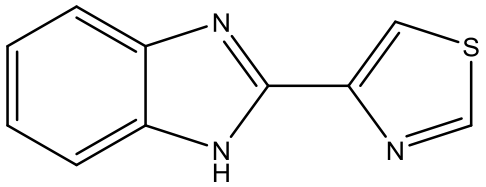
m/z	93	125	282	63	79	47	173	188
%	100	40	20	20	20	20	10	10

282 (20) – M^+
188 (10) – [M-94] loss of $C_2H_6O_2S$ to $C_2H_6O_2P_2S_2^+$ m/z 187.9284
173 (10) – [M-109] O/S scramble and loss of $(CH_3O)_2P\underline{O}$ to $C_2H_6OPS_3^+$ m/z 172.9318
125 (40) – [M-157] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
93 (100) – [M-189] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
79 (20) – [M-203] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (20) – [M-219] PS^+ m/z 62.9458
47 (20) – [M-235] PO^+ m/z 46.9687 (and/or CH_3S+ m/z 46.9956)

No NIST spectrum available.

Thiabendazole **$C_{10}H_7N_3S$** **M:201(100%)**

Theoretical molecular ion: m/z 201.0361 (100%), 202.0394 (11%), 203.0319 (4.5%)
Average MW: 201.25



Benzimidazole fungicide. Used mainly for post-harvest control of a wide range of diseases including *Aspergillus, Botrytis, Cladosporium* and *Fusarium*. Approved for use in EU. Also used as a food preservative, E233.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

Often poor GC peak shape.

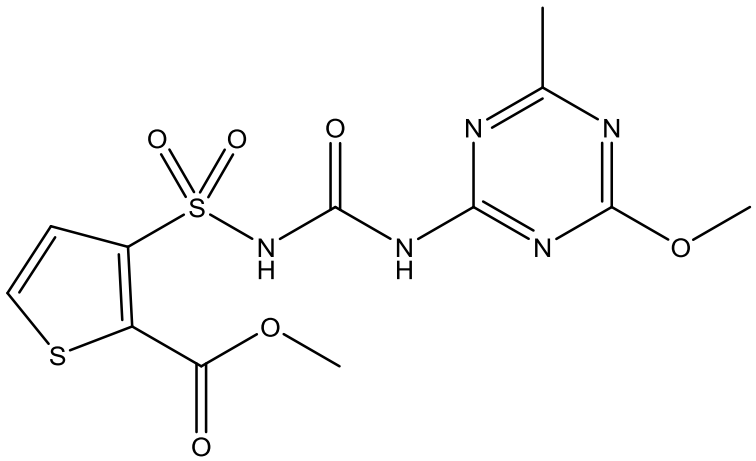
m/z	201	174	202	63	90	129	175	100
%	100	75	15	15	10	10	10	10

201 (100) – M^+
174 (75) – [M-27] loss of HCN to $C_9H_6N_2S^+$ m/z 174.0252

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C148798&Units=SI&Mask=200#Mass-Spec

Thifensulfuron-methyl **$C_{12}H_{13}N_5O_6S_2$** **M:387(0%)**

Theoretical molecular ion: m/z 387.0307 (100%), 388.0341 (13%), 389.0265 (9.0%)
Average MW: 387.39



Triazine sulphonylurea herbicide. Used for post-emergence control of grass and broad-leaved weeds. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

Not amenable to GC. Degradation may produce 2-amino-4-methoxy-6-methyl-1,3,5-triazine, see chlorsulfuron related compound (i).

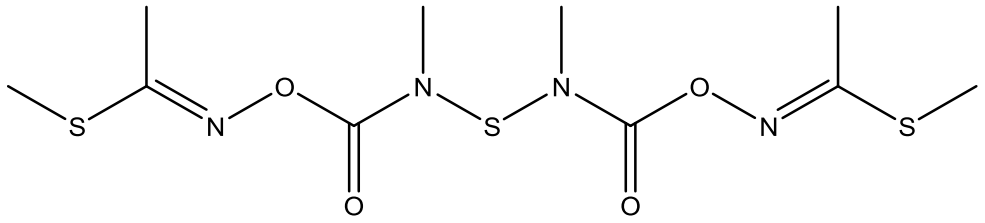
m/z	216	69	140	110	42	247	205	126
%	100	90	80	65	55	45	45	40

387 (0) – M^+
247 (45) – [M-140] loss of triazine to $C_7H_5NO_5S_2^+$ m/z 246.9609
216 (100) – [M-171] $(C_4H_2S)(SO_2NCO)CO^+$ $C_6H_2NO_4S_2^+$ m/z 215.9425
140 (80) –[M-247] $(CH_3O)(CH_3)C_3N_3.NH_2^+$ $C_5H_8N_4O^+$ m/z 140.0698
110 (65) – [M-277] $(CH_3)C_3HN_3.NH_2^+$ $C_4H_6N_4^+$ m/z 110.0593
69 (90) [M-318] $(CH3)C=NCNH_2^+$ $C_3H_5N_2^+$ m/z 69.0453

No NIST spectrum available, but cf. **metsulfuron-methyl** which exhibits similar fragmentation.

Thiodicarb **$C_{10}H_{18}N_4O_4S_3$** **M:354(1%)**

Theoretical molecular ion: m/z 354.0490 (100%), 355.0524 (11%), 356.0448 (14%)
Average MW: 354.46



Oxime carbamate insecticide and molluscicide. Not approved for use in EU.

Acute oral LD50 for rat 50 mg/kg (high toxicity).

Not amenable to GC. May be oxidised to sulphoxide(s) and sulphone(s).

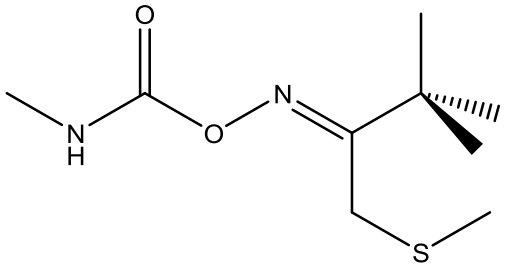
m/z	41	44	47	40	45	61	88	30
%	100	85	55	45	45	45	35	30

354 (1) – M^+
193 (5) – [M-161] $C_5H_9N_2O_2S_2^+$ m/z 193.0105
88 (35) – [M-266] $CH_3S(CH_3)C=N^+$ $C_3H_6NS^+$ m/z 88.0221
61 (45) – [M-293] CH_3NS^+ m/z 60.9986
47 (55) – [M-307] CH_3S^+ m/z 46.9956
44 (85) – [M-310] CO_2^+ m/z 43.9898
41 (100) – [M-313] $N=CCH_3^+$ $C_2H_3N^+$ m/z 41.0266
30 (30) – [M-324] NO^+ m/z 29.9980

No NIST spectrum available.

Thiofanox **$C_9H_{18}N_2O_2S$** **M:218(0%)**

Theoretical molecular ion: m/z 218.1089 (100%), 219.1123 (9.7%), 220.10470 (4.5%)
Average MW: 218.31



Oxime carbamate insecticide and acaricide. Not approved for use in EU.

Acute oral LD50 for rat approx. 5 mg/kg (high toxicity).

May be metabolised to **thiofanox oxime**, and to thiofanox sulphoxide and sulphone.

Poor transmission through GC. May degrade to oxime (by loss of methyl isocyanate), and pivalonitrile, $(CH_3)_3CCN$, on heating in presence of stainless steel (Corkins1982 & Middleditch 1989).

See Corkins (1980) for MS study.

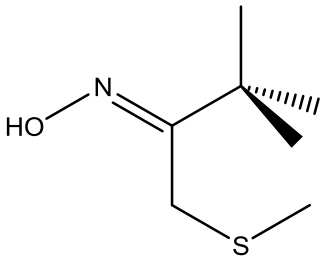
m/z	115	41	57	83	61	55	42	87
%	100	95	90	65	65	60	45	35

218 (0) – M^+ absent $C_9H_{18}N_2O_2S^+$
172 (10) – [M-46] loss of CH_2S to $C_8H_{16}N_2O_2^+$ m/z 172.1212
161 (5) – [M-57] loss of methyl isocyanate CH_3NCO to oxime $C_7H_{15}NOS^+$ m/z 161.0874
144 (5) – [M-74] loss of CH_3NCO & HO to $C_7H_{14}NS^+$ m/z 144.0847
143 (5) – [M-75] loss of CH_3NCO & H_2O to $C_7H_{13}NS^+$ m/z 143.0769
115 (100) – [M-103] loss of CH_3NCO & CH_2S to $C_6H_{13}NO^+$ m/z 115.0997
83 (90) – [M-135] $(CH_3)_3C.C{\equiv}N^+$ $C_5H_9N^+$ m/z 83.0735
61 (65) – [M-157] $CH_2SCH_3^+$ $C_2H_5S^+$ m/z 61.0112
57 (90) – [M-161] $(CH_3)_3C^+$ $C_4H_9^+$ m/z 57.0704 and/or CH_3NCO^+ $C_2H_3NO^+$ m/z 57.0215
41 (95) – [M-177] $C_3H_5^+$ m/z 41.0730

Cf. noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C39196184&Mask=200#Mass-Spec which exhibits some similar abundant ions (m/z 115, 83, 57, 61), but m/z 161 and 55 are much stronger and, critically, m/z 172 is absent. It also displays uninformative background ions to m/z 550. This appears to be a spectrum of a thiofanox degradation product – thiofanox oxime.

Thiofanox oxime $C_7H_{15}NOS$ **M:161(50%)**

Theoretical molecular ion: m/z 161.0874 (100%), 162.0908 (7.6%), 163.0832 (4.5%)
Average MW: 161.26



Thiofanox degradation product. Usually poor GC peak shape.

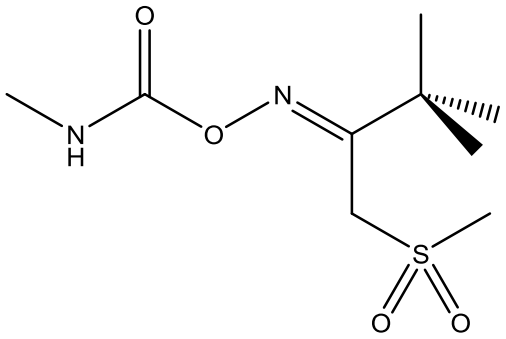
m/z	41	55	60	83	115	161	40	57
%	100	95	90	90	85	50	40	35

Assignments confirmed by accurate mass (Cardiff GCT).
161 (50) – M^+ $C_7H_{15}NOS^+$ m/z 161.0874
144 (5) – [M-17] loss of OH to $C_7H_{14}NS^+$ m/z 144.0847
115 (85) – [M-46] loss of CH_2S to $C_6H_{13}NO^+$ m/z 115.0997
100 (10) – [M-61] loss of C_2H_5S to $C_5H_{10}NO^+$ m/z 100.0762
87 (40) – [M-74] $C_3H_5NS^+$ m/z 87.0861
83 (90) – [M-78] $C_6H_{11}^+$ m/z 83.0735
68 (45) – [M-93] $C_4H_6N^+$ m/z68.0500
61 (80) – [M-100] $C_2H_5S^+$ m/z 61.0108
60 (90) – [M-101] $CHSCH_3^+$ $C_2H_4S^+$ m/z 60.0034
57 (100) – [M-104] $C_4H_9^+$ m/z 57.0704
55 (95) – [M-106] $C_4H_7^+$ m/z 55.0548
45 (50) – [M-78] CHS^+ m/z 44.9799
41 (100) – [M-120] $C_3H_5^+$ m/z 41.0730

No NIST spectrum available.

Thiofanox sulphone $C_9H_{18}N_2O_4S$ **M:250(0%)**

Theoretical molecular ion: m/z 250.0987 (100%), 251.1021 (9.7%), 252.0945 (4.5%)
Average MW: 250.31



Thiofanox metabolite. Not amenable to GC.
Note: Data obtained using VG7070 MS (with JEOL DX300 MS m/z 79 was base peak (ca. 5% in VG spectrum).

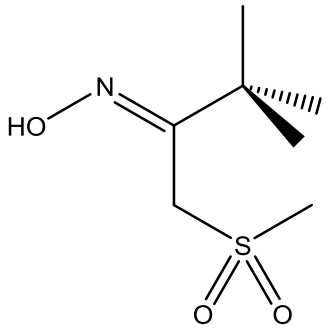
m/z	83	55	41	57	113	58	45	81
%	100	55	35	30	25	25	25	15

250 (0) – M^+
193 (5) – [M-57] loss of methyl isocyanate CH_3NCO to oxime $C_7H_{15}NO_3S^+$ m/z 193.0773
176 (5) – [M-74] loss of CH_3NCO & HO to $C_7H_{14}NO_2S^+$ m/z 176.0745
83 (90) – [M-167] $(CH_3)_3C.C{\equiv}N^+$ $C_5H_9N^+$ m/z 83.0735
79 (5 to 100) – [M-171] $CH_3SO_2^+$ m/z 78.9854
55 (95) – [M-195] $C_4H_7^+$ m/z 55.0548
41 (100) – [M-209] $C_3H_5^+$ m/z 41.0730

No NIST spectrum available.

Thiofanox sulphone oxime **$C_7H_{15}NO3S$** **M:193(0%)**

Theoretical molecular ion: m/z 193.0773 (100%), 194.0806 (7.6%), 195.0731 (4.5%)
Average MW: 193.26



Usually poor GC peak shape.

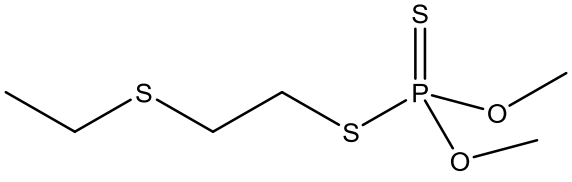
m/z	83	55	41	57	29	81	113	120
%	100	85	65	30	25	20	15	10

193 (0) – M+
176 (3) – [M-17] loss of OH to C7H14NO2S+ m/z 176.0745
120 (10) – [M-73] loss of OH & C4H8 to C3H6NO2S+ m/z 120.0119
113 (15) – [M-80] loss of CH_3SO_2H to $C_6H_{11}NO^+$ m/z 113.0841
83 (100) – [M-110] $(CH_3)_3C.C{\equiv}N^+$ $C_5H_9N^+$ m/z 83.0735
55 (95) – [M-138] $C_4H_7^+$ m/z 55.0548
41 (100) – [M-152] $C_3H_5^+$ m/z 41.0730

No NIST spectrum available.

Thiometon **$C_6H_{15}O_2PS_3$** **M:246(5%)**

Theoretical molecular ion: m/z 245.9972 (100%), 247.9930 (14%), 247.0005 (6.5%)
Average MW: 246.34



Organophosphorus insecticide and acaricicide.

Acute oral LD50 for rat approx 40 mg/kg (high toxicity).

Several oxidative metabolites.

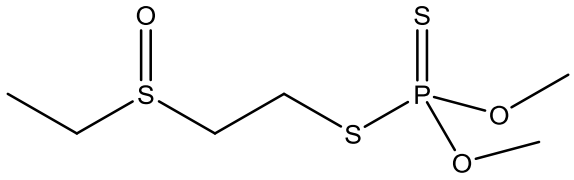
"Thiometon oxon" is equivalent to demeton-S-methyl.

m/z	88	89	60	125	61	246	90	158
%	100	20	20	10	10	5	5	5

246 (5) – M^+
158 (5) – [M-86] $(CH_3O)_2(HS)P{=}S^+$ $C_2H_7O_2PS_2^+$ m/z 158.9625
125 (10) – [M-121] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
93 (5) – [M-153] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.1054
88 (100) – [M-157] $CH_3CH_2SCH{=}CH_2^+$ $C_4H_8S^+$ m/z 88.0347

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C640153&Mask=200

Thiometon sulphoxide **$C_6H_{15}O_2PS_3$** **M:262(0%)**
Theoretical molecular ion: m/z 261.9921 (100%), 262.9955 (6.5%), 263.9879 (14%)
Average MW: 262.34

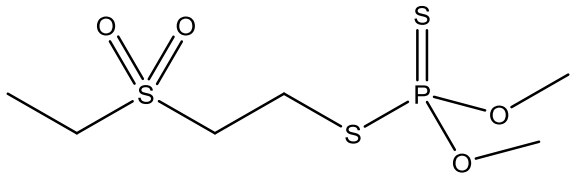


Not amenable to GC analysis.

m/z	125	185	157	93	59	159	187	88
%	100	85	80	15	15	10	10	5

262 (0) – M+ absent
185 (85) – [M-77] loss of CH_3CH_2SO to $CH_2CH_2SPS(OCH_3)_2^+$ $C_4H_{10}O_2PS_2^+$ m/z 184.9860
125 (100) – [M-137] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826

Thiometon sulphone **$C_6H_{15}O_2PS_3$** **M:278(0.5%)**
Theoretical molecular ion: m/z 277.9870 (100%), 278.9904 (6.5%), 279.9828 (13.6%)
Average MW: 278.34



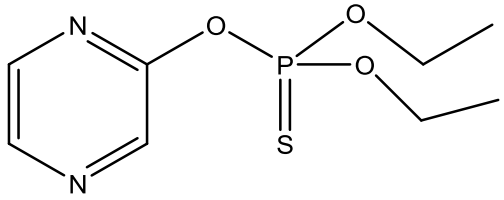
m/z	125	185	93	157	29	158	186	61
%	100	55	35	20	15	10	10	10

278 (0.5) – M^+ weak
185 (55) [M-93] loss of $CH_3CH_2SO_2$ to $CH_2CH_2SPS(OCH_3)_2^+$ $C_4H_{10}O_2PS_2^+$ m/z 184.9860
125 (100) – [M-153] $(CH_3O)_2P{=}S^+$ m/z 124.9826
93 (35) – [M-185] probably due to $(CH_3O)_2P^+$ ($C_2H_6O_2P^+$, m/z 93.0105), rather than $CH_3CH_2SO_2^+$ (m/z 93.0010), as also observed in sulphide spectrum.

Thiometon oxon, see Demeton-S-methyl

Thionazin **$C_8H_{13}N_2O_3PS$** **M:248(20%)**

Theoretical molecular ion: m/z 248.03845 (100%), 249.0418 (8.7%), 250.03425 (4.5%)
Average MW: 248.24



Organophosphorus nematicide. No longer approved for use in EU.

Acute oral LD50 for rat approx 3.5 mg/kg (high toxicity)

May exhibit poor GC transmission. Complex MS fragmentation.

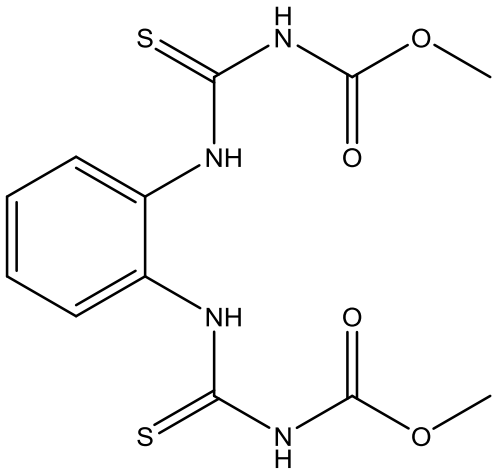
m/z	96	97	107	143	68	79	29	106
%	100	85	80	50	50	50	40	35

Assignments confirmed by accurate mass (Cardiff GCT)
248 (20) – M^+ $C_8H_{13}N_2O_3PS^+$ m/z 238.0385
220 (15) – [M-28] loss of C_2H_4 to $C_6H_9N_2O_3PS^+$ m/z 220.1828
215 (10) – [M-33] loss of SH to $C_8H_{12}N_2O_3P^+$ m/z 215.05855
203 (10) – [M-45] loss of C_2H_5O to $C_6H_8N_2O_2PS^+$ m/z 203.0044
192 (20) – [M-56] loss of $2C_2H_4$ to $C_4H_5N_2O_3PS^+$ m/z 192.1288
175 (20) – [M-73] loss of C_2H_5O & C_2H_4 to $C_4H_4N_2O_2PS^+$ m/z 174.9731
171 (20) – [M-77] loss of C_2H_5OS to $C_6H_8N_2O_2P^+$ m/z 171.0323
159 (10) – [M-89] loss of C_4H_9S to $C_4H_4N_2O_3P^+$ m/z 158.9960
143 (50) – [M-105] $(C_4H_3N_2)OPOH^+$ $C_4H_4N_2O_2P^+$ m/z 143.0010
128(20) – [M-120] $(C_4H_3N_2)SOH^+$ $C_4H_4N_2OS^+$ m/z 128.0043
112(20) – [M-136] $(C_4H_3N_2)SH^+$ $C_4H_4N_2S^+$ m/z 112.0095
107 (80) – [M-141] loss of $C_2H_6O_3PS$ to $(C_4H_3N_2)C_2H_4^+$ $C_6H_7N_2^+$ m/z 107.0609 (ethyl transfer)
97 (85) – [M-151] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
96 (100) – [M-152] pyrazinol $(C_4H_3N_2)OH^+$ $C_4H_4N_2O^+$ m/z 96.0324
79 (50) – [M-169] pyrazine moiety $C_4H_3N_2^+$ m/z 79.0296
68 (50) – [M-180] $C_3H_4N_2^+$ m/z 68.0375
65 (20) – [M-183] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
52(25) – [M-196] C3H2N+ m/z 52.0187

Cf. similar (though weak/noisy) spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C297972&Mask=200#Mass-Spec

Thiophanate-methyl $C_{12}H_{14}N_4O_4S_2$ **M:342(0%)**

Theoretical molecular ion: m/z 342.04565 (100%), 343.0490 (13%), 344.0414 (9.0%)
Average MW: 342.39



Benzimidazole precursor fungicide. Used to control a broad spectrum of diseases in fruit, vegetables, turf and other crops, including eyespot, scab, powdery mildew and grey mould. Approved for use in EU.

Thiophanate-methyl is not amenable to GC analysis. Metabolised to **carbendazim**.

Acute oral LD50 for rat approx >5,000 mg/kg (low toxicity)

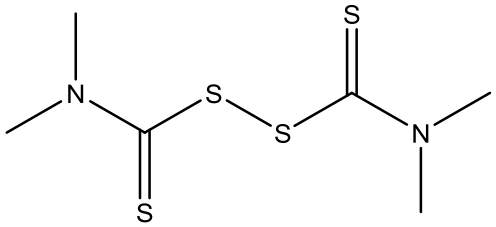
m/z	150	73	44	72	86	159	43	30
%	100	40	25	20	20	20	20	20

324 (0) M^+ absent
209 (10) – [M-115] $C_6H_4(NCS)(NHCSNH2)^+$ $C_8H_7N_3S_2^+$ m/z 209.0081
192 (10) – [M-132] $C_6H_4(NCS)_2^+$ $C_8H_4N_2S_2^+$ m/z 191.9816
150 (100) – [M-175] $C_6H_4(NCS)NH_2^+$ $C_7H_6N_2S_2^+$ m/z 150.0252
73 (40) – [M-251] $NCSNH^+$ CHN_2S+ m/z 73.0930
44 (25) – [M-281] NH_2CO^+ CH_2NO^+ m/z 44.0136

No NIST spectrum available.

Thiram $C_6H_{12}N_2S_4$ **M:240(35%)**

Theoretical molecular ion: m/z 239.9883 (100%), 240.9917 (6.5%), 241.9841 (18.1%)
Average MW: 240.42



Dithiocarbamate fungicide and bird repellent. Used as a seed treatment to control "damping off" (*Pithium sp*) and as a spray to control other fungi such as Botrytis. Also pesticide transformation product.

Acute oral LD50 for rat >1,800 mg/kg (moderate toxicity).

Very poor GC transmission.

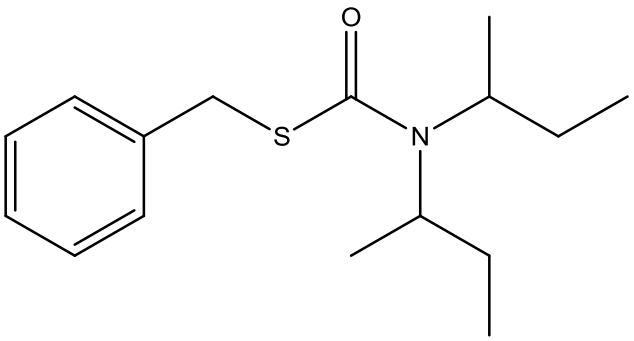
m/z	88	43	240	44	120	42	73	121
%	100	40	35	35	30	30	20	20

240 (35) – M^+
208 (10) – [M-32] loss of S to $C_6H_{12}N_2S_3^+$ m/z 208.0163
120 (30) – [M-120] $C_3H_6NS_2^+$ m/z 119.9942
88 (100) – [M-152] $S{=}C.N(CH_3)_2^+$ $C_3H_6NS^+$ m/z 88.0221
44 (35) – [M-196] $(CH_3)_2N^+$ $C_2H_6N^+$ 44.0500
43 (40) – [M-197] CH_3NCH2^+ $C_2H_5N^+$ m/z 43.0422

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C137268&Units=SI&Mask=200#Mass-Spec apart from absence of m/z 43.

Tiocarbazil **$C_{16}H_{25}NOS$** **M:279(20%)**

Theoretical molecular ion: m/z 279.1657 (100%), 280.1690 (17%), 281.1615 (4.5%)
Average MW: 279.17



Thiocarbamate herbicide. Used to control grasses in submerged rice fields. Not approved for use in EU.

Acute oral LD50 for rat >10,000 mg/kg (low toxicity)

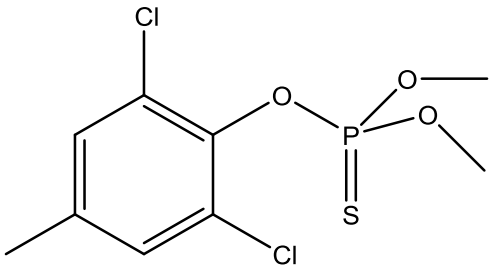
Poor GC transmission/peak shape.

m/z	156	100	57	91	279	250	190	134
%	100	65	60	50	20	15	10	10

279 (20) – M^+ $C_{16}H_{25}NOS^+$
156 (100) – [M-123] loss of $C_6H_5CH_2S$ to $C_9H_{18}NO^+$ m/z 156.1388
100 (65) – [M-179] $CH_3CH_2CH(CH_3)NHCHCH_3^+$ $C_6H_{14}N^+$ m/z 100.1126
91 (50) – [M-188] $C_6H_5CH_2^+$ $C_7H_7^+$ m/z 91.0548
57 (60) – [M-222] $CH_3CH_2CHCH_3^+$ $C_4H_9^+$ m/z 57.0704

No NIST spectrum available.

Tolclofos-methyl **$C_9H_{11}Cl_2O_3PS$** **M:300(0%)**
Theoretical molecular ion: m/z 299.9544 (100%), 301.9514 (64%), 303.9485 (10%)
Average MW: 301.12



Organophosphorus fungicide. Used against soil-borne diseases caused by *Rhizoctonia*, *Corticium*, *Sclerotium* and *Typhula spp*.

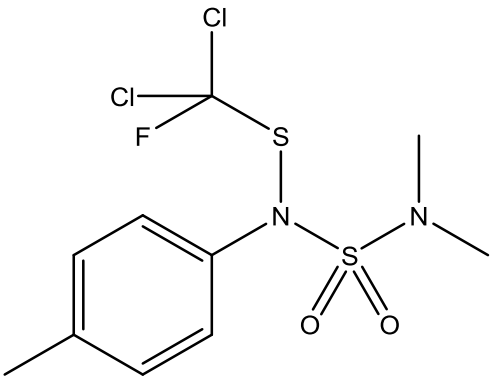
Acute oral LD50 for rat > 5,000 mg/kg (low toxicity).

m/z	265	267	125	79	93	250	47	63
%	100	35	30	20	15	15	10	10

300 (0) – M^+ absent
265,267 (100,35) – [M-35] loss of Cl to give $C_9H_{11}ClO_3PS^+$ m/z 265.9855 etc.
250,252 (15,5) – [M-50] loss of Cl & CH_3 to give $C_8H_8ClO_3PS^+$ m/z 249.9620 etc.
125 (30) – [M-175] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
79 (20) – [M-221] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
63 (10) – [M-237] PS^+ m/z 62.9458

Cf. Similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C57018049&Mask=200#Mass-Spec

Tolylfluanid **$C_{10}H_{13}Cl_2FN_2O_2S_2$** **M:346,348 (5,3%)**
Theoretical molecular ion: m/z 345.9780 (100%), 347.9750 (64%), 349.9721 (10.2%)
Average MW: 347.24



Phenylsulfamide fungicide. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

Tolylfluanid may contain low levels of impurities differing in structure from tolylfluanid in their halogen substituents, i.e. Cl_3CS- and ClF_2CS-, vs. Cl_2FCS- of tolylfluanid. The spectra of these analogues all exhibit m/z137 as base peak.

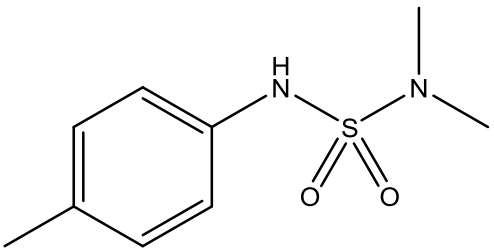
Cf. **dichlofluanid** (homologue).

m/z	137	238	181	240	106	45	214	92
%	100	40	35	25	15	15	10	10

346,348 (5,3) – M^+
238,240,242 (40,25,10) – [M-108] loss of $SO_2N(CH_3)_2$ to $C_8H_7Cl_2FNS^+$ m/z 237.9660 etc.
181 (35) – [M-165] loss of $CFCl_2$ & SO_2(!) to $C_9H_{13}N_2S^+$ m/z 181.0799 [rearrangement]
137 (100) – [M-209] $C_6H_5NS^+$ $C_7H_7NS^+$ m/z 137.0299

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C731271&Mask=200

Tolylfluanid related **$C_9H_{14}N_2O_2S$** **M:214(50%)**
N-(dimethylsulphamoyl)-*p*-toluidine
Theoretical molecular ion: m/z 214.0776 (100%), 215.0810 (9.7%), 216.0734 (4.5%)
Average MW: 214.08



GC degradation product:

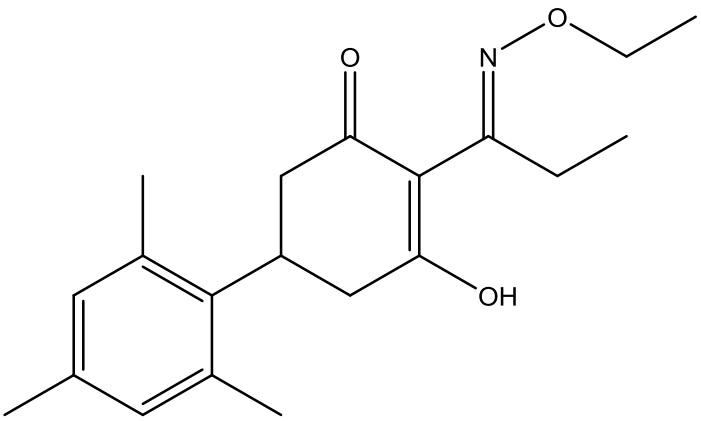
m/z	106	214	79	77	107	78	135	92
%	100	50	40	25	15	10	5	5

214 (40) – M+
106 (100) – [M-108] $CH_3C_6H_4NH^+$ $C_7H_8N^+$ m/z 106.0657

Toxaphene, see Camphechlor

Tralkoxydim $C_{20}H_{27}NO_3$ **M:329(1%)**

Theoretical molecular ion: m/z 329.1991 (100%), 330.20245 (21.6%)
Average MW: 329.44



Cyclohexene oxime herbicide. Used as foliar applied agent for grass weed control in cereals. Approved for use in EU. (Cf. **cycloxydim**.)

Acute oral LD50 for rat approx. 900 mg/kg (moderate toxicity).

Poor GC transmission.

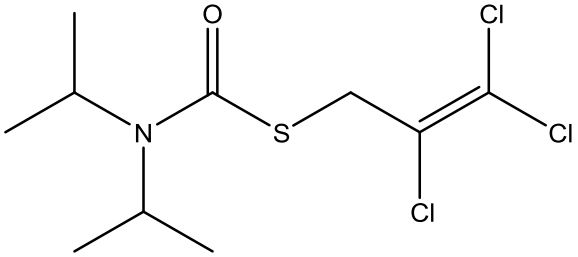
m/z	284	29	138	126	146	285	43	91
%	100	80	55	25	25	20	20	20

329 (1) – M^+
284 (100) – [M-45] loss of CH_3CH_2O to $C_{18}H_{22}NO_2^+$ m/z 284.16505
138 (55) – [M-191] cyclohexene core $C_6H_5(O)(OH)CN/H_2^+$ $C_7H_8NO_2^+$ m/z 138.0555
29 (80) – [M-300] $CH_3CH_2^+$ $C_2H_5^+$ m/z 29.0391

No NIST spectrum available.

Tri-allate $C_{10}H_{16}Cl_3NOS$ **M:303,305,307(0,0,0%)**

Theoretical molecular ion: m/z 303.0018 (100%), 304.9989 (96%), 306.9959 (31%)
Average MW: 304.65



Thiocarbamate herbicide. Soil-acting, post-sowing, pre-emergence agent for control of wild oat and some annual grass weeds in cereal crops. Approved for use in EU.

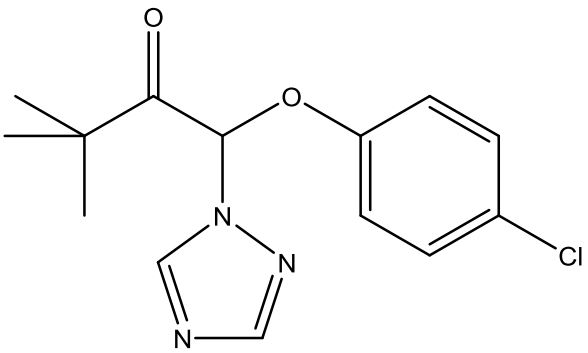
Acute oral LD50 for rat approx. 1,000 mg/kg (moderate toxicity).

m/z	43	86	268	128	270	143	145	84
%	100	85	20	20	15	10	10	5

303,305,307 (0,0,0) – M^+ absent $C_{10}H_{16}Cl_3NOS^+$
268,270,272 (20,15,3) – [M-35] loss of Cl to $C_{10}H_{16}Cl_2NOS^+$ m/z 268.0330
143,145,147 (10,10,5) – [M-160] $(CH_2)ClC{=}CCl_2^+$ $C_3H_2Cl_3^+$ m/z 142.9222 etc.
128 (20) – [M-175] $[(CH_3)_2CH]_2NCO^+$ $C_7H_{14}NO^+$ m/z 128.1075
86 (85) – [M-217] $(CH_3)_2CHNCOH^+$ $C_4H_8NO^+$ m/z 86.0606
43 (100) – [M-260] $(CH_3)_2CH^+$ $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2303175&Mask=200#Mass-Spec

Triadimefon **$C_{14}H_{16}ClN_3O_2$** **M:293,295(2,1%)**
Theoretical molecular ion: m/z 293.0931 (100.0%), 294.0965 (15%), 295.09015 (32%)
Average MW: 293.75



Fungicide. Used to control powdery mildew, rusts, and other infections in many crops. No longer approved for use in EU.

Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

Oxidation product of **triadimenol**.

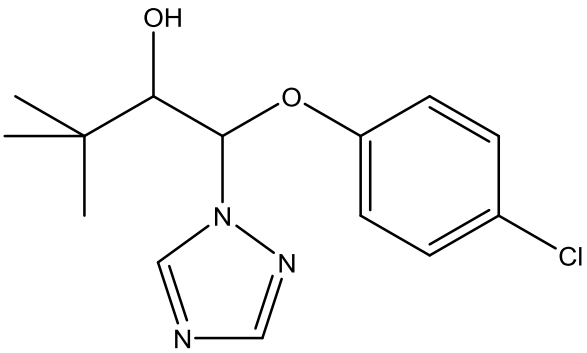
m/z	57	208	41	85	29	128	110	181
%	100	50	40	35	30	20	20	20

293,295 (2,1) – M^+
236,238 (3,2) – [M-57] loss of $(CH_3)_3C$ to $C_{10}H_7ClN_3O_2^+$ m/z 236.0227 etc.
208,210 (50,15) – [M-85] loss of $(CH_3)_3C.CO$ to $C_9H_7ClN_3O^+$ m/z 208.0278
85 (35) – [M-208] $(CH_3)_3CCO^+$ $C_5H_9O^+$ m/z 85.0653
57 (100) – [M-236] $(CH_3)_3C^+$ $C_4H_9^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C43121433&Mask=200#Mass-Spec and in Flamini (2010).

Triadimenol **$C_{14}H_{18}ClN_3O_2$** **M:295(0%)**

Theoretical molecular ion: m/z 295.10875 (100%), 296.1121 (15%), 297.1058 (32%)
Average MW: 295.75



Fungicide. Used on cereals, beet and brassicas to control a range of diseases including powdery mildew, rusts, bunts and smuts. Approved for use in EU.

Acute oral LD50 for rat approx. 700 mg/kg (moderate toxicity).

Poor GC transmission/peak shape.

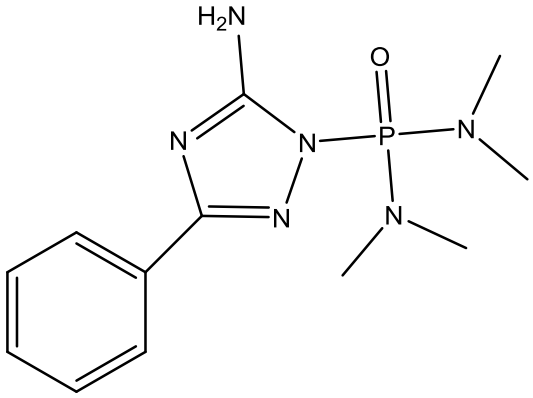
m/z	112	168	128	70	57	43	130	169
%	100	90	35	35	30	15	10	10

295,297 (0,0) – M^+ absent
238,240 (5,2) – [M-57] loss of $(CH_3)_3C$ to $C_{10}H_9ClN_3O_2^+$ m/z 238.0383
168 (90) – [M-127] loss of ClC_6H_4O to $C_8H_{14}N_3O^+$ m/z 168.1137
128 (35) – [M-167] $ClC_6H_4OH^+$ $C_6H_5ClO^+$ m/z 128.0029
112 (100) – [M-183] $(C_2H_2N_3)C_2H_3OH^+$ $C_4H_6N_3O^+$ m/z 112.0511
70 (35) – [M-225] triazole moiety $C_2H_4N_3^+$ m/z 70.0405
57 (30) – [M-238] $(CH_3)_3C^+$ $C_4H_9^+$ m/z 57.0704

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C55219653&Mask=200#Mass-Spec apart from different relative intensities (e.g. m/z 168 weaker and m/z 41 stronger)

Triamiphos **$C_{12}H_{19}N_6OP$** **M:294(20%)**

Theoretical molecular ion: m/z 294.1358 (100%), 295.13915 (13%), 295.1328 (2.2%)
Average MW: 294.29



Organophosphorus fungicide. Not approved for use in EU.

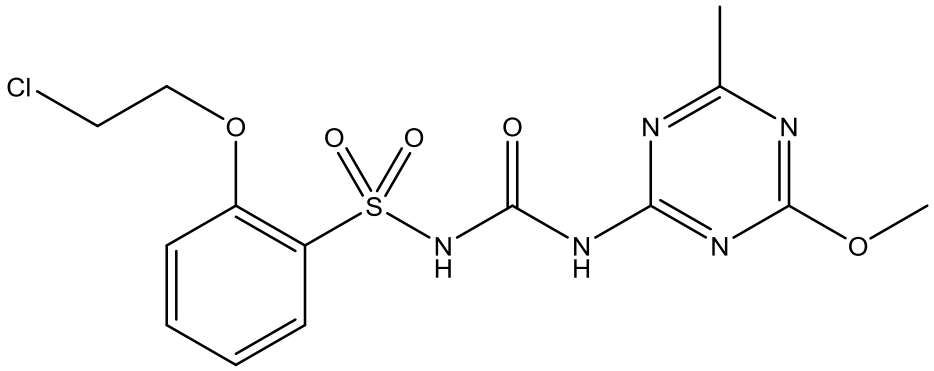
Acute oral LD50 for rat approx. 20 mg/kg (high toxicity).

m/z	160	44	135	294	92	161	104	251
%	100	40	40	20	15	15	10	5

294 (20) – M^+
160 (100) – [M-134] $C_6H_5.C_2N_3.NH_2/H^+$ $C_8H_8N_4^+$ m/z 160.0749
135 (40) – [M-159] $[(CH_3)_2N]_2P{=}O^+$ $C_4H_{12}N_2OP^+$ m/z 135.0687
104 (10) – [M-190] $C_6H_5.CNH^+$ $C_7H_6N^+$ m/z 104.0500
92 (15) – [M-202] $[(CH_3)_2N]P{=}OH^+$ $C_2H_7NOP^+$ m/z 92.0265
44 (40) – [M-250] $(CH_3)_2N^+$ $C_2H_6N^+$ m/z 44.0500

Cf. similar, but weak, spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1031476&Mask=200#Mass-Spec

Triasulfuron **$C_{14}H_{16}ClN_5O_5S$** **M:401,403(0,0%)**
Theoretical molecular ion: m/z 401.0561 (100%), 402.0594 (15%), 403.0531 (32%)
Average MW: 401.82



Herbicide. Used to control annual broad-leaved weeds in cereals. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

Not amenable to GC. Degradation may produce 2-amino-4-methoxy-6-methyl-1,3,5-triazine, see chlorsulfuron related compound (i).

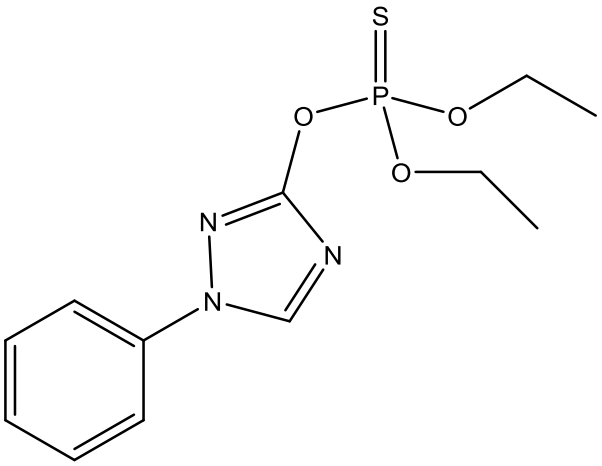
m/z	63	69	156	42	140	65	110	92
%	100	90	85	85	65	50	50	50

401,403 (0,0) – M^+ absent
261,263 (20,5) – [M-140] $ClC_2H_4OC_6H_4SO_2NCO^+$ $C_9H_8ClNO_4S^+$ m/z 260.9863 etc.
156 (85) – [M-245] $OC_6H_4SO_2^+$ $C_6H_4O_3S^+$ m/z 155.9882
140 (65) – [M-261] $CH_3(CH_3O)(C_3N_3)NH_2^+$ $C_5H_8N_4O^+$ m/z 140.0698
69 (90) – [M-332] $(CH3)C{=}NCNH2^+$ $C_3H_5N_2^+$ m/z 69.0453
63 (100) – [M-338] $ClCH_2CH_2^+$ $C_2H_4Cl^+$ m/z 63.0002 etc.
42 (30) – [M-353] NCO^+ m/z 41.9980

No NIST spectrum available.

Triazophos $C_{12}H_{16}N_3O_3PS$ **M:313(5%)**

Theoretical molecular ion: m/z 313.0650 (100%), 314.0684 (13%), 315.0608 (4.5%)
Average MW: 313.31



Organophosphorus insecticide and acaricide, used for the control of a range of insects including aphids, thrips, midges, beetles and other soil insects in a wide range of crops.

Acute oral LD50 for rat approx. 50 mg/kg (high toxicity).

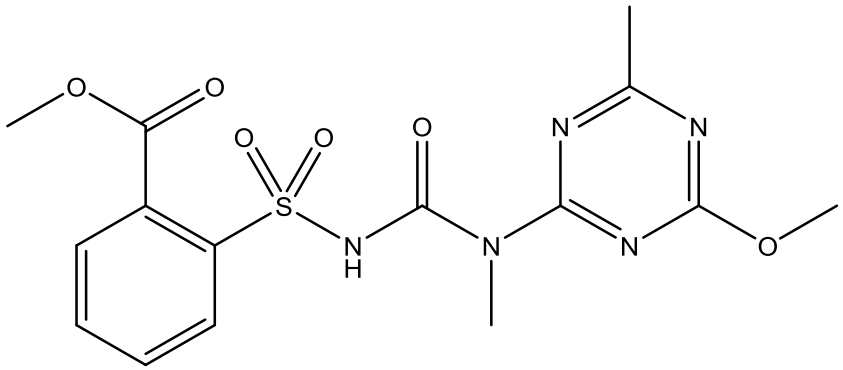
m/z	161	162	172	177	257	97	285	91
%	100	75	50	30	30	25	25	25

Assignments confirmed by accurate mass (Cardiff GCT).
313 (5) – M^+ $C_{12}H_{16}N_3O_3PS^+$ m/z 313.0650
285 (25) – [M-28] loss of C_2H_4 to $C_{10}H_{12}N_3O_3PS^+$ m/z 285.0337
257 (30) – [M-56] loss of $2C_2H_4$ to $C_8H_8N_3O_3PS^+$ m/z 257.0024
240 (10) – [M-73] loss of C_4H_9O to $C_8H_7N_3O_2PS^+$ m/z 239.9997
224 (5) – [M-89] loss of C_4H_9S to $C_8H_7N_3O_3P^+$ m/z 224.0225
208 (20) – [M-105] loss of C_4H_9OS to $C_8H_7N_3O_2P^+$ m/z 208.0276
177 (30) – [M-136] loss of $C_4H_9O_3P$ to $C_8H_7N_3S^+$ m/z 177.0361
172 (50) – [M-141] loss of $C_2H_6O_3PS$ to $C_{10}H_{10}N_3^+$ m/z 172.0875 (ethyl transfer from OP)
162 (100) – [M-151] $C_6H_5.C_2N_3H.OH/H^+$ $C_8H_8N_3O^+$ m/z 162.0667
161 (100) – [M-152] $C_6H_5.C_2N_3H.OH^+$ $C_8H_7N_3O^+$ m/z 161.0589
153 (20) – [M-160] $C_4H_{10}O_2PS^+$ m/z 153.0139
134 (20) – [M-179] $C_6H_5.N_2COH^+$ $C_7H_6N_2O^+$ m/z 134.0480
125 (15) – [M-188] $(CH_3CH_2O)(HO)P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
105 (15) – [M-179] $C_6H_5.N_2^+$ $C_6H_5N_2^+$ m/z 105.0452
97 (25) – [M-216] $(HO)_2PS^+$ $H_2O_2PS^+$ m/z 96.9513
91 (25) – [M-210] $C_6H_5N^+$ m/z 91.0422
77 (25) – [M-236] $C_6H_5^+$ m/z 77.0391
65 (20) – [M-248] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792
51 (20) – [M-262] $C_4H_3^+$ m/z 51.0235

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C24017478&Mask=200#Mass-Spec

Tribenuron-methyl $C_{15}H_{17}N_5O_6S$ **M:395(0%)**

Theoretical molecular ion: m/z 395.08995 (100%), 396.0933 (16%), 397.08575 (4.5%)
Average MW: 395.39



Triazylsulphonylurea herbicide. Foliar acting, post-emergence action used to control broad-leaved weeds in cereals. Approved for use in EU. Also free acid.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity)

Not amenable to GC.

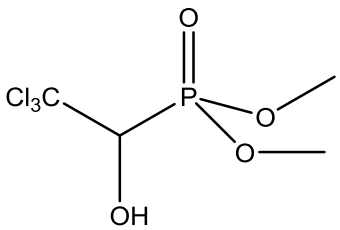
m/z	210	154	42	56	124	90	69	77
%	100	75	30	30	30	25	20	20

395 (0) – M^+ absent
241 (15) – [M-154] $CH_3OCO.C_6H_4.SO_2NCO^+$ $C_9H_7NO_5S+$ m/z 241.0045
210 (100) – [M-185] $CO.C_6H_4.SO_2NCO^+$ $C_8H_5NO_4S+$ m/z 241.0045
154 (75) – [M-241] $CH_3NH(C_3N_3)(CH_3)(OCH_3)^+$ $C_6H_{10}N_4O^+$ m/z 154.0855
42 (30) – [M-353] NCO^+ m/z 41.9980

No NIST spectrum available.

Trichlorfon / Metrifonate $C_4H_8Cl_3O_4P$ **M:256(0%)**

Theoretical molecular ion: m/z 255.9226 (100%), 257.9196 (96%), 259.9167 (31%)
Average MW: 257.43



Organophosphorus insecticide. No longer registered for use in EU.

Acute oral LD50 for rat approx. 25 mg/kg (high toxicity)

Trichlorfon may undergo degradation on GC to produce **dichlorvos** (-HCl) and/or **dimethyl phosphite** (see below)

$Cl_3C\text{-}CH(OH)\text{-}P{=}O(OCH_3)_2 \rightarrow Cl_2C{=}CH\text{-}P{=}O(OCH_3)_2$ and/or $HP{=}O(OCH_3)_2$

m/z	109	79	110	145	80	139	112	82
%	100	85	45	35	30	30	25	20

256 (0) – M^+ absent $C_4H_8Cl_3O_4P^+$
221,223 (5,3) – [M-35] loss of Cl to give $C_4H_8Cl_2O_4P^+$ m/z 220.9537 etc.
185,187 (6,2) – [M-71] loss of HCl_2 to give $C_4H_7ClO_4P^+$ m/z 184.9771
145,147 (35,10) – [M-111] loss of Cl_2CCOH to $(CH_3O)_2(HO)PCl^+$ $C_2H_7ClO_3P^+$ m/z 144.9821 – rearrangement
139 (30) – [M-117] loss of CCl_3 to give $(CH_3O)_2PO.CHOH^+$ $C_3H_8O_4P^+$ m/z 139.0160
110 (100) – [M-146] $(CH_3O)_2P(OH)^+$ $C_2H_7O_3P^+$ m/z 110.0133
109 (100) – [M-147] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
79 (85) – [M-177] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949
47 (15) – [M-209] PO^+ m/z 46.9687

Cf. http://webbook.nist.gov/cgi/cbook.cgi?ID=C52686&Mask=200

Trichlorfon related **$C_2H_7O_3P$** **M:110(5%)**

Dimethyl phosphite (GC degradation product)
Theoretical molecular ion: m/z 110.0133 (100%)
Average MW: 110.29

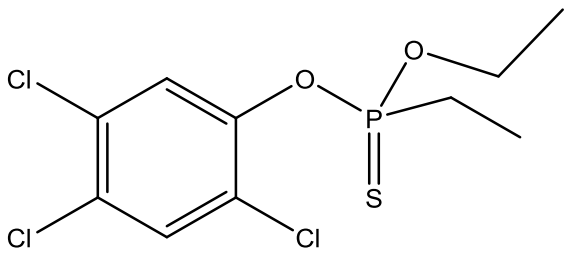
$(CH_3O)_2HP{=}O$

m/z	80	79	47	95	31	110	109	65
%	100	90	30	15	15	5	5	5

110 (5) – M^+
80 (100) – [M-30] loss of CH_2O to $(CH_3O)(HO)HP{=}O^+$ $CH_5O_2P^+$ m/z 80.0027
79 (90) – [M-31] loss of CH_2O to $(CH_3O)(HO)P{=}O^+$ $CH_4O_2P^+$ m/z 78.9949

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C868859&Mask=200#Mass-Spec
Listed under "Phosphonic acid, dimethyl ester"

Trichloronat **$C_{10}H_{12}Cl_3O_2PS$** **M:332,334(0,0%)**
Theoretical molecular ion: m/z 331.9361 (100%), 333.9332 (96%), 335.9302 (31%)
Average MW: 333.59



Organophosphorus (phenyl ethylphosphonothiate) insecticide. No longer approved for use in EU.

Acute oral LD50 for rat approx. 20 mg/kg (high toxicity)

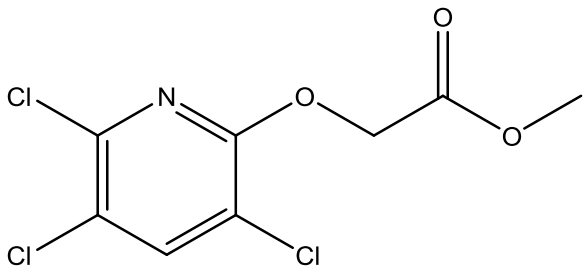
m/z	109	297	269	93	299	271	81	137
%	100	40	30	25	20	20	20	15

332,334 (0,0) – M^+ absent

297,299,301(40,20,5) – [M-35] loss of Cl to give $C_{10}H_{12}Cl_2O_2PS^+$ m/z 296.9673 etc.
269,271,273 (30,20,5) – [M-63] loss of Cl+C2H4 to give $C_8H_8Cl_2O_2PS^+$ m/z 268.9360 etc.
137 (15) – [M-195] $(C_2H_5)(C_2H_5O)P{=}S^+$ $C_4H_{10}OPS^+$ m/z 137.0190
109 (100) – [M-223] $(C_2H_5)(HO)P{=}S^+$ $C_2H_6OPS^+$ m/z 108.9877
93 (25) – [M-239] $(C_2H_5O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C327980&Mask=200#Mass-Spec

Triclopyr-methyl **$C_8H_6Cl_3NO_3$** **M:269,271,273(30,30,5%)**
Theoretical molecular ion: m/z 268.9413 (100%), 270.9384 (96%), 272.9354 (31%)
Average MW: 270.49



Pyridine herbicide. Used for perennial broad-leaved and woody weed control on uncultivated areas, grassland, plantations and rice fields. Approved for use in EU.

Acute oral LD50 for rat approx. 600 mg/kg (moderate toxicity) for triclopyr acid.

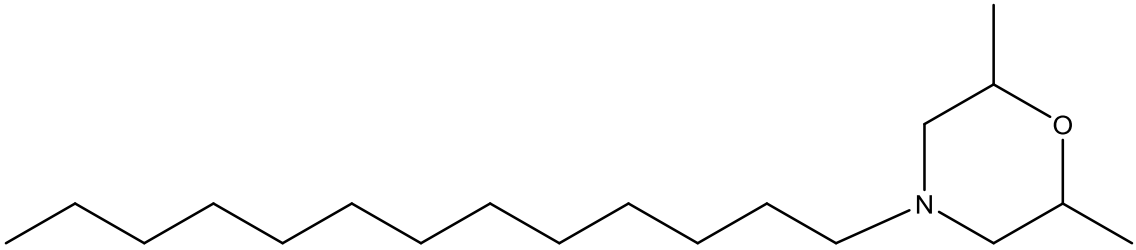
The metabolite 3,5,6-trichloropyridinol (also associated with chlorpyrifos) is of toxicological concern regarding human male reproductive health.

m/z	210	212	182	146	45	269	271	59
%	100	90	40	40	40	30	30	25

269,271 (30,30) – M^+
210,212 (100,90) – [M-59] loss of $COOCH_3$ to $C_6H_3Cl_3NO^+$ m/z 209.9280 etc.
180,182 (35,40) – [M-89] loss of OCH_2COOCH_3 to $C_5HCl_3N^+$ m/z 179.9175 etc.
146,148 (40,15) – [M-123] $C_5H_2Cl_2N^+$ m/z 145.9564 etc.

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C60825265&Mask=200
listed under "Acetic acid, [(3,5,6-trichloro-2-pyridinyl)oxy]-, methyl ester"

Tridemorph **$C_{19}H_{39}NO$** **M:297(2%)**
Theoretical molecular ion: m/z 297.3032 (100%), 298.3065 (21%)
Average MW: 297.53



Major component of Tridemorph (2,6-dimethyl-4-tridecylmorpholine)

Systemic morpholine fungicide. Used to control *Erysiphe graminis* in cereals, and a range of other diseases. No longer approved for use in EU.

Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity).

A mixture of C_{10}-C_{14} alkyl chain isomers is present with the tridecyl being the major component. They have similar MS fragmentation pathways. They elute as a broad envelope of peaks on GC. KI(CPSil19) = 18-20

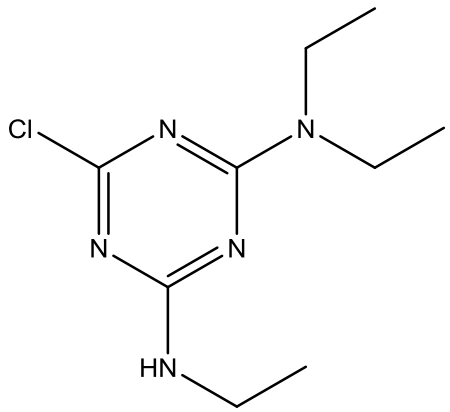
m/z	128	129	43	55	115	70	84	297
%	100	10	5	5	5	5	5	2

297 (2) – M^+
128 (100) – [M-169] loss of $C_{12}H_{25}$ to give $CH_2{=}N(C_4H_6O_2)(CH_3)_2^+$ $C_7H_{14}NO^+$ m/z 128.1075
43 (5) – [M-254] CH_3CO^+ $C_2H_3O^+$ m/z 43.0184

No NIST spectrum available.

Trietazine **$C_9H_{16}ClN_5$** **M:229,231(65,20%)**

Theoretical molecular ion: m/z 229.1094 (100%), 231.1065 (32%)
Average MW: 229.71



Chlorotriazine herbicide. Used, often with linuron, for weed control in potatoes and legumes.

Acute oral LD50 for rat approx. 500 mg/kg (moderate toxicity)

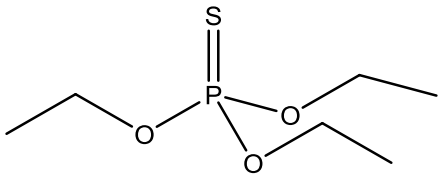
m/z	200	229	214	186	202	68	72	231
%	100	65	60	55	35	25	25	20

229,231 (65,20) – M^+
214,216 (60,20) – [M-15] loss of CH_3 to give $C_8H_{13}ClN_5^+$ m/z 214.08599 etc.
200,202 (100,35) – [M-29] loss of CH_3CH_2 to give $C_7H_{11}ClN_5^+$ m/z 200.0703 etc.
186,188 (55,15) – [M-43] loss of CH_3+CH_3CH_2 to give $C_6H_9ClN_5^+$ m/z 186.05465 etc.
72 (25) – [M-157] $(CH_3CH_2)_2N^+$ $C_4H_{10}N^+$ m/z 72.0813
68 (25) – [M-161] triazole fragment HN-C=N-C=NH^+ $H_2C_2N_3^+$ m/z 68.0249

http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912261&Mask=200

Triethyl-(O,O,O) phosphorothioate $C_6H_{15}O_3PS$ **M:198(100%)**

Theoretical molecular ion: m/z 198.0480 (100%), 199.0513 (6.5%)
Average MW: 198.22



A formulation contaminant of demeton etc.

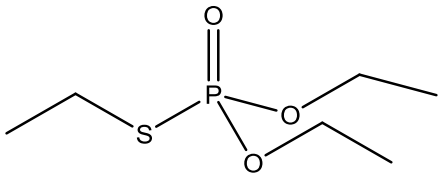
m/z	198	121	93	109	115	114	126	65
%	100	95	75	40	40	40	40	35

Assignments confirmed by accurate mass study (Cardiff GCT)
198 (100) – M^+ $C_6H_{15}O_3PS^+$ m/z 125.9904
126 (40) – [M-72] $(CH_3CH_2O)(HO)P{=}SH^+$ $C_2H_7O_2PS^+$ m/z 125.9904
121 (95) – [M-77] $(CH_3CH_2O)_2P^+$ $C_4H_{10}O_2P^+$ m/z 121.0418
115 (40) – [M-83] $(HO)_3P{=}SH^+$ $H_4O_3PS^+$ m/z 114.9619
114 (40) – [M-84] $(HO)_3P{=}S^+$ $H_3O_3PS^+$ m/z 113.9506
109 (40) – [M-89] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
97 (30) – [M-101] $(HO_2)_2P{=}S^+$ $H_2O_2PS^+$ m/z 96.9513
93 (75) – [M-105] $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105
81 (30) – [M-117] $(HO)_2P{=}O^+$ $H_2O_3P^+$m/z 80.9742
65 (35) – [M-133] $(HO)_2P^+$ $H_2O_2P^+$ m/z 64.9792

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C126681&Units=SI&Mask=200#Mass-Spec

Triethyl-(O,O,S) phosphorothioate $C_6H_{15}O_3PS$ **M:198(60%)**

Theoretical molecular ion: m/z 198.0480 (100%), 199.0513 (6.5%)
Average MW: 198.22



A formulation contaminant of demeton etc.

m/z	138	111	198	170	109	82	93	142
%	100	80	60	55	50	35	35	30

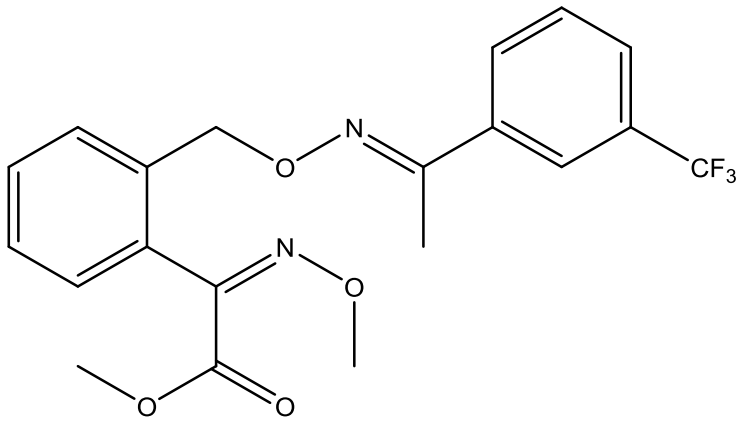
198 (60) – M^+
170 (55) – [M-28] loss of C_2H_4 to give $(CH_3CH_2O)_2(HS)P{=}O^+$ $C_4H_{11}O_3PS^+$ m/z 170.0167
142 (30) – [M-56] loss of $2C_2H_4$ to give$(CH_3CH_2O)(HS)(HO)P{=}O^+$ $C_2H_7O_3PS^+$ m/z 141.9854
138 (100) – [M-60] loss of C_2H_4S to give $(CH_3CH_2O)_2(HO)P^+$ $C_4H_{11}O_3P^+$ m/z 138.0446
111 (80) – [M-87] loss of $(CH_3CH_2O)(HO)_2PH^+$ $C_2H_8O_3P^+$ m/z 111.02111 (?)
109 (50) – [M-89] $(CH_3CH_2O)(HO)P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
93 (75) – [M-105] $(CH_3CH_2O)(HO)P^+$ $C_2H_6O_2P^+$ m/z 93.0105
82 (35) – [M-116] $(HO)_3P^+$ $H_3O_3P^+$ m/z 81.9820

Fascinating differences between these 2 isomers.

Cf. very poor spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1186090&Units=SI&Mask=200#Mass-Spec

Trifloxystrobin **$C_{20}H_{19}F3N_2O_4$** **M:408(0,0%)**

Theoretical molecular ion: m/z 387.0986 (100%), 389.0956 (32%)
Average MW: 408.37



Strobilurin fungicide. Protective and curative action. Approved for use in EU.

Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

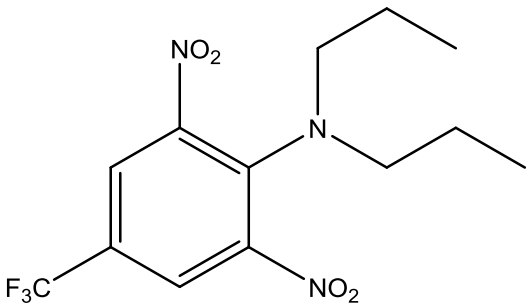
m/z	116	131	59	132	145	222	186	206
%	100	60	45	30	25	20	20	20

408 (0) – M^+ absent
377 (2) – [M-31] loss of CH_3O to $C_{19}H_{16}F_3N_3O^+$ m/z 377.1113
222 (20) – [M-223] $C_8H_6CNO_3^+$ m/z 164.00348?
145 (25) – [M-263] $C_6H_4.CF_3^+$ $C_7H_4F_3^+$ m/z 145.0265
131 (60) – [M-276] $NC.C_6H_4.CHO^+$ $C_8H_5NO^+$ m/z 131.0371
116 (100) – [M-292] $NC.C_6H_4.CH_2^+$ $C_8H_6N^+$ m/z 116.0500
59 (45) – [M-349] $COOCH_3^+$ $C_2H_3O_2^+$ m/z 59.0133

No NIST spectrum. Data from NJ DEP collection:
http://www.nj.gov/dep/enforcement/pcp/bpo/pem/spectras/eispectra/Trifloxystrobin.pdf

Trifluralin **$C_{13}H_{16}F_3N_3O_4$** **M:335(15%)**

Theoretical molecular ion: m/z 335.1093 (100%), 336.11265 (14%)
Average MW: 335.28



Dinitroaniline herbicide. Used as a pre-emergence, soil-incorporated agent in various crops to control annual grasses and broad-leaved weeds. Not approved for use in EU.

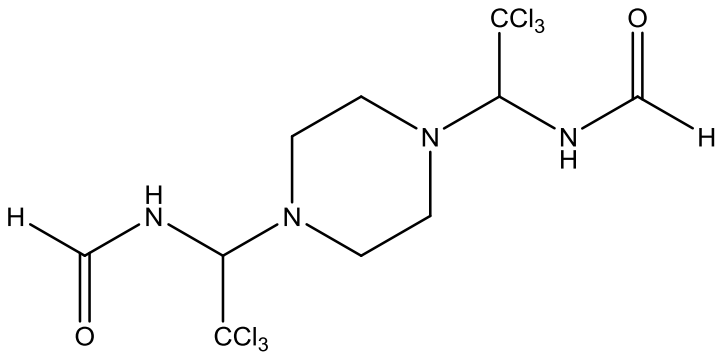
Acute oral LD50 for rat >5,000 mg/kg (low toxicity).

m/z	306	264	43	41	290	335	307	248
%	100	80	65	35	15	15	15	15

335 (15) – M^+
318 (5) – [M-17] loss of OH from $–NO_2$ to $C_{13}H_{15}F_3N_3O_3^+$ m/z 318.1066
316 (5) – [M-19] loss of F from $-CF_3$ to give $C_{13}H_{16}F_2N_3O_4^+$ m/z 316.1109
306 (100) – [M-29] loss of CH_3CH_2 to give $C_{11}H_{11}F_3N_3O_4^+$ m/z 306.0702
290 (15) – [M-45] loss of $OH+C_2H_5$ $C_{11}H_{11}F_3N_3O_3^+$ m/z 290.0753
264 (80) – [M-71] loss of $C_2H_5+C_3H_8$ to $C_8H_5F_3N_3O_4^+$ m/z 264.0232
43 (65) – [M-293] $C_3H_7^+$ m/z 43.0548

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C1582098&Mask=200#Mass-Spec

Triforine **$C_{10}H_{14}Cl_6N_4O_2$** **M:432,434,436(0,0,0%)**
Theoretical molecular ion: m/z 431.9248 (70%), 433.9218 (89%), 435.9189 (100%), 437.9159 (37%) etc.
Average MW: 434.95



Amide fungicide. Used to control a range of diseases including powdery mildew, scab and rust. Not approved for use in EU.

Acute oral LD50 for rat >16,000 mg/kg (low toxicity).

Not amenable to GC analysis. The main ions observed by direct insertion MS are due to HCl (m/z 36 and 38).

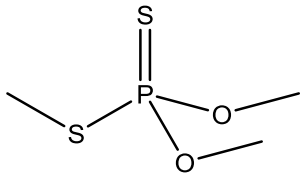
m/z	36	38	56	270	272	243	142	29
%	100	35	25	15	15	10	10	10

432,434,436 (0.1,0.2,0.1) – M^+
388,390,392 (1,2,1) – [M-44] loss of HCONH to $C_9H_{12}Cl_6N_3O^+$ m/z 387.9112 etc.
360,362,364 (1,2,1) – [M-72] loss of 2HCl to $C_{10}H_{12}Cl_4N_4O_2^+$ m/z 359.9714 etc.
352,353,354,355,356 (1,1,2,2,1,1) – [M-80] loss of HCONH+HCl to $C_9H_{11}Cl_5N_3O^+$ m/z 351.9345 etc.
315,317,319 (25,25,10) – [M-117] loss of CCl_3 to $C_9H_{14}Cl_3N_2O_2^+$ m/z 315.0182 etc.
270,272 (15,15) – [M-162] loss of $HNCHO+CHCl_3$ to $C_8H_{11}Cl_3N_3O^+$ m/z 269.9968 etc.
56 (25) – [M-376] $CNHCHO^+$ $C_2H_2NO^+$ m/z 56.0136

36,38 (100,35 [M-396] HCl m/z 35.9767 etc.

No NIST spectrum available.

Trimethyl-(O,O,S) phosphorodithioate $C_3H_9O_2PS_2$ M:172(100%)
Theoretical molecular ion: m/z 171.978 (100%), 172.9815 (3.2%), 173.97395 (4.5%)
Average MW: 172.20



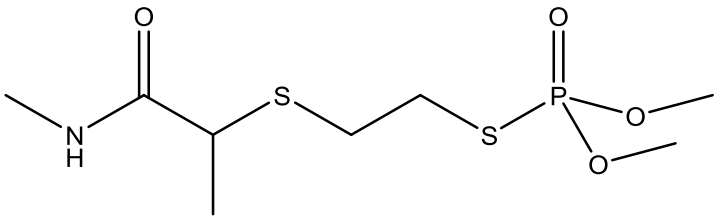
A formulation contaminant of malathion etc.

m/z	172	93	125	47	63	79	109	174
%	100	95	70	30	20	20	20	10

172 (100) – M^+
125 (70) – [M-47] loss of CH_3S to give $C_2H_6O_2PS^+$ m/z 124.9826
93 (05) – [M-79] $(CH_3O)_2P^+$ $C_2H_6O_2P^+$ m/z 93.0105
47 (30) – [M-125] CH_3S^+ m/z 46.9956

Cf. Similar but weak and noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2953299&Mask=200#Mass-Spec

Vamidothion $C_8H_{18}NO_4PS_2$ M:287(1%)
Theoretical molecular ion: m/z 287.0415 (100%), 288.0448 (8.7%), 289.0373 (9.0%)
Average MW: 287.33



Organophosphorus insecticide and acaricide. Provides persistent control of the woolly apple aphid, *Eriosoma lanigerum,* and other piercing and sucking *Homoptera*.

Acute oral LD50 for rat approx 60 mg/kg (high toxicity).

May be oxidised to the sulphoxide and sulphone metabolites, which are included in MRLs.

Sometimes poor GC transmission.

m/z	87	145	146	142	109	88	58	60
%	100	45	20	15	15	15	10	10

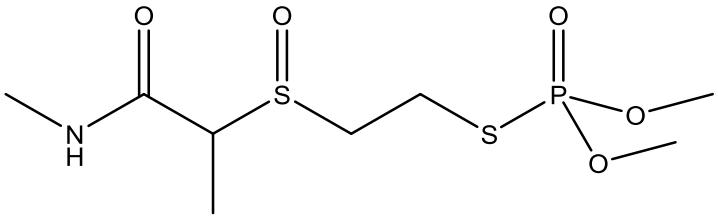
287 (1) – M^+
169 (5) – [M-118] $(CH_3O)_2P{=}S.SCH_2CH_2^+$ $C_2H_7O_3PS^+$ m/z 169.0088

145 (45) – [M-142] $CH_3NHCOCH(CH_3)SCH{=}CH_2^+$ $C_6H_{11}NOS^+$ m/z 145.0561
142 (15) – [M-145] $(CH_3O)_2(HO)PS^+$ $C_2H_7O_3PS^+$ m/z 141.9854
109 (15) – [M-178] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
87 (100) – [M-200] $CH_3NHCOCH(CH_3)/H^+$ $C_4H_9NO^+$ m/z 87.0684
58 (10) – [M-229] CH_3NHCO^+ $C_2H_4NO^+$ m/z 58.0293

Cf. Similar but weak and noisy spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2275232&Mask=200

Vamidothion sulphoxide **$C_8H_{18}NO_5PS_2$** **M:303(0%)**

Theoretical molecular ion: m/z 303.0364 (100%), 304.0398 (8.7%), 305.0322 (9.0%)
Average MW: 303.33



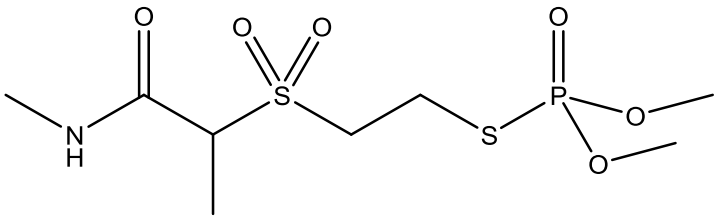
Vamidothion oxidative metabolite. Not amenable to GC.

m/z	169	109	125	58	87	143	142	86
%	100	50	25	20	20	15	15	10

303 (0) – M^+ absent
217 (5) – [M-86] $\cdot S{=}O.CH_2CH_2S.P{=}S.(OCH_3)_2^+$ $C_4H_{10}O_4PS_2^+$ m/z 216.9758
199 (5) – [M-104] $C_4H_8O_3PS_2^+$ m/z 198.9653
169 (100) – [M-134] $(CH_3O)_2P{=}O.SCH_2CH_2^+$ $C_2H_7O_3PS^+$ m/z 169.0088
125 (25) – [M-178] $(CH_3O)_2P{=}S^+$ $C_2H_6O_2PS^+$ m/z 124.9826
58 (0) – [M-245] CH_3NHCO^+ $C_2H_4NO^+$ m/z 58.0293

Vamidothion sulphone **$C_8H_{18}NO_6PS_2$** **M:319(1%)**

Theoretical molecular ion: m/z 319.0313 (100%), 320.0347 (8.7%), 321.0271 (9.0%)
Average MW: 319.33



Vamidothion oxidative metabolite. Poor GC transmission.

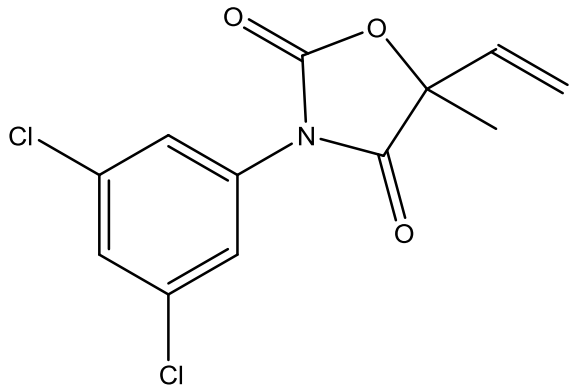
m/z	87	169	109	125	58	142	86	79
%	100	40	25	20	15	10	10	10

319 (1) – M^+ weak
169 (40) – [M-150] $(CH_3O)_2P{=}O.SCH_2CH_2^+$ $C_2H_7O_3PS^+$ m/z 169.0088
142 (10) – [M-177] $(CH_3O)_2(HO)PS^+$ $C_2H_7O_3PS^+$ m/z 141.9854
109 (25) – [M-210] $(CH_3O)_2P{=}O^+$ $C_2H_6O_3P^+$ m/z 109.0055
87 (100) – [M-232] $CH_3NHCOCH(CH_3)/H^+$ $C_4H_9NO^+$ m/z 87.0684
79 (10) – [M-240] $(CH_3O)(HO)P^+$ $CH_4O_2P^+$ m/z 78.9949

Vinclozolin **$C_{12}H_9Cl_2NO_3$** **M:285,287(80,50%)**

Theoretical molecular ion: m/z

Average MW:



Dichlorophenyl dicarboximide fungicide used mainly on oilseed rape, vines, fruit and vegetables to control *Botrytis*, *Monolinia* and *Sclerotinia* spp. Not approved for use in EU.

Acute oral LD50 for rat >15,000 mg/kg (low toxicity).

The metabolite **3,5-dichloroaniline** may be important. See **iprodione degradation (ii)**.

KI (SE-30) = 18.2

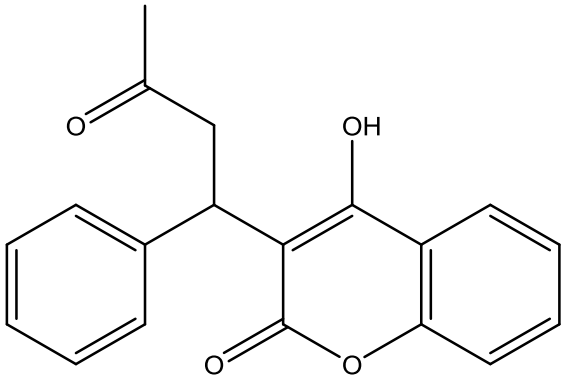
m/z	39	54	187	213	285	212	53	198
%	100	90	85	80	80	80	73	65

285,287 (80,50) – M^+
241,243 (15,10) – [M-44] loss of CO_2 to give $C_{11}H_9Cl_2NO^+$ m/z 241.0061 etc.
213,215,217 (80,60,20) – [M-72] loss of CO_2/C_2H_4 to $C_9H_5Cl_2NO^+$ m/z 212.9748 etc.
(or loss of CO_2/CO with rearrangement to $C_{10}H_9Cl_2N^+$ m/z 213.0112 etc.)
212,214,216 (80,60,20) – [M-73] loss of CO_2 & C_2H_5 to $C_9H_4Cl_2NO^+$ m/z 211.9670 etc.
198,200,202 (65,45,15) – [M-87] rearrangement and loss of CO_2/CO/CH_3 to $C_9H_6Cl_2N^+$ m/z 197.9877 etc.
187,189,191 (85) – [M-98] $Cl_2C_6H_3NCO^+$ dichlorophenyl isocyanate $C_7H_3Cl_2NO^+$ m/z 186.9592 etc.
159,161 (20,10) – [M-126] $C_6H_3Cl_2N^+$ m/z 158.9643 etc.
145,147 (20,10) – [M-140] $C_6H_3Cl_2^+$ m/z 144.9612 etc.
124,126 (60,20) – [M-161] $C_6H_3ClN^+$ m/z 123.9954 etc.
39 (100) – [M-246] $C_3H_3^+$ m/z 39.0235

Cf. similar spectrum in NIST MS http://webbook.nist.gov/cgi/cbook.cgi?ID=C50471448&Mask=200

Warfarin **$C_{19}H_{16}O_4$** **M:308(45%)**

Theoretical molecular ion: m/z 308.1049 (100%), 309.1082 (21%)
Average MW: 308.33



Anticoagulant rodenticide. Acute oral LD50 for rat approx. 2 mg/kg.

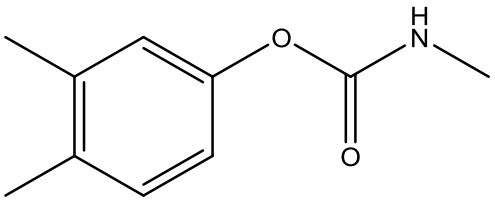
Poor GC transmission.

m/z	265	43	121	45	308	266	187	213
%	100	65	60	55	45	35	30	25

308 (35) – M^+
265 (100) – [M-43] loss of CH_3CO to give $C_{17}H_{13}O_3^+$ m/z 265.0865
121 (60) – [M-187] $C_7H_5O_2^+$ m/z 121.0290
43 (65) – [M-265] CH_3CO^+ m/z 43.0185

Xylylcarb **$C_{10}H_{13}NO_2$** **M:179(2%)**

Theoretical molecular ion: m/z 179.09463 (100.0%), 180.09798 (10.8%)
Average MW: 179.22



Carbamate insecticide, used for the control of hoppers and other sucking insects on rice, and leafhoppers, planthoppers, and scale insects on fruit. Not approved for use in EU.

Acute oral LD50 for rat approx. 300 mg/kg (moderate toxicity).

m/z	122	107	121	77	79	57	91	123
%	100	45	15	15	10	5	5	5

179 (2) – M^+
122 (100) – [M-57] loss of methyl isocyanate CH_3NCO to phenol $C_8H_{10}O^+$ m/z 122.0732
107 (45) – [M-72] loss of CH_3NCO & CH_3 to $C_7H_7O^+$ m/z 107.0497

Cf. similar spectrum at http://webbook.nist.gov/cgi/cbook.cgi?ID=C2425107&Mask=200#Mass-Spec
listed under “Phenol, 3,4-dimethyl-, methylcarbamate”

Zineb, see Dithiocarbamates

Ziram, see Dithiocarbamates

GC contaminants/artefacts

acetyl tri*-n-*butyl citrate **$C_{20}H_{35}O_8$** **M:402(0%)**

m/z	185	129	259	43	57	41	157	139
%	100	60	50	40	30	25	20	10

m/z 329 (7%) distinguishes from tri-n-butyl citrate (below)

"Antioxidant 2246" **$C_{23}H_{32}O_2$** **M:340(40%)**

m/z	177	161	164	149	340	41	57	284
%	100	75	50	40	40	25	25	20

"Antioxidant 425" **$C_{25}H_{36}O_2$** **M:368(45%)**

KI(OV-17) = 27.2

m/z	191	175	178	368	163	57	135	169
%	100	70	60	45	40	35	25	20

benzothiazole **C_7H_5NS** **M:135(100%)**

m/z	135	108	69	82	63	91	45	54
%	100	40	25	15	10	10	10	10

"BHA" butylated hydroxy anisole **$C_{11}H_{16}O_2$** **M:180(50%)**

m/z	165	180	137	166	91	124	181	77
%	100	50	50	10	10	5	5	5

"BHT" butylated hydroxy toluene **$C_{15}H_{24}O$** **M:220(25%)**

m/z	205	220	57	206	145	105	177	55
%	100	25	25	15	15	10	10	5

bis(2-ethylhexyl) phthalate **$C_{24}H_{38}O_4$** **M:390(0%)**

KI(OV-17) = 27.1

m/z	149	167	57	71	43	70	279	113
%	100	45	35	25	25	20	20	15

bis(2-ethylhexyl) adipate/hexanedioate **$C_{22}H_{42}O_4$** **M:370(1%)**

m/z	129	57	70	71	112	147	113	55
%	100	40	35	30	25	15	15	15

m/z 259 (10%), m/z 241 (10%)

dibromopentane isomers **$C_5H_{10}Br_2$** **M:228(0%)**

Diethyl ether contaminant. Several GC peaks due to different isomers.

m/z	69	149	151	41	55	70	121	123
%	100	85	85	40	15	10	5	5

di-n-butyl phthalate **$C_{16}H_{22}O_4$** **M:278(1%)**

KI(OV-17) = 22.1

m/z	149	29	150	41	57	56	223	205
%	100	10	10	10	5	5	5	5

dibutyl sebacate/decanedioate **$C_{18}H_{34}O_4$** **M:314(0.1%)**

m/z	241	185	56	57	98	41	123	125
%	100	75	65	55	40	40	35	35

diethyl phthalate **$C_{12}H_{14}O_4$** **M:222(5%)**

KI(OV-17) = 17.9

m/z	149	177	150	65	176	76	105	29
%	100	25	10	10	10	10	10	5

dimethyl phthalate **$C_{10}H_{10}O_4$** **M:194(10%)**

m/z	163	77	76	135	92	50	164	194
%	100	25	15	10	10	10	10	10

dimethylsilanediol (silicone related) **$C_2H_8O_2Si$** **M:92(0%)**

$(CH_3)_2Si(OH)_2$ - Hydrolysis product of polydimethylsiloxanes.

m/z	77	78	79	-	-	-	-	-
%	100	6	4	-	-	-	-	-

N-butyl benzenesulphonamide **$C_{10}H_{15}NO_2S$** **M:213(5%)**

m/z	141	77	170	30	158	171	78	213
%	100	95	85	20	15	10	10	5

oleamide **$C_{18}H_{35}NO$** **M:281(5%)**

KI(OV-17) = 25.8

m/z	59	72	55	41	67	83	126	98
%	100	45	35	25	15	15	10	10

silicones, cyclic (e.g. Si9) **$C_{18}H_{54}O_9Si_9$** **M:666(0%)**

Frequently observed, characteristic "envelope" of peaks due to cyclic dimethylsiloxanes, $[(CH_3O)_2Si]_n$, either material dislodged from the GC injector and/or column, or contaminant (usually ex GC vial septum).

m/z	73	429	147	221	355	281	430	431
%	100	45	35	25	25	15	15	15

silicones, linear (e.g. Si6) **$C_{14}H_{42}O_7Si_6$** **M:490(0%)**

These compounds, $CH_3O\text{-}[(CH_3)_2SiO]_n\text{-}CH_3$ are sometimes observed in the presence of the cyclic silicones, $[(CH_3O)_2Si]_n$, as a less abundant series. Several ions are common to both series, but the presence of an ion at m/z 89, due to $(CH_3O)Si(CH_3)_2^+$, serves to distinguish the linear species.

m/z	73	163	237	89	341	59	253	429
%	100	65	60	35	30	25	20	20

m/z 475 (10%) M-CH_3

tri*-n-*butyl citrate **$C_{18}H_{32}O_7$** **M:360(0%)**

m/z	185	129	57	259	29	111	147	56
%	100	80	45	35	25	15	15	10

m/z 259 (35%) distinguishes from acetyl tri-n-butyl citrate

tri*-n-*butyl phosphate **$C_{12}H_{27}O_4P$** **M:266(0%)**

m/z	99	155	211	125	57	41	137	56
%	100	25	10	5	5	5	5	2

triphenyl phosphate **$C_{18}H_{15}O_4P$** **M:326(100%)**

KI(SE-30) = 23.4

m/z	326	325	77	170	94	233	215	65
%	100	65	45	35	30	25	20	20

tris-(2-chloroethyl) phosphate **$C_6H_{12}Cl_3O_4P$** **M:284,286(0,0%)**

KI (CPSil19) = 17.8

m/z	63	249	251	27	143	205	65	223
%	100	85	45	45	40	40	35	25

unidentified GC vial septum contaminant **$C_?H_?O_?$** **M:292(5%)**

Probably an octyl-substituted compound as m/z180 may be due to $(M\text{-}C_8H_{16})^+$.

m/z	97	57	99	43	83	123	69	137
%	100	60	20	20	15	15	15	10

179,180 (10,10)

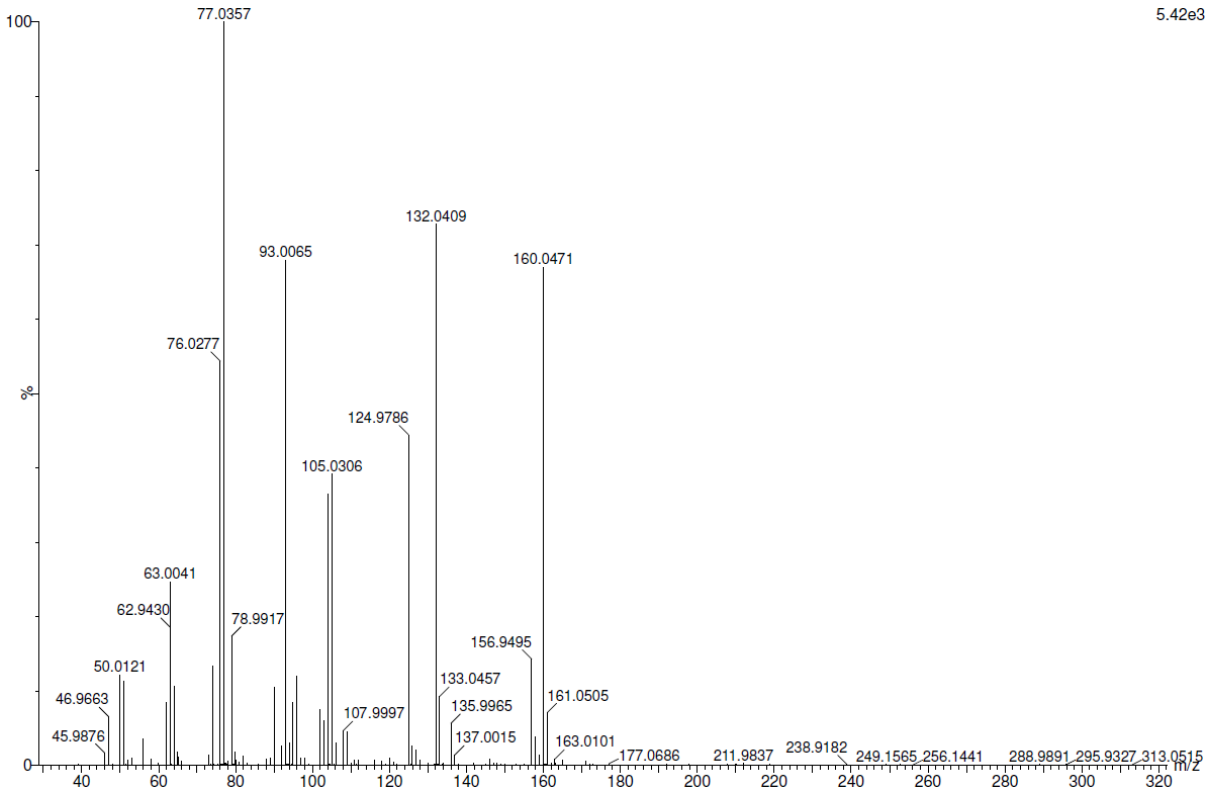
Appendix I. Supplement

Accurate mass data for selected pesticides

Acquired using Cardiff GCT OA TOF MS (Spring 2015)
With assigned empirical formula and assignment notes.

GCT Spectrum	Pesticide
1	Azinphos methyl
2	Butocarboxim & oxime degradation product
3	Chlorpyrifos
4	Diazinon
5	Dichlorvos
6	Dimethoate
7	Disulfoton
8	Ethoprophos
9	Famphur
10	Fenamiphos
11	Isofenphos
12	Methiocarb sulphoxide degradation product
13	Parathion
14	Parathion methyl
15	Pirimiphos methyl
16	Prothiofos
17	Pyraclostrobin
18	Pyrazophos
19	Pyridaphenthion
20	Quinalphos
21	Sulfotep
22	Thiofanox oxime
23	Thionazin
24	Triazophos
25	Triethyl thiophosphate

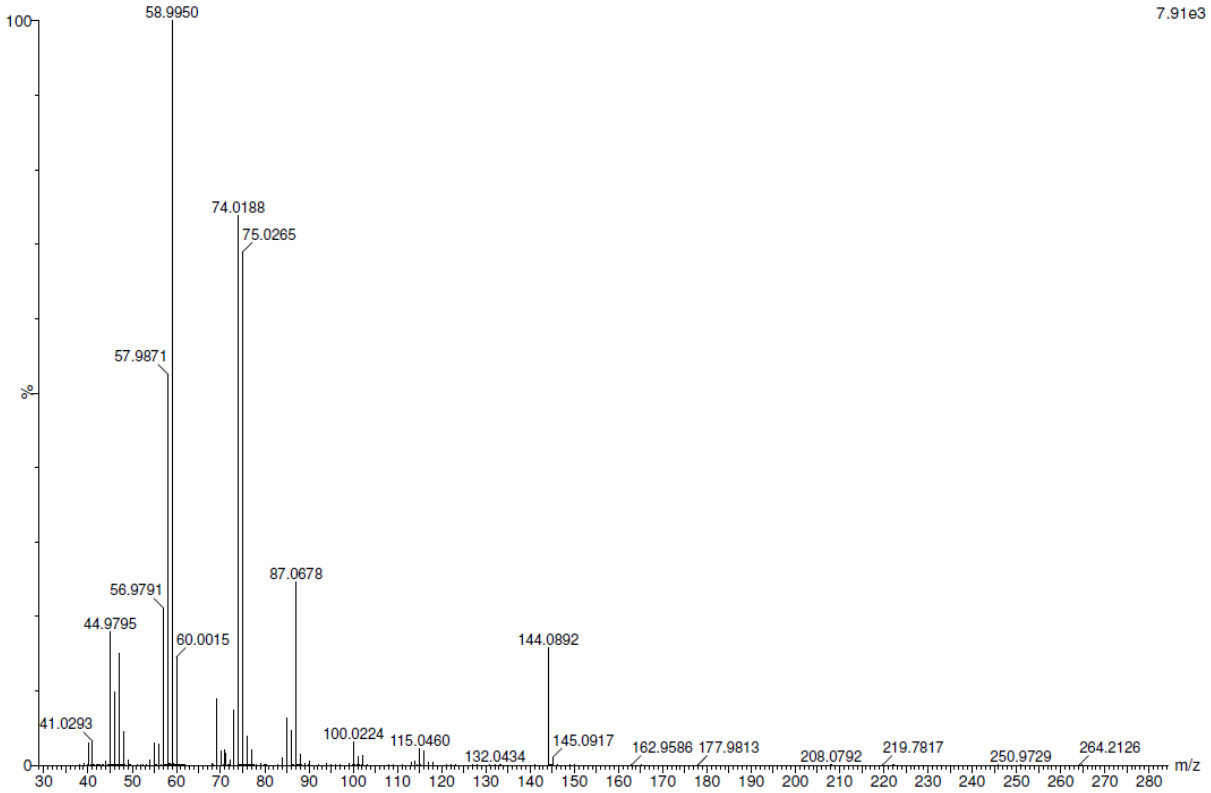
GCT Spectrum #1 – Azinphos Methyl, Guthion



Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
317	0	n/a	345.0371	-	C10H12N3O3PS2	M
160	157	160.0471	160.0511	-0.0040	C8H6N3O	M-C2H8O2PS2
157	160	156.9495	156.9547	-0.0052	C2H6O2PS2	OP ion
	„	„	*156.9533*	*-0.0038*	*H4N3OPS2*	*possible alternative*
132	185	132.0409	132.0449	-0.0040	C8H6NO	M-C2H8O2PS2 & N2
125	192	124.9786	124.9826	-0.0040	C2H6O2PS	OP ion
105	212	105.0306	105.034	-0.0034	C7H5O	C6H5CO
104	213	104.0352	104.0375	-0.0023	C6H4N2	aromatic ion
	„	„	*104.0262*	*-0.0009*	*C6H4CO*	*Not predicted ion*
93	224	93.0065	93.0105	-0.0040	C2H6O2P	OP ion
79	238	78.9917	78.9949	-0.0032	CH4O2P	OP ion
77	240	77.0357	77.0391	-0.0034	C6H5	phenyl group
76	241	76.0277	76.0313	-0.0036	C6H4	aromatic
63	252	63.0041	63.0082	-0.0041	CH3O3	rather unlikely
		„	*63.0109*	*-0.0068*	*C4HN*	*alternative*
		„	*63.0017*	*+0.0024*	*H3N2S*	„
		„	*63.0000*	*+0.0041*	*CH4HOP*	„
		„	*62.9956*	*+0.0085*	*HNO3*	„
63	252	62.9430	62.9458	-0.0028	PS	OP ion
50	267	50.0121	50.0157	-0.0036	C4H2	Aromatic ion
47	270	46.9663	46.9687	-0.0024	PO	OP ion

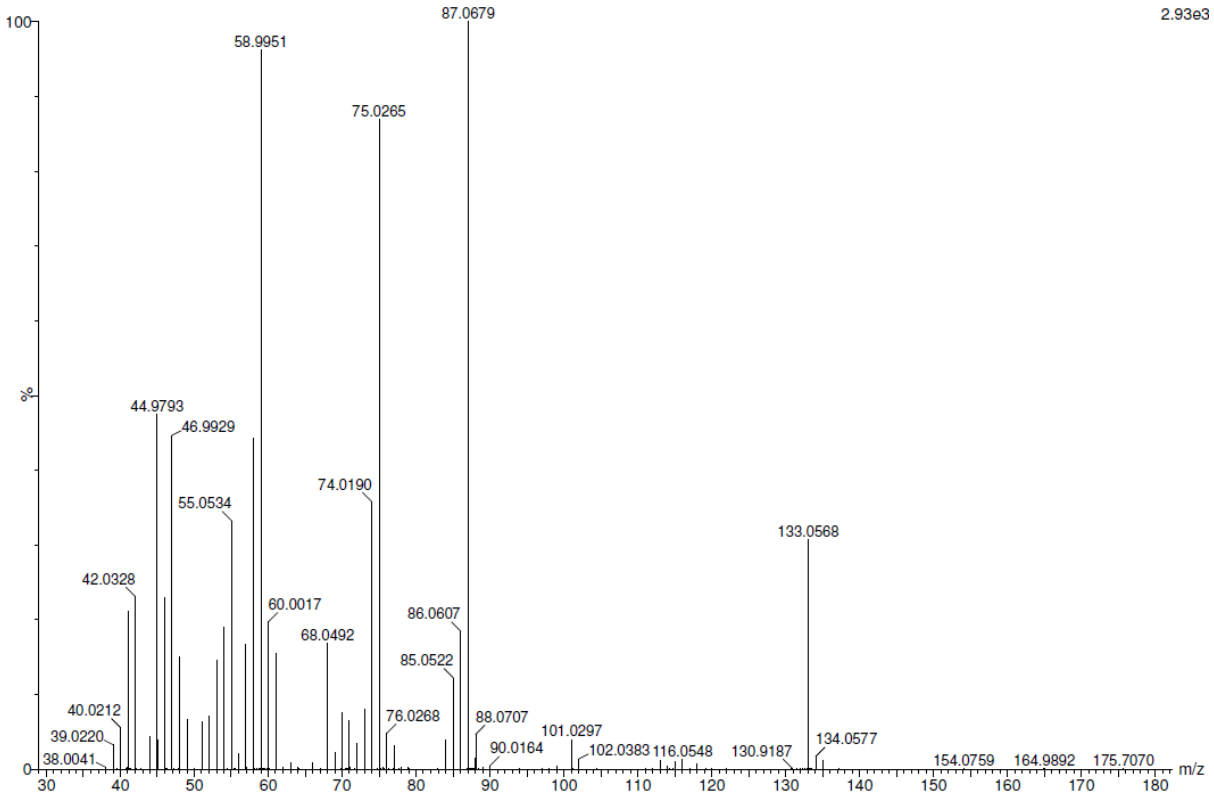
GCT Spectrum #2a – Butocarboxim (intact)

See degradation product (oxime) overleaf



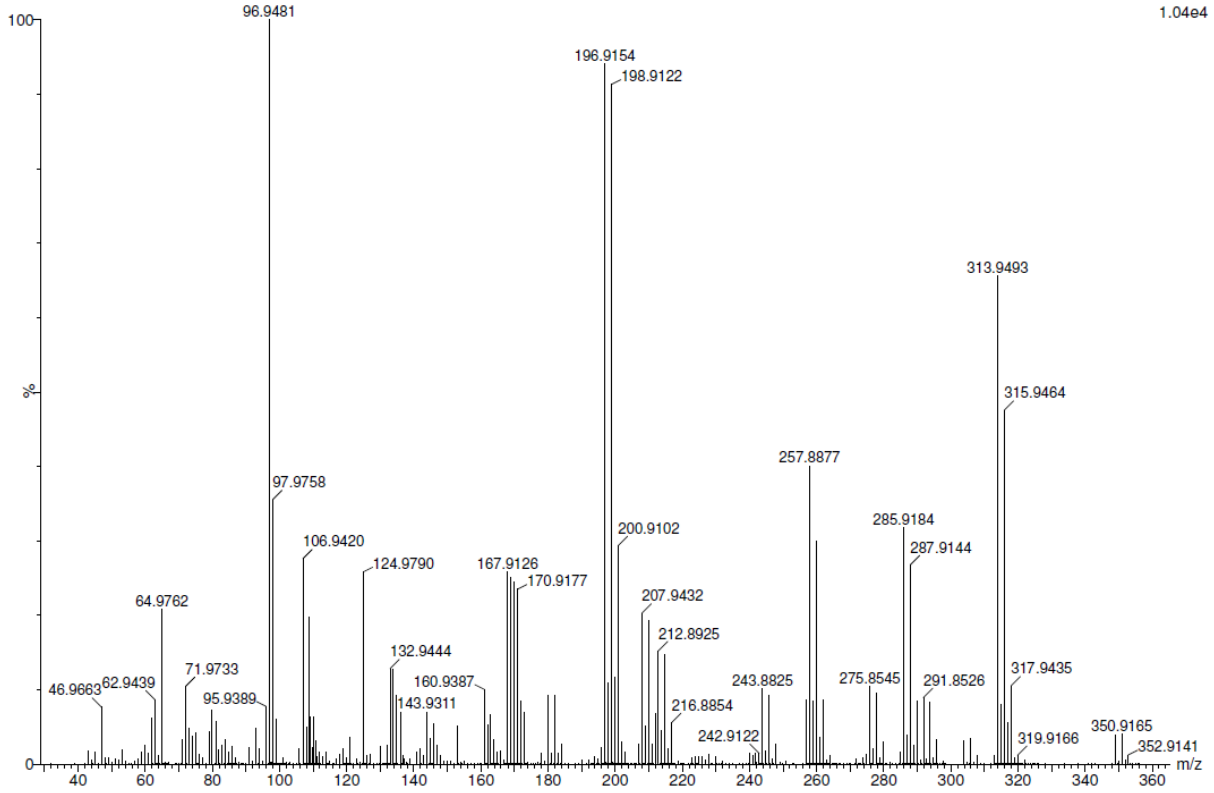
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
190	0	not present	-	-	C7H14N2O2S	M
144	46	144.0892	144.0899	-0.0007	C6H12N2O2	M-CH2S
115	75	115.046	115.0456	0.0004	C5H9NS	M-C2H5O2
100	90	100.0224	100.0221	0.0003	C4H6NS	M-C3H8NO2
87	103	87.0678	87.0684	-0.0006	C4H9NO	
75	115	75.0265	75.0268	-0.0003	C3H7S	
74	116	74.0188	74.019	-0.0002	C3H6S	
59	131	58.995	58.9955	-0.0005	C2H3S	
58	132	57.9871	57.9877	-0.0006	C2H2S	
45	145	44.9795	44.9799	-0.0004	CHS	

GCT Spectrum #2b – Butocarboxim oxime (GC degradation)



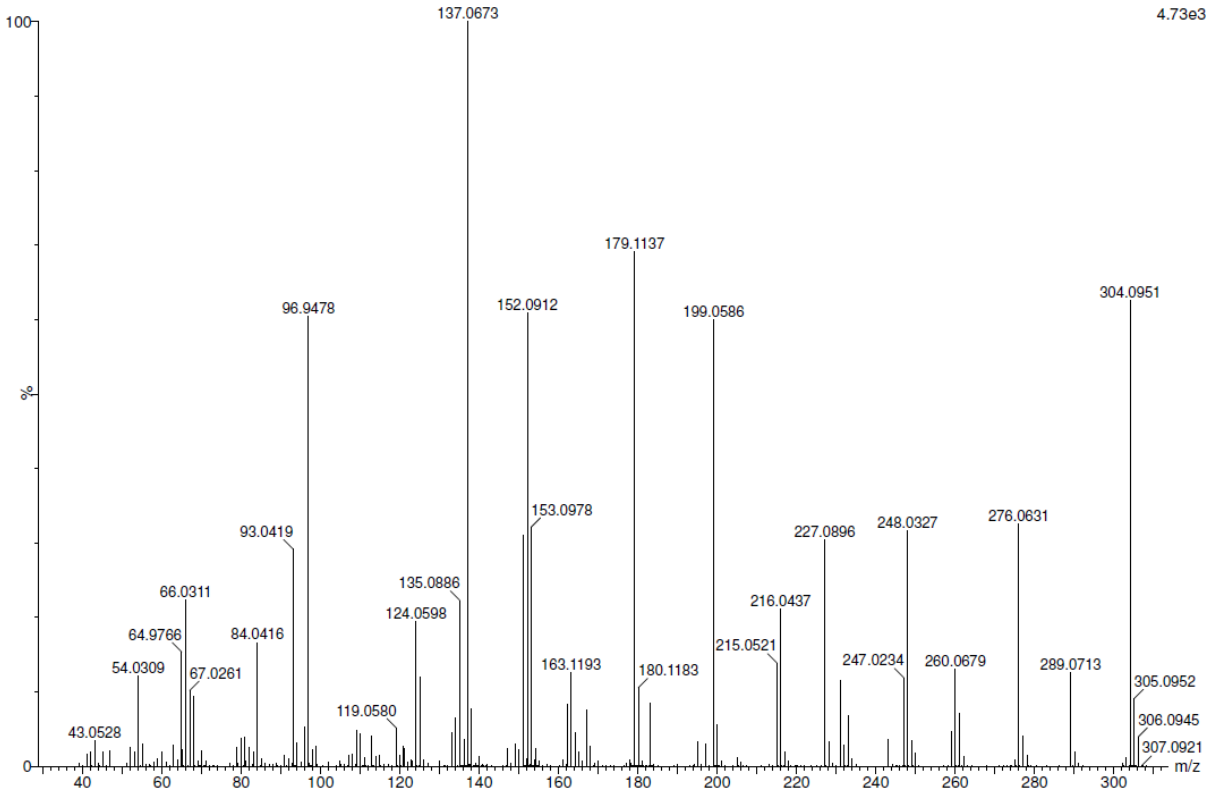
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
133	0	133.0568	133.0561	0.0007	C5H11NOS	M
101	32	101.0297	101.0299	-0.0002	C4H7NS	M-CH3OH
87	46	87.0679	87.0684	-0.0005	C4H9NO	M-CH2S
75	58	75.0265	75.0268	-0.0003	C3H7S	
68	65	68.0492	68.0500	-0.0008	C4H6N	
59	74	58.9951	58.9955	-0.0004	C2H3S	
55	78	55.0534	55.0548	-0.0014	C4H7	
47	86	46.9929	46.9955	-0.0026	CH3S	
45	88	44.9793	44.9799	-0.0006	CHS	

GCT Spectrum #3 – Chlorpyrifos “Dursban”



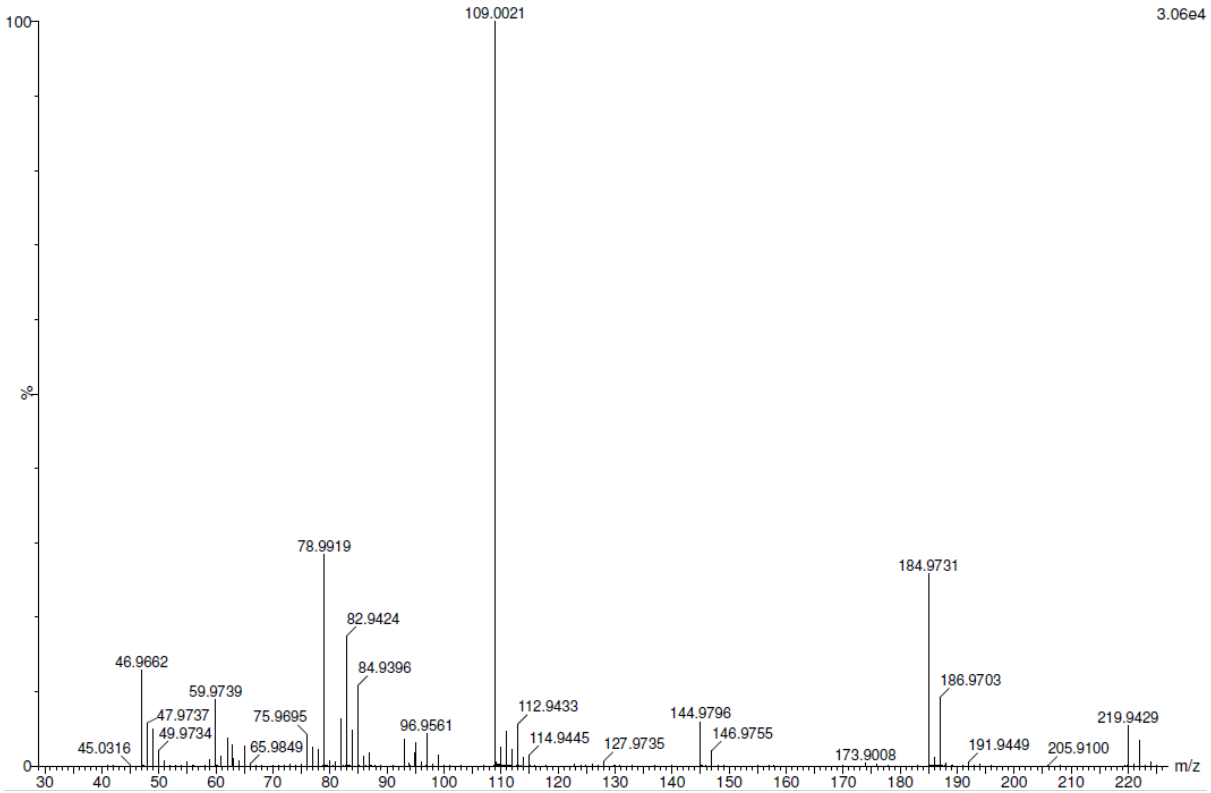
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
349	0	348.9183	348.9263	-0.0080	C9H11Cl3NO3PS	M
314	35	313.9493	313.9574	-0.0081	C9H11Cl2NO3PS	M-Cl
292	57	291.8526	291.8559	-0.0033	C5H2Cl3NO3PS	M-C4H9
286	63	285.9184	285.9261	-0.0077	C7H7Cl2NO3PS	M-C2H4Cl
276	73	275.8545	275.8609	-0.0064	C5H2Cl3NO2PS	M-C4H9O
258	91	257.8877	257.8948	-0.0071	C5H3Cl2NO3PS	M-C4H8Cl
244	105	243.8825	243.8889	-0.0064	C5H2Cl3NO2P	M-C4H9OS
213	136	212.8925	212.8974	-0.0049	C5H2Cl3NS	M-C4H9O3P
208	141	207.9432	207.9488	-0.0056	C7H5Cl3N	M-C2H6O3PS
197	152	196.9154	196.9202	-0.0048	C5H2Cl3NO	M-C4H9O2PS
180	169	179.9125	179.9175	-0.0050	C5HCl3N	M-C4H10O3PS
169	180	168.9201	168.9253	-0.0052	C4H2Cl3N	M-C5H9OPS
168	181	167.9126	167.9175	-0.0049	C4HCl3N	M-C5H8OPS
125	224	124.979	124.9826	-0.0036	C2H6O2PS	OP ion
107	242	106.942	106.9455	-0.0035	C3HCl2	
98	251	97.9758	97.9798	-0.0040	C4HClN	m/z 168-Cl2
97	252	96.9481	96.9513	-0.0032	H2O2PS	
65	284	64.9762	64.9792	-0.0030	H2O2P	
63	286	62.9439	62.9458	-0.0019	PS	
47	302	46.9663	46.9687	-0.0024	PO	

GCT Spectrum #4 – Diazinon



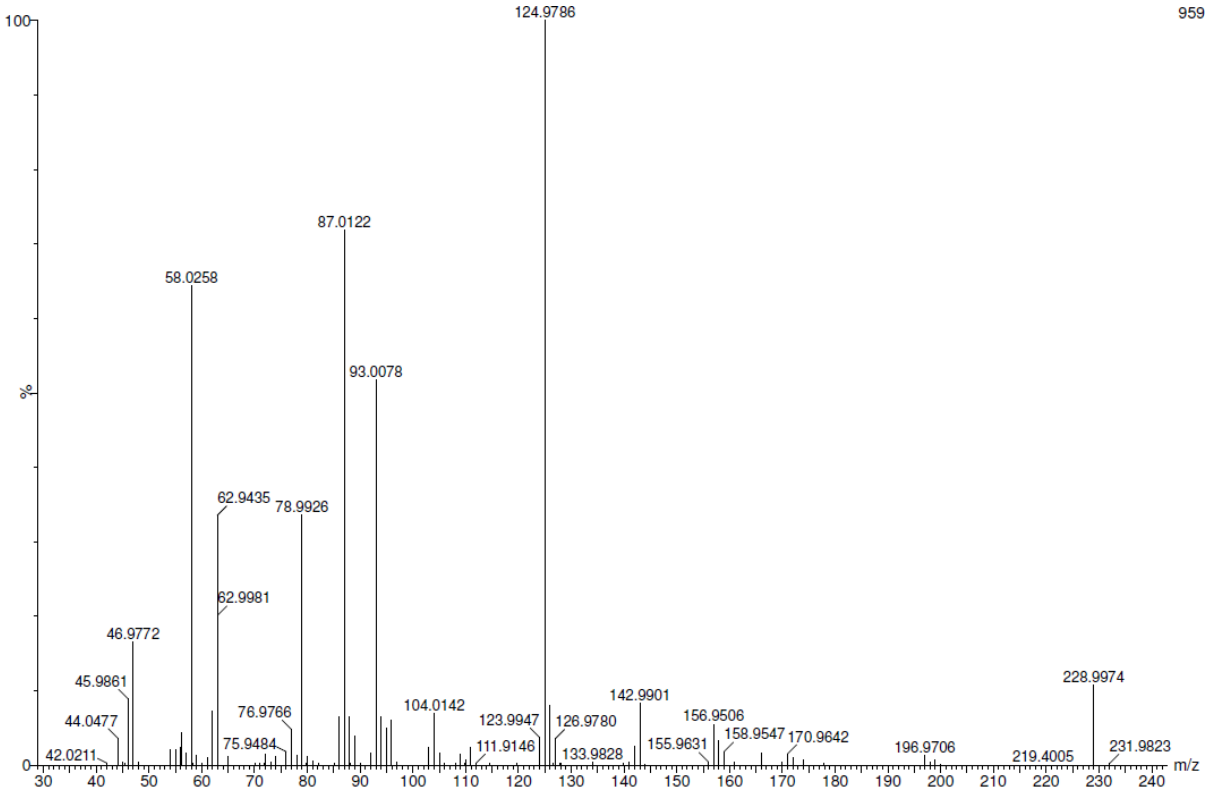
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
304	0	304.0951	304.1010	-0.0060	C12H21N2O3PS	M
289	15	289.0713	289.0776	-0.0063	C11H18N2O3PS	M-CH3
276	28	276.0631	276.0698	-0.0067	C10H17N2O3PS	M-C2H4
260	44	260.0679	260.0748	-0.0069	C10H17N2O2PS	M-C2H4O
248	56	248.0327	248.0385	-0.0058	C8H13N2O3PS	M-2C2H4
227	77	227.0896	227.0949	-0.0053	C10H16N2O2P	M-C2H5OS
216	88	216.0437	216.0486	-0.0049	C8H13N2OPS	M-C4H8O2
215	89	215.0521	215.0586	-0.0065	C8H12N2OPS	M-C4H9S
199	105	199.0586	199.0636	-0.0050	C8H12N2O2P	M-C4H9OS
179	125	179.1137	179.1184	-0.0047	C10H15N2O	M-C2H6O2PS
163	141	163.1193	163.1235	-0.0042	C10H15N2	M-C2H6O3PS
153	151	153.0978	153.1028	-0.0050	C8H13N2O	loss of OP
152	152	152.0912	152.0950	-0.0038	C8H12N2O	loss of OP
137	167	137.0673	137.0715	-0.0042	C7H9N2O	
135	169	135.0886	135.0922	-0.0036	C8H11N2	
124	180	124.0598	124.0637	-0.0039	C6H8N2O	loss of OP & CH3
97	207	96.9478	96.9513	-0.0035	H2O2PS	(HO)2PS
93	211	93.0419	93.0453	-0.0034	C5H5N2	
	,,	,,	*93.0105*	*-0.0314*	*C2H6O2P*	*NOT expected OP ion*
84	220	84.0416	84.0449	-0.0033	C4H6NO	
66	238	66.0311	66.0344	-0.0033	C4H4N	
65	239	64.9766	64.9792	-0.0026	H2O2P	(HO)2P
54	250	54.0309	54.0344	-0.0035	C3H4N	

GCT Spectrum #5 – Dichlorvos, DDVP, Vapona



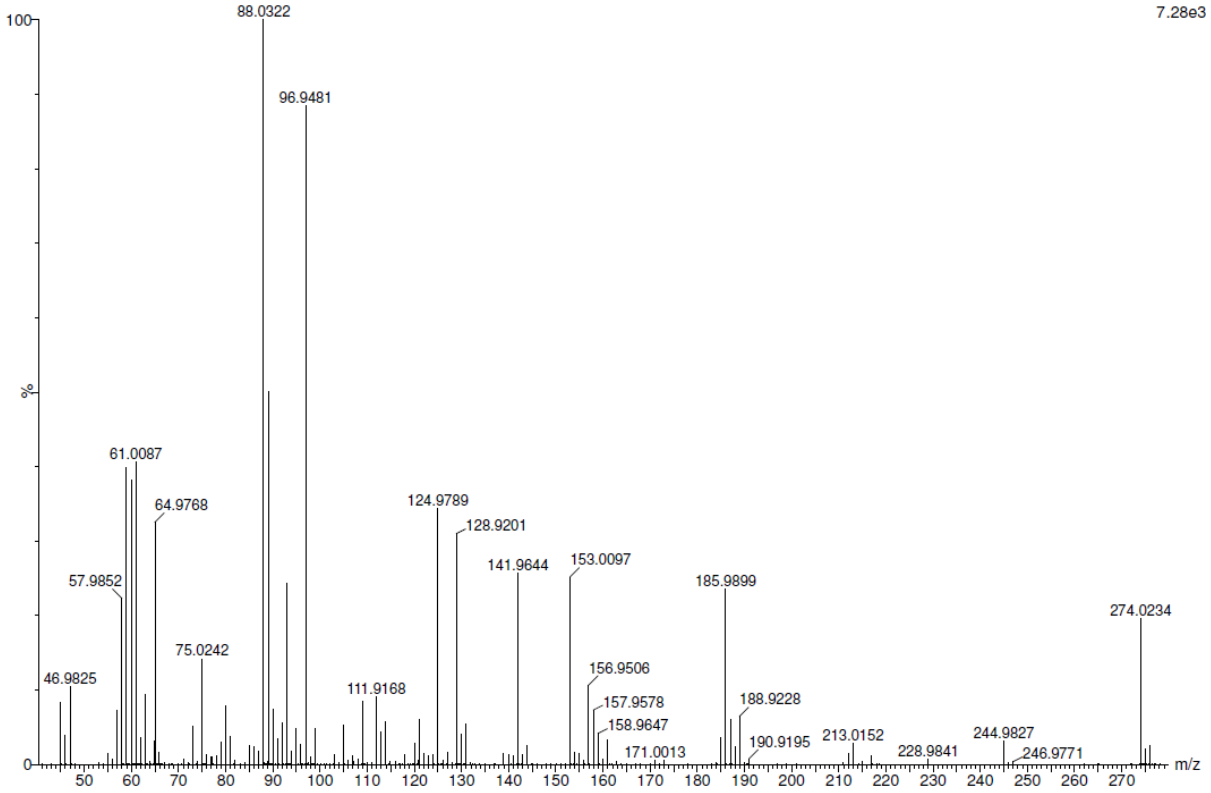
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
220	0	219.9429	219.9459	-0.0030	C4H7Cl2O4P	M
185	35	184.9731	184.9771	-0.0040	C4H7ClO4P	M-Cl
145	75	144.9796	144.9821	-0.0025	C2H7ClO3P	(CH3O)2POCl
109	111	109.0021	109.0055	-0.0034	C2H6O3P	(CH3O)2PO
83	138	82.9424	82.9455	-0.0031	CHCl2	CHCl2
79	141	78.9919	78.9949	-0.0028	CH2Cl	CH2Cl
47	173	46.9662	46.9687	-0.0025	PO	PO

GCT Spectrum #6 – Dimethoate



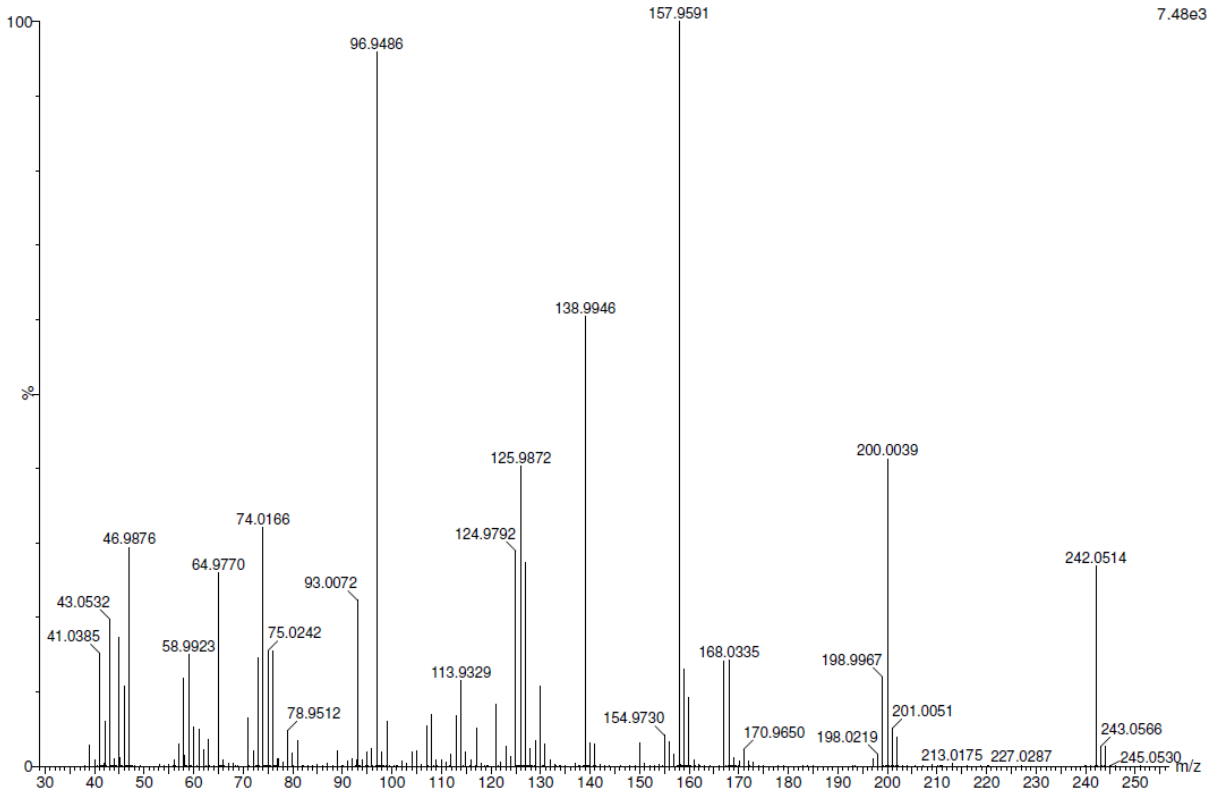
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
229	0	228.9974	228.9996	-0.0022	C5H12NO3PS2	M
157	72	156.9506	156.9547	-0.0041	C2H6O2PS2	OP ion
143	86	142.9901	142.9932	-0.0031	C2H8O3PS	Rearrangement & loss of C3H4NS
125	104	124.9786	124.9826	-0.0040	C2H6O2PS	Complementary OP ion to m/z 104
104	125	104.0142	104.017	-0.0028	C3H6NOS	Complementary to m/z 125
93	136	93.0078	93.0105	-0.0027	C2H6O2P	OP ion
87	142	87.0122	87.0143	-0.0021	C3H5NS	≡ m/z 104-OH
79	150	78.9926	78.9949	-0.0023	CH4O2P	OP ion
63	166	62.9435	62.94584	-0.0023	PO	OP ion
58	171	58.0258	58.0293	-0.0035	C2H4NO	Amide ion CH3NHCO

GCT Spectrum #7 – Disulfoton



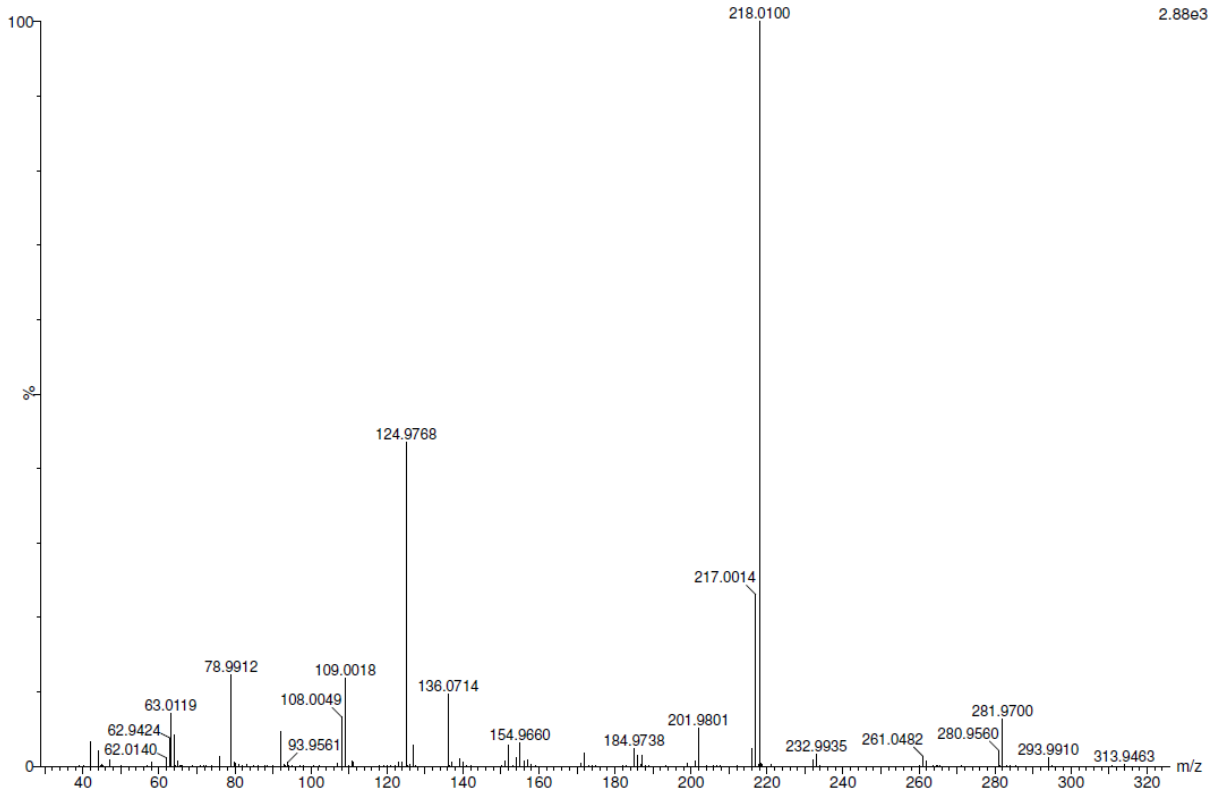
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
274	0	274.0234	274.0285	-0.0051	C8H19O2PS3	M
245	29	244.9827	244.9894	-0.0067	C6H14O2PS3	M-C2H5
213	61	213.0152	213.0173	-0.0021	C6H14O2PS2	M-C2H5S
186	88	185.9899	185.9938	-0.0039	C4H11O2PS2	OP ion
153	121	153.0097	153.0139	-0.0042	C4H10O2PS	OP ion
142	132	141.9644	141.9676	-0.0032	C2H7OPS2	
129	145	128.9201	128.9234	-0.0034	H2O2PS2	
125	149	124.9789	124.9827	-0.0038	C2H6O2PS	
112	162	111.9168	111.9206	-0.0038	HOPS2	OP ion (129-OH)
97	177	96.9481	96.9513	-0.0032	H2O2PS	OP ion
93	181	92.9809	92.9833	-0.0024	C2H5S2	
	„	„	*93.0105*	*-0.0296*	*C2H6O2P*	*NOT expected OP ion*
89	185	??	89.0425	??	C4H9S	
88	186	88.0322	88.0347	-0.0025	C4H8S	
75	199	75.0242	75.0268	-0.0026	C3H7S	
65	209	64.9768	64.9792	-0.0024	H2O2P	OP ion
60	214	60.0013	60.0034	-0.0020	C2H4S	
59	215	58.993	58.9955	-0.0025	C2H3S	

GCT Spectrum #8 – Ethoprophos, Mocap



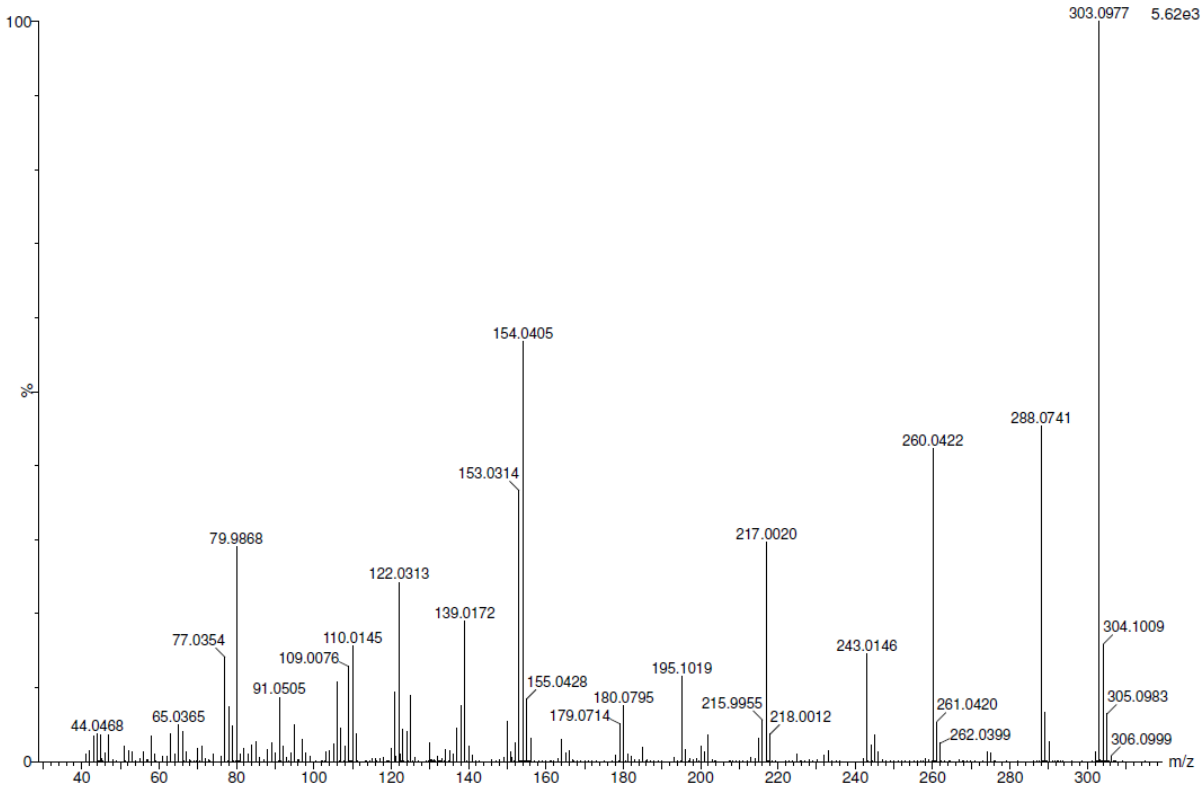
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
242	0	242.0514	242.0564	-0.0050	C8H19O2PS2	M
200	42	200.0039	200.0095	-0.0056	C5H13O2PS2	M-C3H6
168	74	168.0335	168.0374	-0.0039	C5H13O2PS	M-C3H6S
158	84	157.9591	157.9625	-0.0034	C2H7O2PS2	OP ion
139	103	138.9946	138.9983	-0.0037	C3H8OPS	
126	116	125.9872	125.9904	-0.0032	C2H7O2PS	
125	117	124.9792	124.9826	-0.0034	C2H6O2PS	
97	145	96.9486	96.9513	-0.0027	H2O2PS	
93	149	93.0072	93.0105	-0.0033	C2H6O2P	
74	168	74.0166	74.019	-0.0024	C3H6S	
65	177	64.977	64.9792	-0.0022	H2O2P	
47	195	46.9876	46.9956	-0.0080	PO	

GCT Spectrum #9 – Famphur



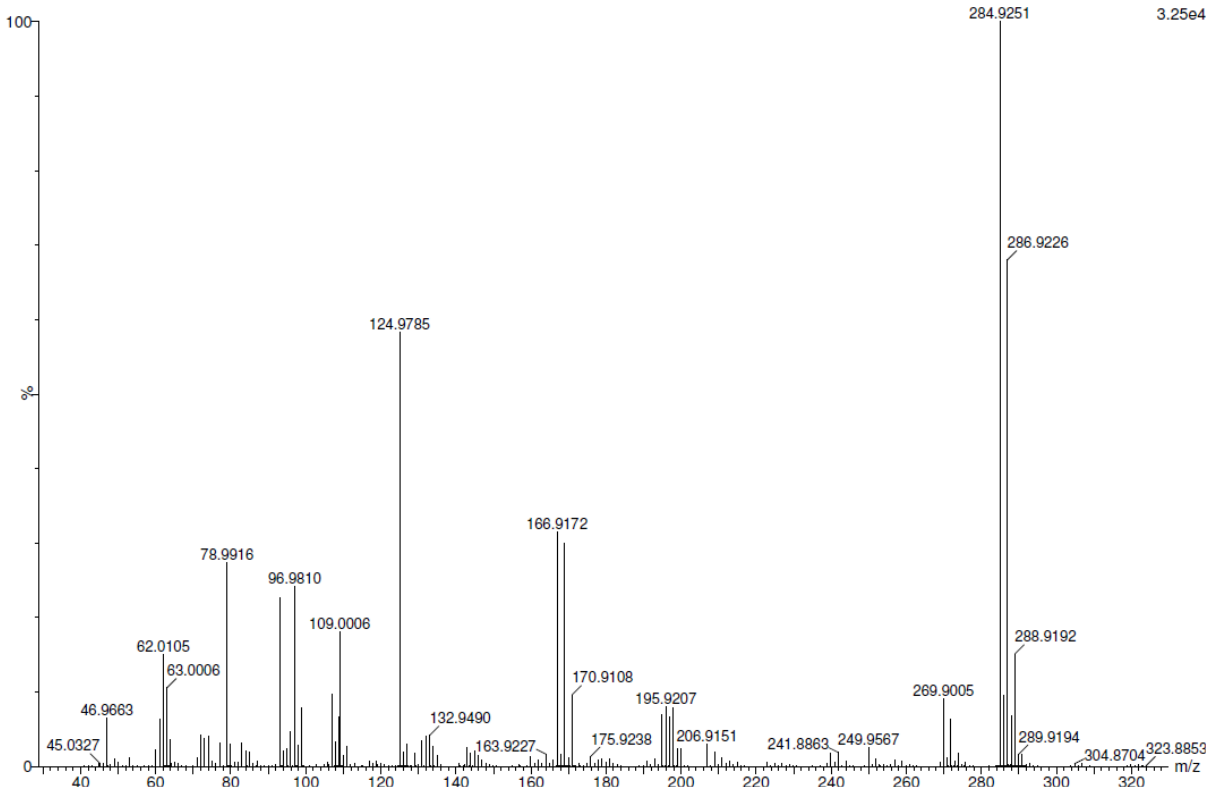
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
325	0	not present	325.0208	-	C10H16NO5PS2	M
282	43	281.9700	281.9786	-0.0086	C8H11O5PS2	M-C2H5N
218	107	218.0088	218.0167	-0.0079	C8H11O3PS	M-C2H5N / SO2
217	108	217.0014	217.0088	-0.0074	C8H10O3PS	M-C2H6N / SO2
202	123	201.9801	201.9854	-0.0053	C7H7O3PS	M-C2H6N/SO2/CH3
136	189	136.0714	136.0762	-0.0048	C8H10NO	(CH3)2NC6H4
125	200	124.9768	124.9826	-0.0058	C2H6O2PS	OP ion
109	216	109.0018	109.0055	-0.0037	C2H6O3P	OP ion
79	246	78.9912	78.9949	-0.0037	CH4O2P	OP ion

GCT Spectrum #10 – Fenamiphos



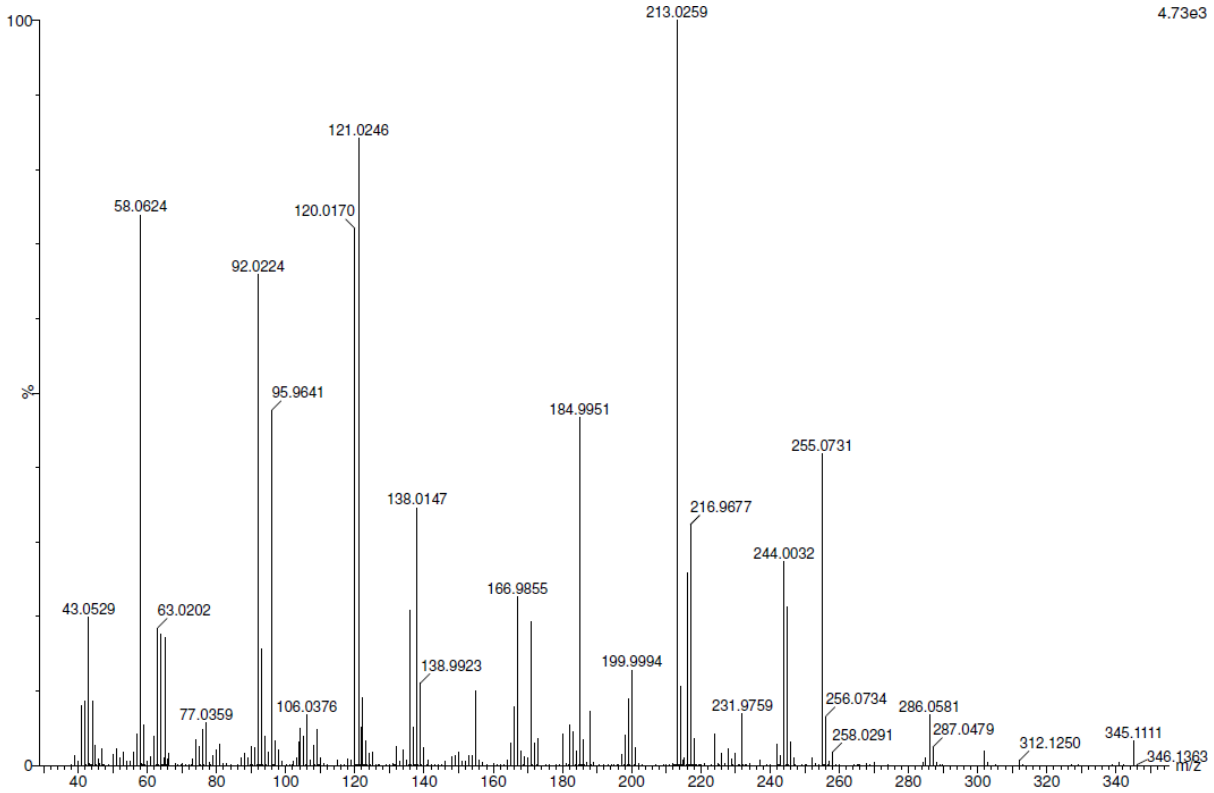
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
303	0	303.0977	303.1058	-0.0081	C13H22NO3PS	M
288	15	288.0741	288.08233	-0.00823	C12H19NO3PS	M-CH3
260	43	260.0422	260.05103	-0.00883	C10H15NO3PS	M-C3H7
243	60	243.0146	243.024476	-0.009876	C10H12O3PS	M-C3H10N
217	86	217.002	217.00883	-0.00683	C8H10O3PS	M-C5H12N
195	108	195.1019	195.10817	-0.00627	C11H17NS	M-C2H5O3P
180	123	180.0795	180.0847	-0.0052	C10H14NS	M-C3H8O3P = C2H5O3P & CH3
154	149	154.0405	154.04524	-0.00474	C8H10OS	M-C5H12NO2P
153	150	153.0314	153.03741	-0.00601	C8H9OS	M-C5H13NO2P
139	164	139.0172	139.02176	-0.00456	C7H7OS	
122	181	122.0313	122.03709	-0.00579	C3H9NO2P	OP-C2H4
110	193	110.0145	110.01902	-0.00452	C6H6S	
109	194	109.0076	109.011196	-0.003596	C6H5S	
91	212	91.0505	91.05478	-0.00428	C7H7	
80	223	79.9868	79.9901	-0.0033	H3NO2P	
77	226	77.0354	77.039125	-0.003725	C6H5	
44	259	44.0468	44.05002	-0.00322	C2H6N	

GCT Spectrum #11 – Fenchlorphos, Ronnel



Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
320	0		319.8997		C8H8Cl3O3PS	M
285	35	284.9251	284.9309	-0.0058	C8H8Cl2O3PS	M-Cl
270	50	269.9005	269.9074	-0.0069	C7H5Cl2O3PS	M-Cl-CH3
167	153	166.9172	166.92221	-0.00501	C5H2Cl3	M-C3H6O3PS
125	195	124.9785	124.9826	-0.0041	C2H6O2PS	
109	211	109.0006	109.0055	-0.0049	C2H6O3P	
97	223	96.9810	96.9845	-0.0035	C5H2Cl	
	,,	,,	*96.9513*	*+0.0297*	*H2O2PS*	*NOT expected OP ion*
79	241	78.9916	78.9949	-0.0033	CH4O2P	
63	257	63.0006	62.99998	0.00062	CH4OP	
62	258	62.0105	62.0157	-0.0052	C5H2	aromatic
47	273	46.9663	46.9687	-0.0024	PO	

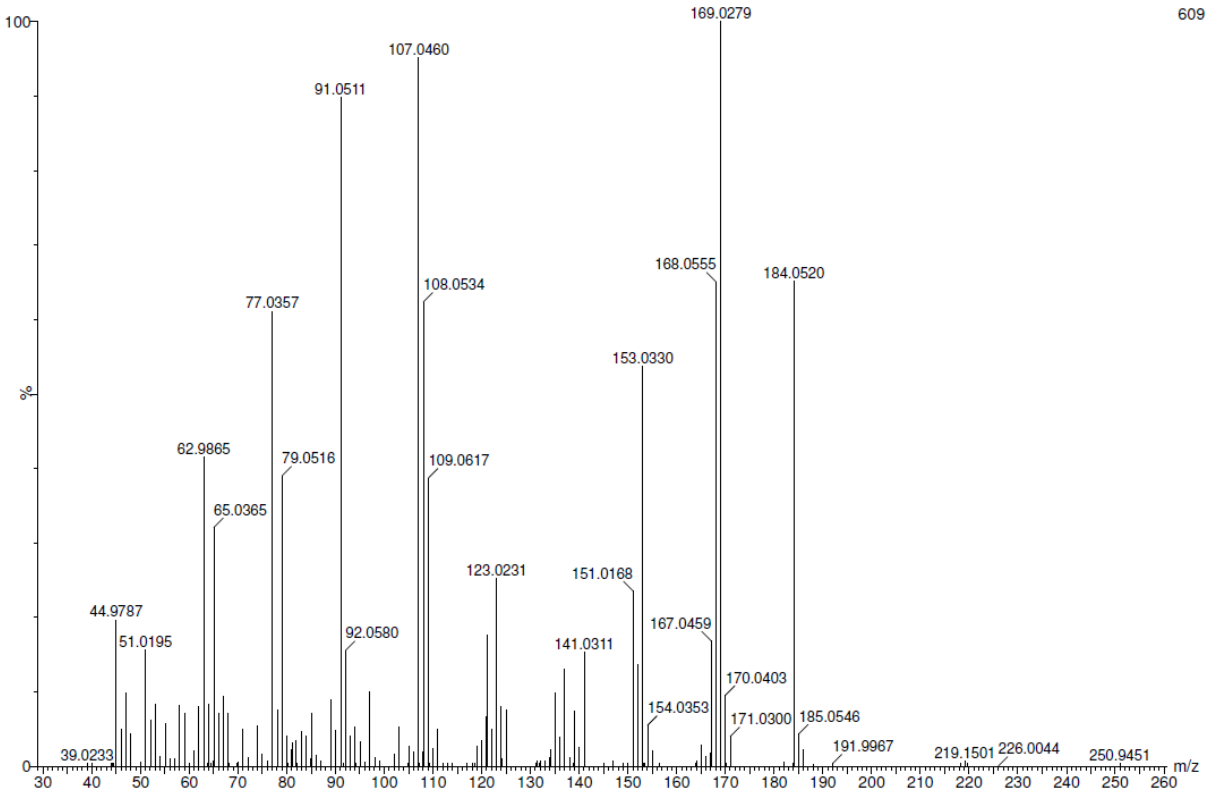
GCT Spectrum #12 – Isofenphos



Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
345	0	345.1111	345.1164	-0.0053	C15H24NO4PS	M
312	33	312.125	312.1365	-0.0115*	C15H23NO4P	M-SH ?
286	59	286.0581	286.0667	-0.0086	C12H17NO3PS	M-C3H7O
	,,	,,	*286.0429*	*+0.0152**	*C12H15O4PS*	*M-C3H9N ?*
255	90	255.0731	255.0786	-0.0055	C12H16O4P	
244	101	244.0032	244.0197	-0.0165	C9H11NO3PS	
217	128	216.9677	216.9724	-0.0047	C7H6O4PS	
213	132	213.0259	213.0317	-0.0058	C9H10O4P	Unlikely?
185	160	184.9951	185.0004	-0.0053	C7H6O4P	
167	178	166.9855	166.9898	-0.0043	C7H4O3P	
138	207	138.0147	138.0191	-0.0044	C6H4NO3	Unlikely?
	,,	,,	138.0143	+0.0004*	C3H9NOPS	More likely structure?
121	224	121.0246	121.0290	-0.0044	C7H5O2	
120	225	120.017	120.0211	-0.0041	C7H4O2	
96	249	95.9641	95.9673	-0.0032	H3NOPS	
92	253	92.0224	92.0262	-0.0038	C6H4O	
58	287	58.0624	58.0657	-0.0033	C3H8N	

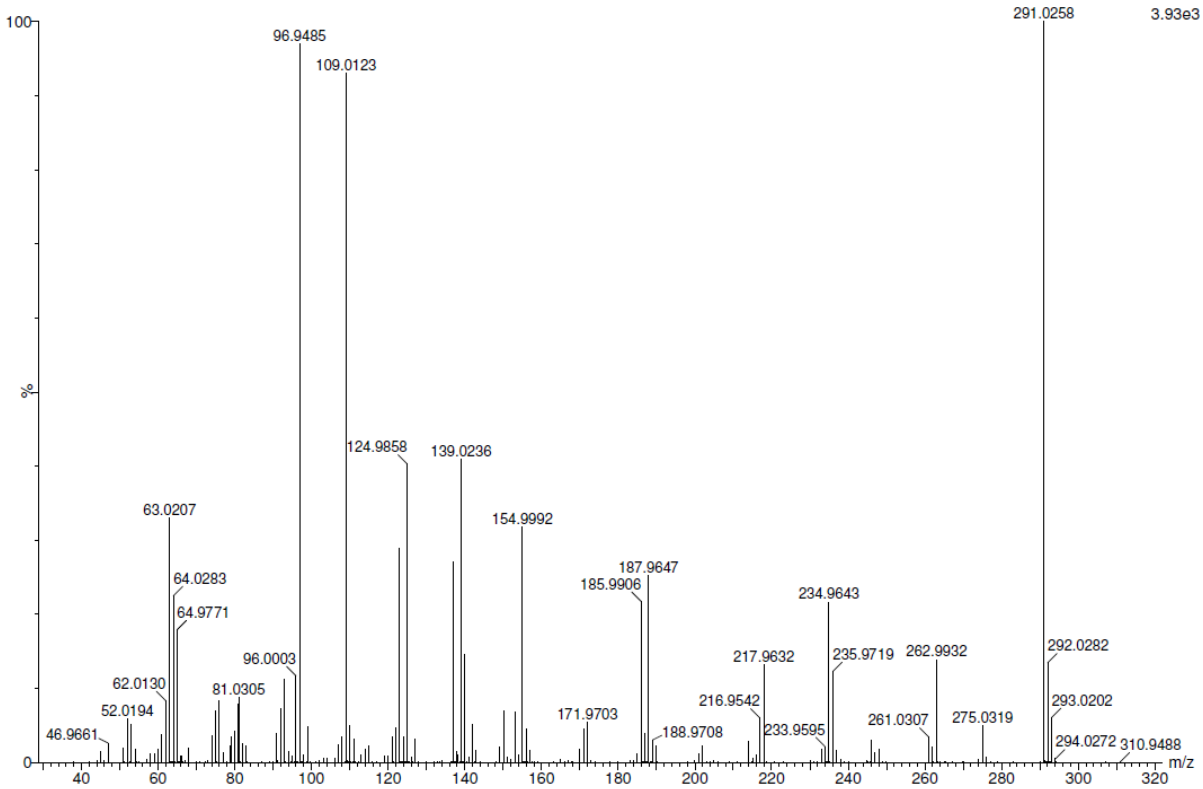
* apparent mass error unexpectedly large

GCT Spectrum #13 – Methiocarb sulphoxide degradation product



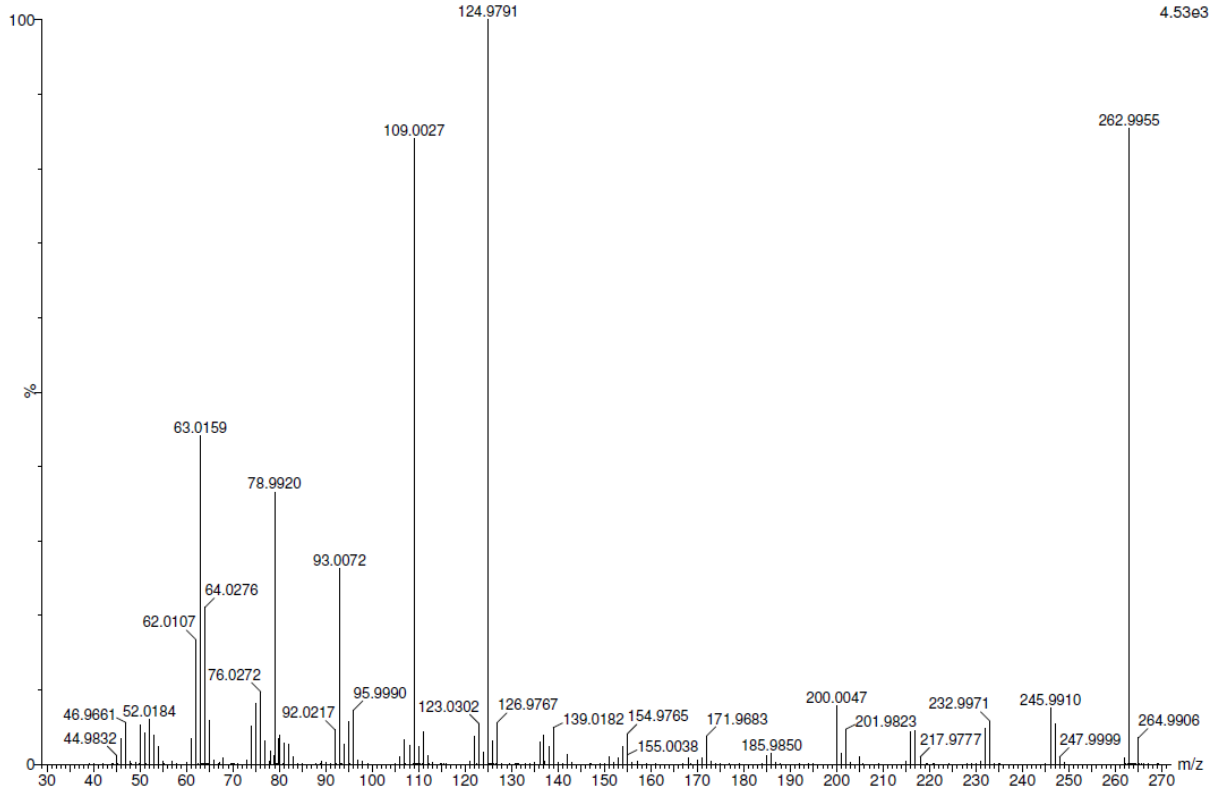
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
184	0	184.052	184.0558	-0.0038	C9H12O2S	M
169	15	169.0279	169.0323	-0.0044	C8H9O2S	M-CH3
168	16	168.05555	168.0609	-0.00535	C9H12OS	M-O
153	31	153.033	153.0374	-0.0044	C8H9OS	M-CH3O
151	33	151.0168	151.0218	-0.005	C8H7OS	M-CH5O
123	61	123.0231	123.0269	-0.0038	C7H7S	M-C2H3O2
109	75	109.0617	109.0653	-0.0036	C7H9O	
108	76	108.0534	108.0575	-0.0041	C7H8O	
107	77	107.046	107.0497	-0.0037	C7H7O	
91	93	91.0511	91.0548	-0.0037	C7H7	
79	105	79.0516	79.0548	-0.0032	C6H7	
77	107	77.0357	77.0391	-0.0034	C6H5	
65	119	65.0365	65.0425	-0.006	C5H5	
63	121	62.9865	62.9905	-0.004	CH3OS	
51	133	51.0195	51.0235	-0.004	C4H3	
45	139	44.9787	44.98	-0.0013	CHS	

GCT Spectrum #14 – Parathion



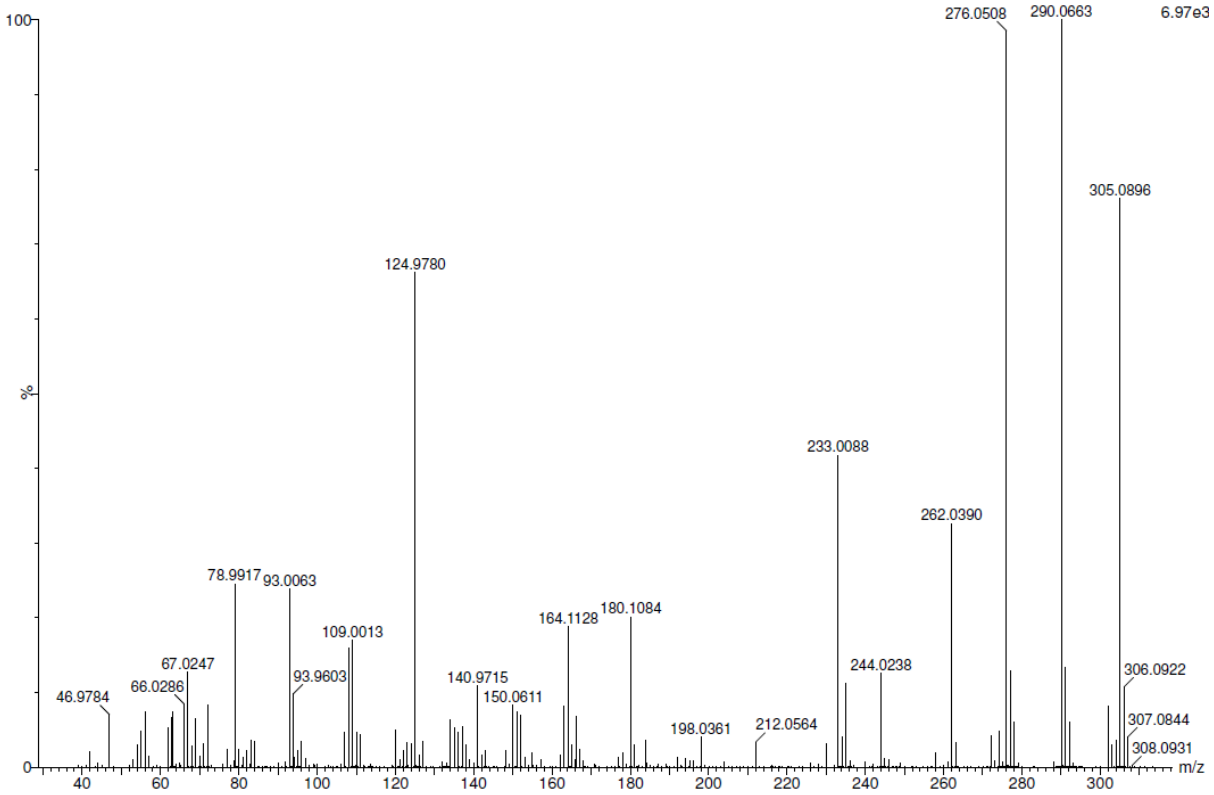
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
291	0	291.0348	291.03303	-0.00723	C10H14NO5PS	M
275	16	275.0394	275.038119	-0.00582	C10H14NO4PS	M-O
263	28	262.9998	263.0017	-0.00840	C8H10NO5PS	M-C2H4
235	56	234.9706	234.9704	-0.00600	C6H4NO5PS	M-2C2H4
218	73	?	217.967694	-0.00459	C6H5NO4PS	M-C2H4/C2H5O
188	103	187.9692	187.969701	-0.00520	C6H5O3PS	M-C2H4/C2H5/NO2
186	105	185.9983	185.995622	-0.00512	C6H5NO4P	M-C2H5S/C2H5O/
155	136	155.0046	155.0041	-0.00480	C6H5NO2S	M-2C2H5O/PO
150	141	?	150.055503		C8H8NO2	M-C2H6O3PS
139	152	139.0253	139.0269	-0.00340		
137	154	137??	137.0368			
125	166	124.9891	124.9826	0.00330		
123	168	123???	123.032			
109	182	109.0136	109.0055	0.00690		
97	194	96.9507	96.9513	-0.00270		
93	198	93.0307	93.010543	0.00836	C2H6O2P	
65	226	64.9793	64.979243	-0.00224		

GCT Spectrum #15 – Parathion methyl



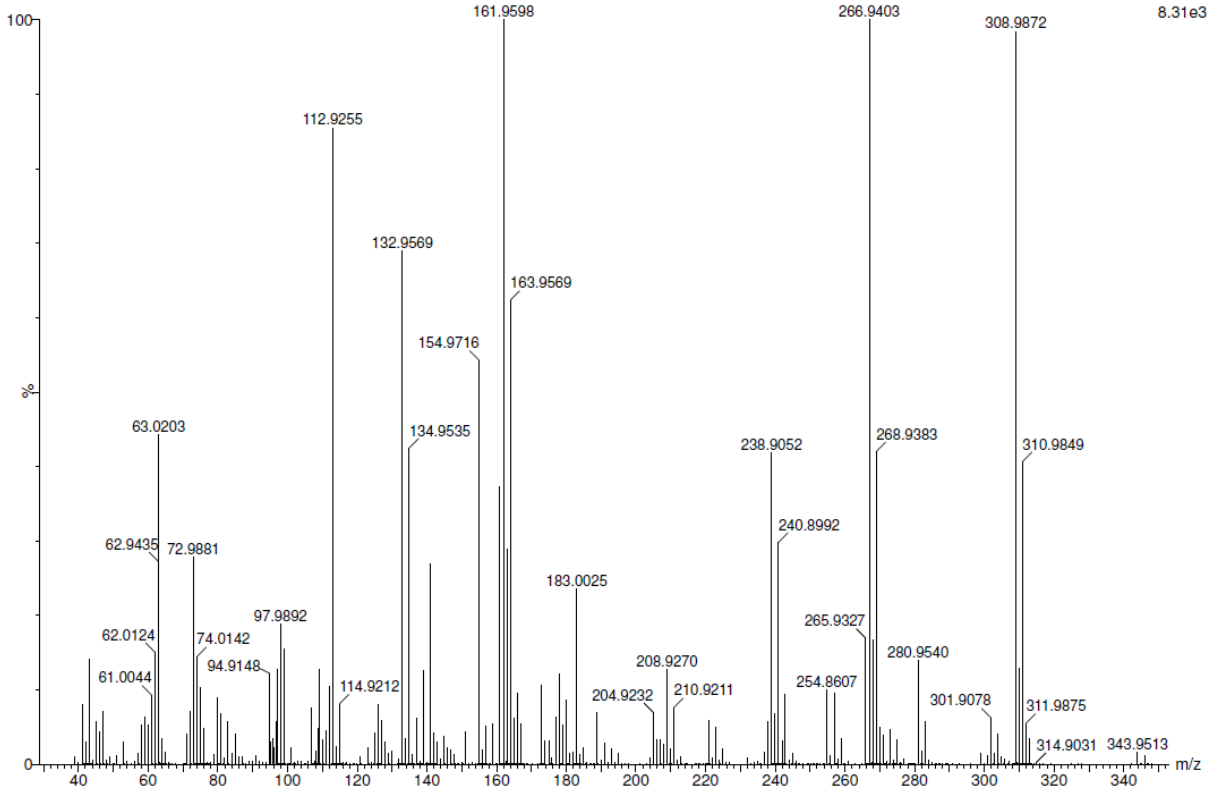
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
263	0	262.9955	263.0017	0.00620	C8H10NO5PS	M
246	17	245.991	245.999	0.00800	C8H9NO4PS	M-OH
233	30	232.9971	233.0037	0.00660	C8H10O4PS	M-NO
202	61	201.9823	201.985355	0.00305	C7H7O3PS	M-NO/CH3O
202	61	201.9823	201.99054	0.00824	C6H5NO5P	M-C2H5S
200	63	200.0047	200.01127	0.00657	C7H7NO4P	M-CH3O/S
125	138	124.9791	124.9826	0.00350		
109	154	109.0027	109.0055	0.00280		
93	170	93.0072	93.010543	0.00334	C2H6O2P	
79	184		78.9949			
63	200	64.9793	64.979243	-0.00006		

GCT Spectrum #16 – Pirimiphos-methyl



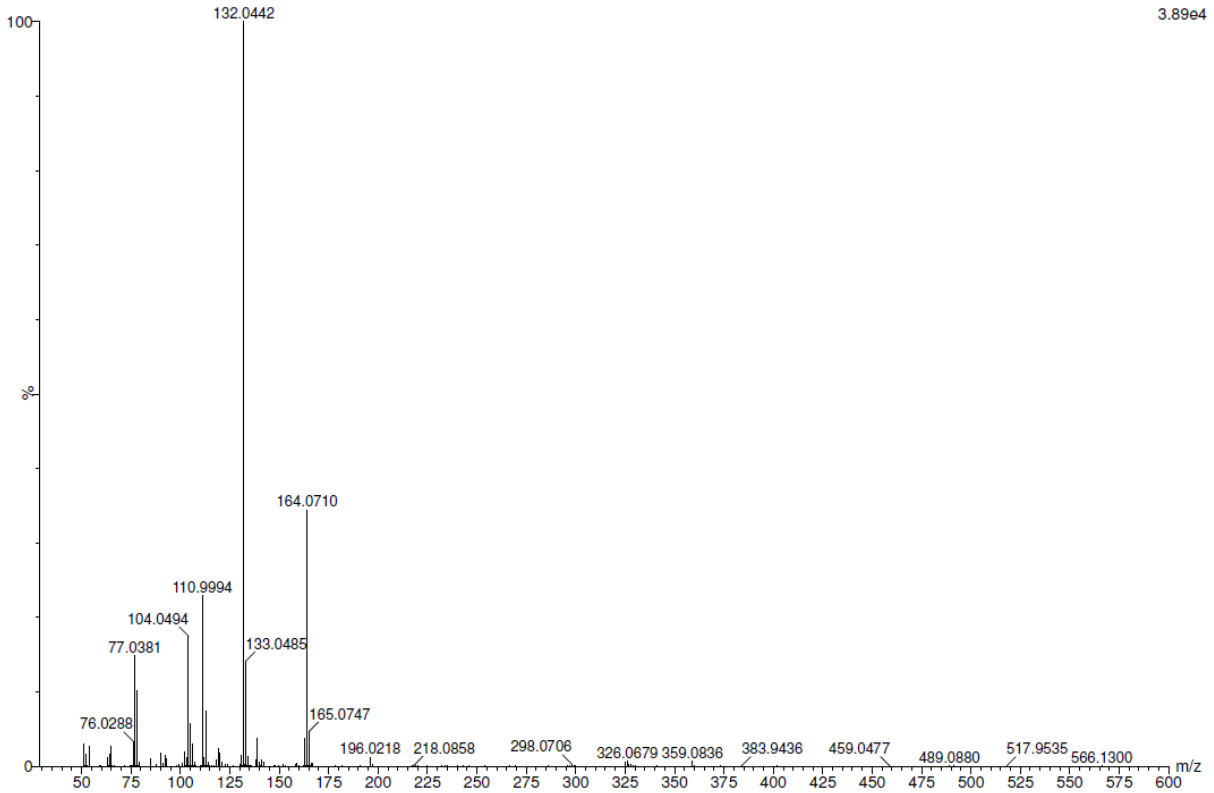
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
305	0	305.0896	305.0963	-0.0067	C11H20N3O3PS	M
290	15	290.0663	290.0728	-0.0065	C10H17N3O3PS	M-CH3
276	29	276.0508	276.0572	-0.0064	C9H15N3O3PS	M-C2H5
262	43	262.039	262.0415	-0.0025	C8H13N3O3PS	M-C3H7
244	61	244.0238	244.031	-0.0072	C8H11N3O2PS	M-C3H9O
233	72	233.0088	233.015	-0.0062	C7H10N2O3PS	M-C4H10N
212	93	212.0564	212.0636	-0.0072	C7H17O3PS	M-C4H3N3!!
198	107	198.0361	198.0432	-0.0071	C7H9N3O2P	M-C4H11OS
180	125	180.1084	180.1137	-0.0053	C9H14N3O	M-C2H6O2PS
164	141	164.1128	164.1188	-0.006	C9H14N3	M-C2H6O3PS
141	164	140.9715	140.9775	-0.006	C2H6O3PS	C9H14N3
125	180	124.978	124.9826	-0.0046	C2H6O2PS	
109	196	109.0013	109.0055	-0.0042	C2H6O3P	
93	212	93.0063	93.0105	-0.0042	C2H6O2P	
79	226	78.9917	78.9949	-0.0032	CH4O2P	
67	238	67.0247	67.0296	-0.0049	C3H3N2	
66	239	66.0286	66.0344	-0.0058	C4H4N	
47	258	46.9784	46.983	-0.0046	PO	

GCT Spectrum #17 – Prothiofos



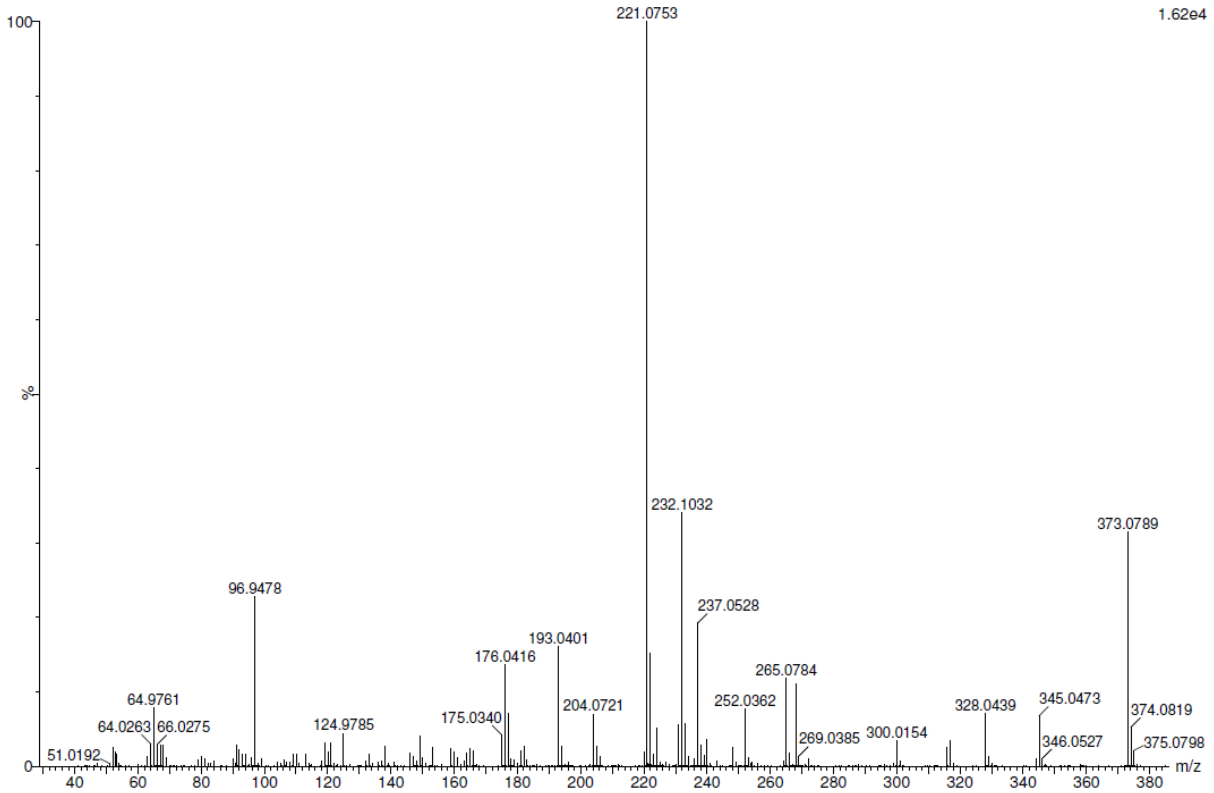
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
344	0	343.9513	343.9628	-0.0115	C11H15Cl2O2PS2	M
309	35	308.9872	308.994	-0.0068	C11H15ClO2PS2	M-Cl
302	42	301.9078	301.9159	-0.0081	C8H9Cl2O2PS2	M-C3H6
281	63	280.954	280.9627	-0.0087		M-Cl-C2H4
267	77	266.9403	266.947	-0.0067	C8H9ClO2PS2	M-Cl-C3H6
255	89	254.8607	254.86617	-0.00547	C6H2Cl2OPS2	M-C5H13O
241	103	240.8992			C6H4Cl2O2PS	
239	105	238.9052	238.91589	-0.01069	C7H5Cl2OS2	M-C5H13S?? WRONG MASS
221	123	??				
209	135	208.927	208.9326	-0.0056	C6H4Cl2O2P	M-C5H11S2
183	161	183.0025	183.0067	-0.0042		C5H12OPS2
162	182	161.9598	161.9639	-0.0041		
155	189	154.9716	154.9754	-0.0038		
141	203					
133	211	132.9569	132.9612	-0.0043		
113	231	112.9255	112.9285	-0.003		
98	246	97.9892				
73	271	72.9881				
63	281	63.0203				
63	281	62.9435	62.9458	-0.0023		

GCT Spectrum #18 – Pyraclostrobin



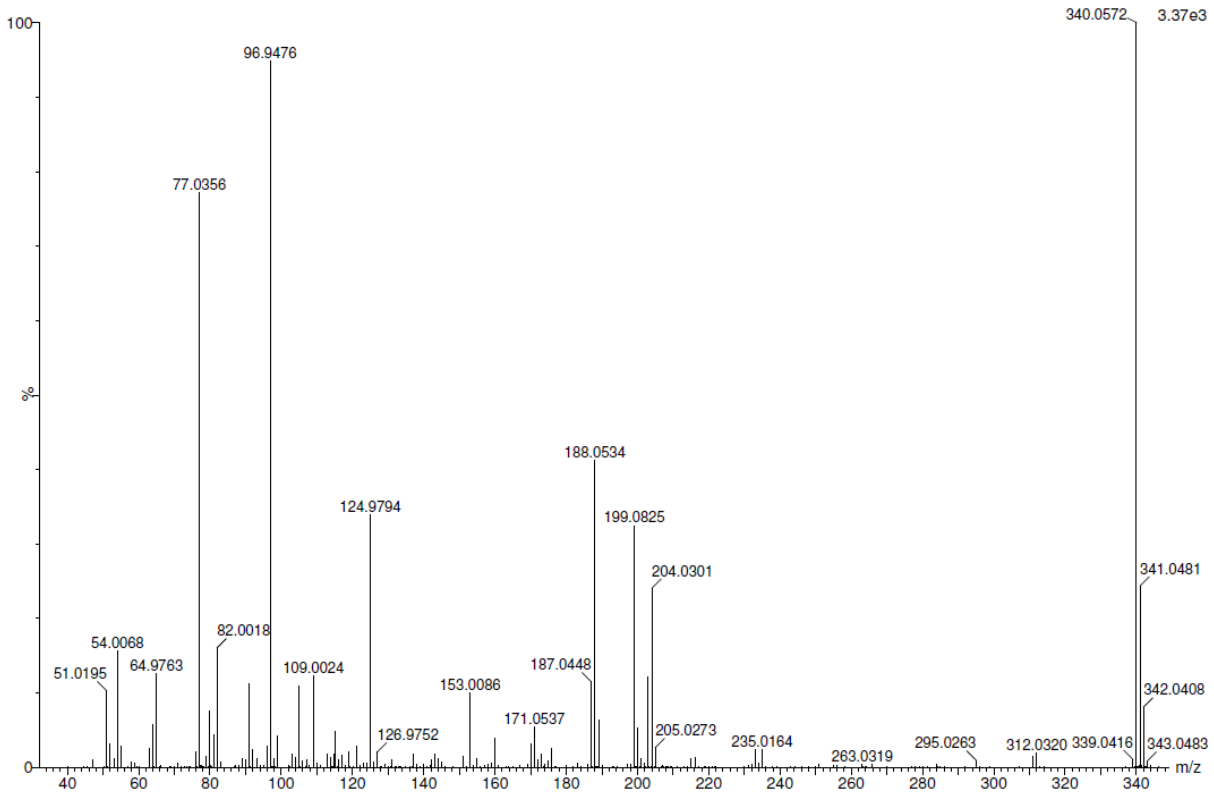
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
387	0	n/a	387.0986	-	C19H18ClN3O4	M
164	223	164.071	164.0712	-0.0002	C9H10NO2	M-C10H8ClN2O2
132	255	132.0442	132.0449	-0.0007	C8H6NO	m/z164-CH3OH
111	276	110.9994	111.0002	-0.0008	C6H4Cl	
104	283	104.0494	104.05	-0.0006	C7H6N	
77	310	77.0381	77.0391	-0.001	C6H5	

GCT Spectrum #19 – Pyrazophos



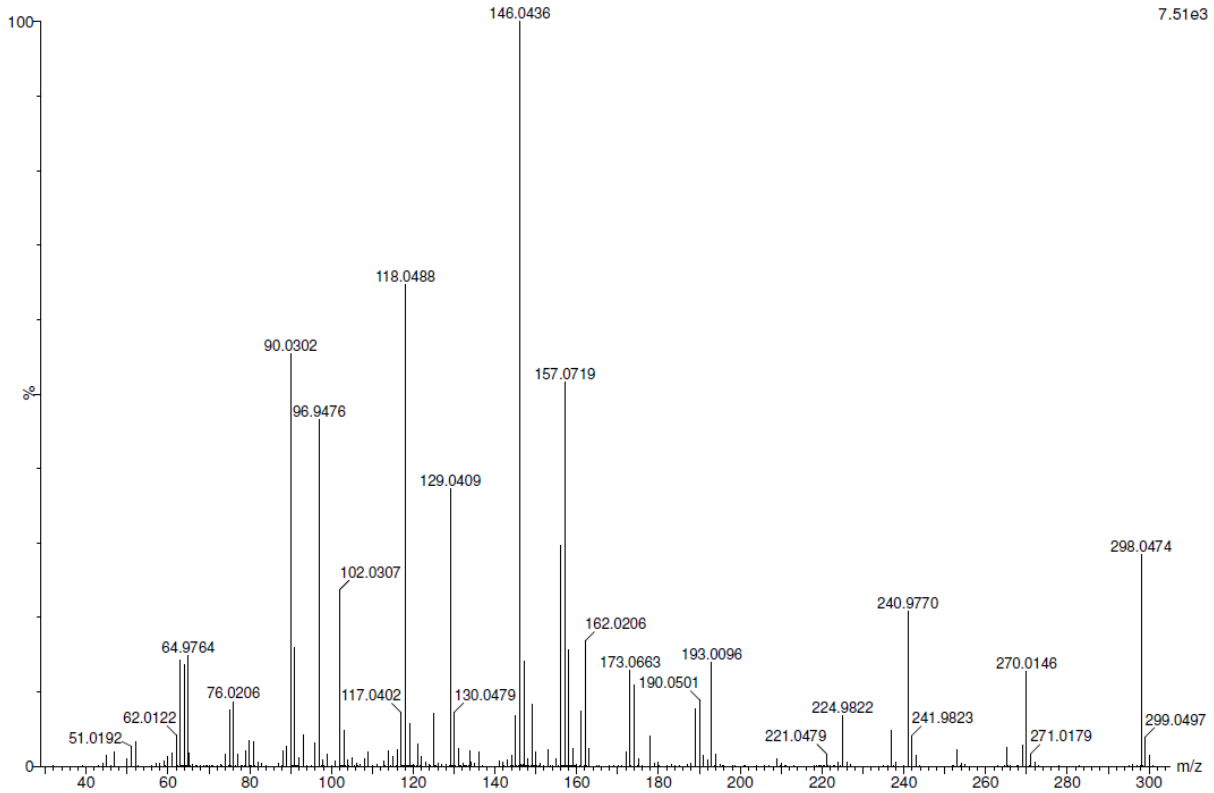
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
373	0	373.0789	373.0861	-0.0072	C14H20N3O5PS	M
345	28	345.0473	345.0548	-0.0075	C12H16N3O5PS	loss of C2H4
328	45	328.0439	328.0521	-0.0082	C12H15N3O4PS	loss of C2H5O
300	73	300.0154	300.02079	-0.00539	C10H11N3O4PS	loss of of 2C2H4+OH (not C2H5OCO)
265	108	265.0784	265.0885	-0.0101		
252	121	252.0362	252.0443	-0.0081		
237	136	237.0528	237.0572	-0.0044	C10H11N3O2S	O/S swap and loss of OP
232	141	232.1032	232.1086	-0.0054	C12H14N3O2	loss of C2H6O3PS = 140.97753
221	152	221.0753	221.08	-0.0047	C10H11N3O3	loss of OP
204	169	204.0721	204.0773	-0.0052	C10H10N3O2	
193	180	193.0401	193.04874	-0.00864	C8H7N3O3	loss of OP & C2H4
176	197	176.0416	176.046	-0.0044	C8H6N3O2	193-17 (OH)
125	248	124.9785	124.9826	-0.0041	C2H6O2PS	(C2H5O)(HO)PS+
97	276	96.9478	96.9513	-0.0035	H2O2PS	(HO)2PS+
65	308	64.9761	64.9792	-0.0031	H2O2P	(HO)2P+

GCT Spectrum #20 – Pyridaphenthion



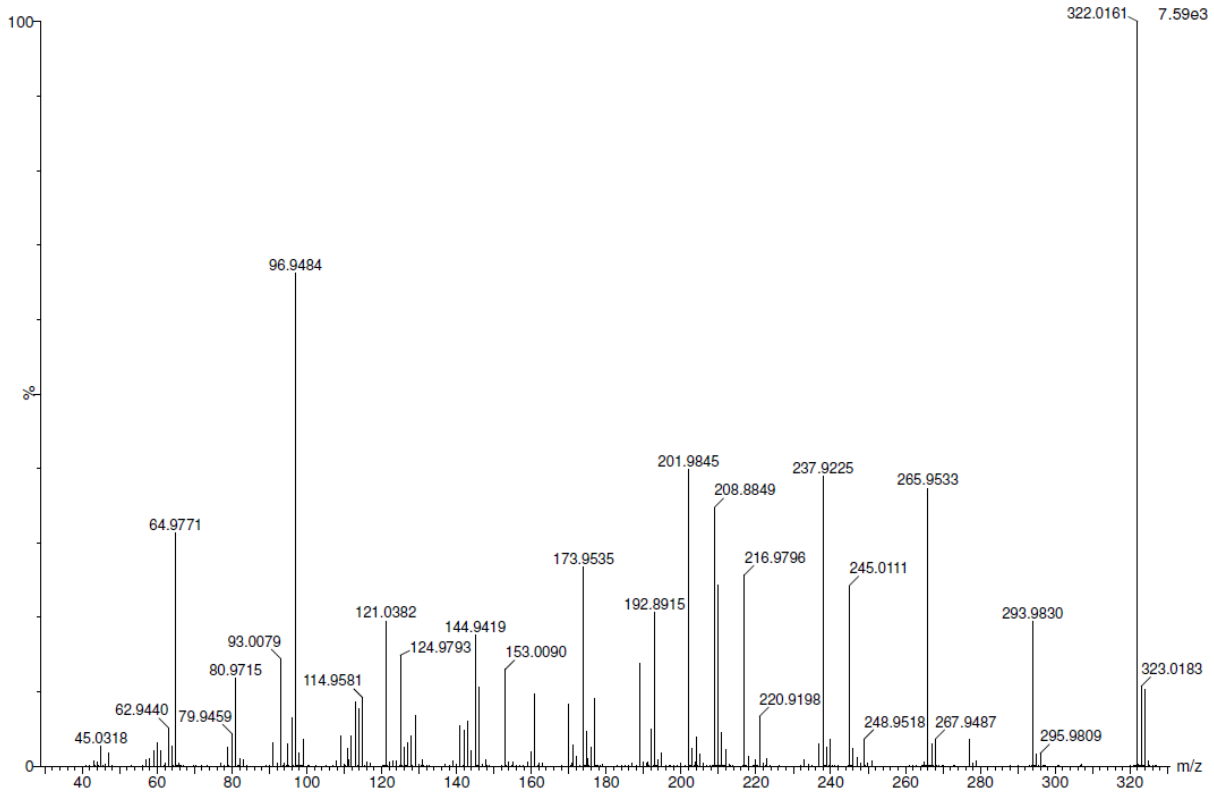
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
340	0	340.0572	340.0647	-0.0075	C14H17N2O4PS	
312	28	312.032	312.0334	-0.0014	C12H13N2O4PS	M-C2H4
295	45	295.0263	295.0306	-0.0043	C12H12N2O3PS	M-C2H5O
235	105	235.0164	235.0273	-0.0109	C10H8N2O3P	M-C4H9OS
204	136	204.0301	204.0357	-0.0056	C10H8N2OS	M-C4H9O3P
199	141	199.0825	199.08714	-0.00464	C12H11N2O	M-C2H6O3PS
188	152	188.0534	188.0586	-0.0052	C10H8N2O2	M-C4H9O2PS
153	187	153.0086	153.0139	-0.0053	C4H10O2PS	M-C10H7N2O2
125	215	124.9794	124.9826	-0.0032	C2H6O2PS	
109	231	109.0024	109.0055	-0.0031	C2H6O3P	
97	243	96.9476	96.9513	-0.0037	H2O2PS	
82	258	82.0018	82.0055	-0.0037	C4H2O2	
77	263	77.0356	77.03913	-0.00353	C6H5	
65	275	64.9763	64.9792	-0.0029	H2O2P	
54	286	54	54.0106	-0.0038	C3H2O	
51	289	51.0195	51.0235	-0.004	C4H3	

GCT Spectrum #21 – Quinalphos



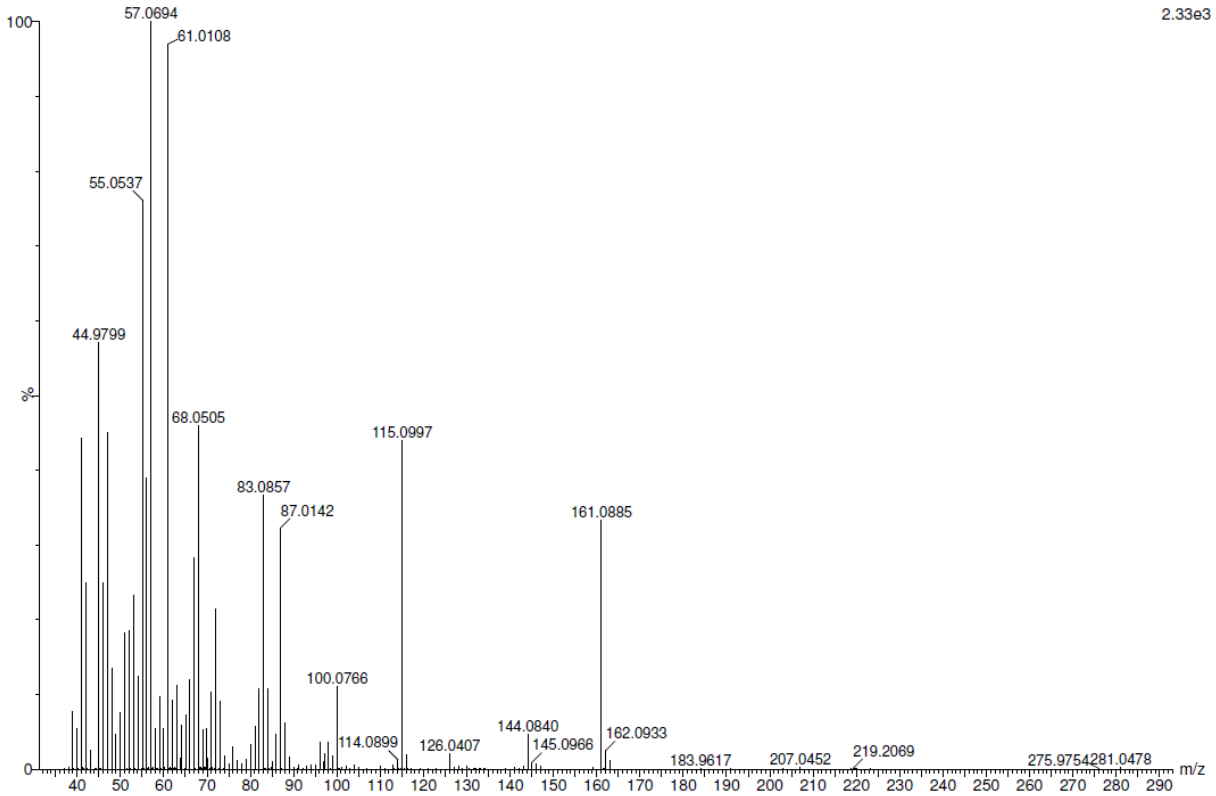
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
298	0	298.0474	298.0541	-0.0067		M
270	28	270.0146	270.0228	-0.0082		loss of C2H4
241	57	240.977	240.9837	-0.0067	M-C4H9	loss of C4H9 = 57.07043
225	73	224.9822	224.9888	-0.0066	C8H6N2O2PS	M-73, loss of C4H9O
193	105	193.0096	193.0164	-0.0068	C8H6N2O2P	M-105
173	125	173.0663	173.0715	-0.0052	C10H9N2+O	loss of C2H6O2PS
162	136	162.0206	162.0252	-0.0046		
157	141	157.0719	157.0766	-0.0047	C10H9N2+	loss of C2H6O3PS = 140.97753
146	152	146.0436	146.048	-0.0044		
129	169	129.0409	129.0453	-0.0044		
118	180	118.0488	118.0531	-0.0043		
102	196	102.0307	102.03437	-0.00367	C7H4N	
97	201	96.9476	96.9513	-0.0037		
90	208	90.0302	90.03437	-0.00417	C6H4N	

GCT Spectrum #22 – Sulfotep



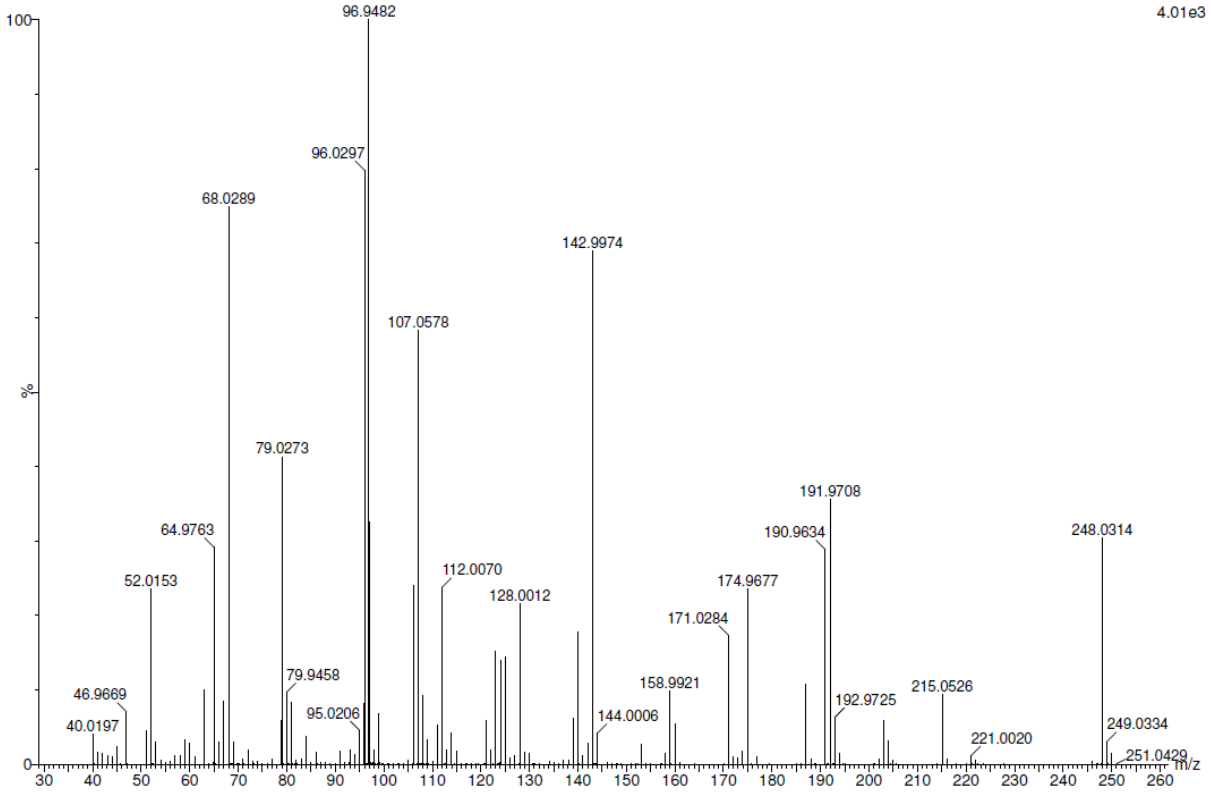
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
322	0	322.0161	322.0227	-0.0066	C8H20O5P2S2	M
294	28	293.983	293.9914	-0.0084	C6H16O5P2S2	M-C2H4
266	56	265.9533	265.9601	-0.0068	C4H12O5P2S2	M-C4H8 = 2C2H4
245	77	245.0111	245.0166	-0.0055	C6H15O4P2S	M-C2H5OS
238	84	237.9225	237.9288	-0.0063	C2H8O5P2S2	M-C6H12 = 3C2H4
221	101	220.9198	220.9261	-0.0063	C2H7O4P2S2	M-C6H13O
217	105	216.9796	216.9853	-0.0057	C4H11O4P2S	M-C4H9OS
209	113	208.8849	208.8897	-0.0048	H3O5P2S2	M-C8H17
202	120	201.9845	201.9887	-0.0042	C4H11O3PS2	M-C4H9O2P
193	129	192.8915	192.8948	-0.0033	H3O4P2S2	M-C8H17O
174	148	173.9535	173.9574	-0.0039	C2H7O3PS2	M-C6H13O2P
153	169	153.009	153.0139	-0.0049	C4H10O2PS	
145	177	144.9419	144.9456	-0.0037	H3O5P2	
125	197	124.9793	124.9826	-0.0033	C2H6O2PS	
121	201	121.0382	121.0418	-0.0036	C4H10O2P	
97	225	96.9484	96.9513	-0.0029	H2O2PS	
93	229	93.0079	93.0105	-0.0026	C2H6O2P	
81	241	80.9715	80.9742	-0.0027	H2O3P	
65	257	64.9771	64.9792	-0.0021	H2O2P	

GCT Spectrum #23 – Thiofanox (probably oxime, MW 161)



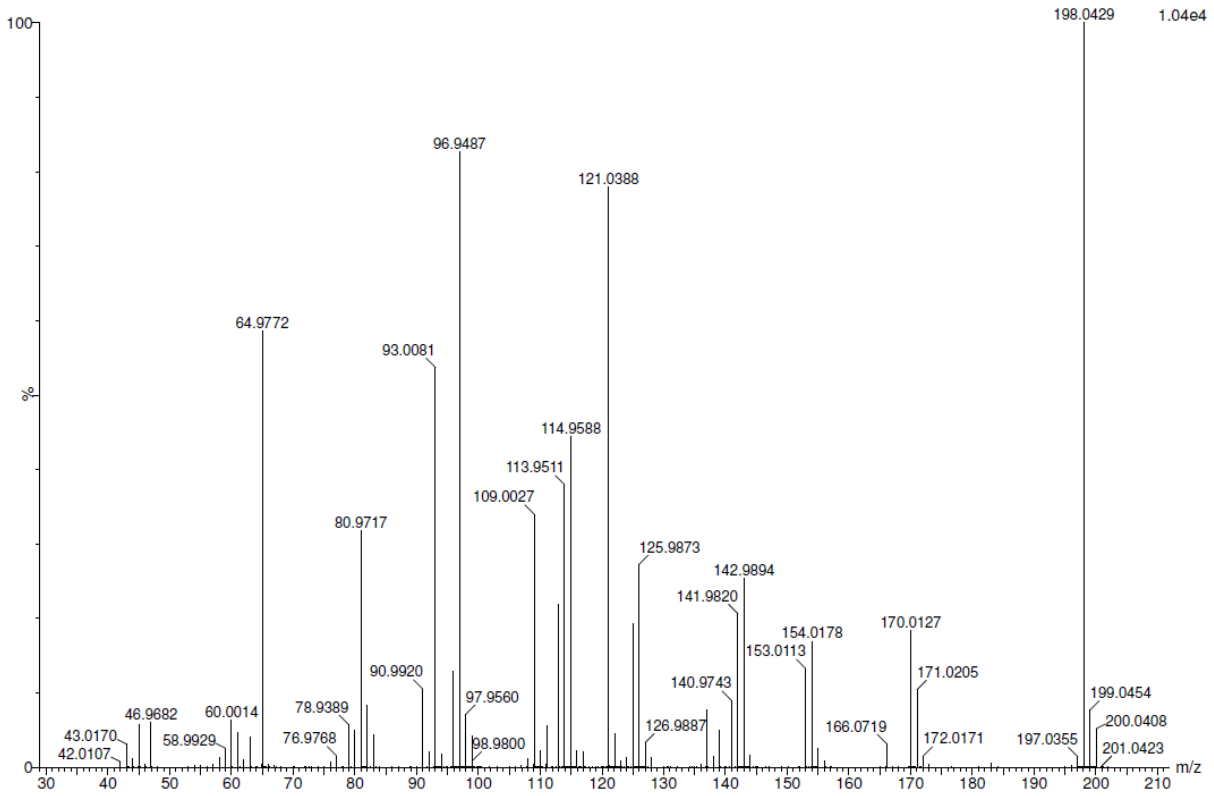
Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
161	0	161.0885	161.0874	0.0011	C7H15NOS	M
144	17	144.084	144.0847	-0.0007	C7H14NS	M-OH
126	35	126.0407			C6H8NS	M-CH7O???
115	46	115.0997	115.0997	0	C6H13NO	M-CH2S
100	61	100.0766	100.0762	0.0004	C5H10NO	M-C2H5S
87	74	87.0142	87.0143	-0.0001	C3H5NS	M-C4H10O
83	78	83.0857	83.0861	-0.0004	C6H11	M-CH4NOS
68	93	68.0505	68.05	0.0005	C4H6N	M-C3H9OS
61	100	61.0108	61.0112	-0.0004	C2H5S	
57	104	57.0694	57.0704	-0.001	C4H9	
45	116	44.9799	44.9799	0	CHS	

GCT Spectrum #24 – Thionazin



Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
248	0	248.0314	248.03845	-0.00705	C8H13N2O3PS	M
221	27	221.002	221.01497	-0.01297	C6H10N2O3PS	M-C2H3
220	28	??	220.00715	??	C6H9N2O3PS	M-C2H4
215	33	215.0526	215.05855	-0.00595	C8H12N2O3P	M-SH
192	56	191.9708	191.97585	-0.00505	C4H5N2O3PS	M-2C2H4
191	57	190.9634	190.96802	-0.00462	C4H4N2O3PS	M-C2H4/C2H5
175	73	174.9677	174.97311	-0.00541	C4H4N2O2PS	M-C2H4/C2H5O
171	77	171.0284	171.03234	-0.00394	C6H8N2O2P	M-C2H5O/S
159	89	158.9921	158.99595	-0.00385	C4H4N2O3P	M-C2H4/C2H5S
143	105	142.9974	143.00104	-0.00364	C4H4N2O2P	M-C2H4/C2H5O/S
128	120	128.0012	128.00443	-0.00323	C4H4N2OS	M-C4H9O2P
112	136	112.007	112.00952	-0.00252	C4H4N2S	
107	141	107.0578	107.06092	-0.00312	C6H7N2	M-C2H6O3PS
106	142	??				
97	151	96.9482	96.95131	-0.00311	H2O2PS	
96	152	96.0297	96.03236	-0.00266	C4H4N2O	
79	169	79.0273	79.02962	-0.00232	C4H3N2	
68	180	68.0289	68.03745	-0.00855	C3H4N2	M-C5H9O3PS
65	183	64.9763	64.97924	-0.00294	H2O2P	
52	196	52.0153	52.01872	-0.00342	C3H2N	

GCT Spectrum #25 – Triethyl phosphorothioate



Nominal mass	Nominal loss	GCT m/z observed	Assigned	Difference	Empirical Formula	Assignment
198	0	198.0429	198.048	-0.0051	C6H15O3PS	M
170	28	170.0127	170.01665	-0.00395	C4H11O3PS	M-C2H4
154	44	154.0178	154.02174	-0.00394	C4H11O2PS	M-C2H4O
153	45	153.0113	153.01391	-0.00261	C4H10O2PS	M-C2H5O
143	55	142.9894	142.99318	-0.00378	C2H8O3PS	M-C4H7
142	56	141.982	141.98535	-0.00335	C2H7O3PS	M-C2H4/C2H4
126	72	125.9873	125.9904	-0.0031	C2H7O2PS	
121	77	121.0388	121.0418	-0.003	C4H10O2P	
115	83	114.9588	114.9619	-0.0031	H4O3PS	
114	84	113.9511	113.9541	-0.003	H3O3PS	
109	89	109.0027	109.0055	-0.0028	C2H6O3P	
97	101	96.9487	96.9513	-0.0026	H2O2PS	
93	105	93.0081	93.0105	-0.0024	C2H6O2P	
81	117	80.9717	80.9742	-0.0025	H2O3P	
65	133	64.9772	64.9792	-0.002	H2O2P	