

*EURL for Cereals and Feeding stuff  
National Food Institute  
Technical University of Denmark*

## **Exact Mass Pesticide Database for use by GC-HRMS**

### **Report 3**

(last version 230318)

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## 1. Introduction

This report describes an exact mass database of 133 pesticides for use with gas chromatography high resolution mass spectrometry (GC-HRMS). For each pesticide the chemical formula and molecular weight is listed as well as the formula and exact mass of a number of characteristic fragment ions.

The database was updated in 2018 with exact mass fragments of 52 pesticides and together with the pesticides included in the database in 2014 and 2015 the total number of pesticides with exact mass fragments are now 133.

The intention is to use the database in conjunction with Agilent MassHunter software. The assigned fragments and their masses have been compared with the masses in the Agilent pesticide PCDL as well as by building a custom PCDL with the 133 pesticides and used that in an analysis of a pesticide mixture.

## 2. Analytical conditions for GC-HRMS

### Gas chromatograph:

Inlet: PTV

Inlet temperature: 60 °C

Injection volume: 5 µl

Carrier gas: Helium

Carrier flow: 1.2 ml/min (column 1) and 1.4 ml/min /column 2)

Columns: 2 identical columns. HP-5MS UI, 15m x 250 µm x 0.25 µm

Oven temperature program: 60 °C in 3 min., 30 °C/min. to 180 °C, hold in 0.8 min, 5 °C/min. to 300 °C. Total run time 31.8 min.

### Mass Spectrometer

Ion source temperature: 230 °C

Transfer line temperature: 300 °C

Ionization: electron impact

Electron energy: 70 eV

Sampling rate: 4 GHz

Mass range: 50 - 500 AMU

### 3. Exact mass database of 81 pesticides for use by GC-HRMS

\*\*\*: included in the database 2017, \*: included in the database 2015, no asterisk: Included in the database in 2014.

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
	2,4-D Butyl ester	94-80-4	12.607	276.03200	C12H14O3Cl2		
	2,4-D Butyl ester	94-80-4	12.607		C8H6O3Cl2	219.968851	219.969399
	2,4-D Butyl ester	94-80-4	12.607		C8H6O3Cl	184.999998	185.000547
	2,4-D Butyl ester	94-80-4	12.607		C7H5OCl2	174.971197	174.971745
	2,4-D Butyl ester	94-80-4	12.607		C6H4OCl2	161.963372	161.963920
	2,4-D Butyl ester	94-80-4	12.607		C6H3Cl2	144.960632	144.961181
	2,4,5-T-methylester	1928-37-6	11.387	267.94610	C9H7O3Cl3		
	2,4,5-T-methylester	1928-37-6	11.387		C9H7O3Cl2	232.976676	232.977225
	2,4,5-T-methylester	1928-37-6	11.387		C7H4OCl3	208.932224	208.932773
	2,4-DB-methylester	18625-12-2	12.196	262.01640	C11H12O3Cl2		
	2,4-DB-methylester	18625-12-2	12.196		C10H9O2Cl2	230.997411	230.997960
	2,4-DB-methylester	18625-12-2	12.196		C6H4OCl2	161.963372	161.963920
	2,4-DB-methylester	18625-12-2	12.196		C5H9O2	101.059706	101.060255
*	2,4-D-methylester	1928-38-7	9.776	233.98500	C9H8O3Cl2		
*	2,4-D-methylester	1928-38-7	9.776		C9H8O3Cl	199.015648	199.016197
*	2,4-D-methylester	1928-38-7	9.776		C7H5OCl2	174.971197	174.971745
*	2,4-D-methylester	1928-38-7	9.776		C6H3OCl2	160.955547	160.956095
	4,4'-Dichlorobenzophenone	90-98-2	14.183	249.99520	C13H8OCl2		
	4,4'-Dichlorobenzophenone	90-98-2	14.183		C13H8OCl	215.025819	215.026368
	4,4'-Dichlorobenzophenone	90-98-2	14.183		C7H4OCl	138.994519	138.995067
	4,4'-Dichlorobenzophenone	90-98-2	14.183		C6H4Cl	110.999604	111.000153
	Acetochlor	34256-82-1	12.709	269.11830	C14H20NO2Cl		
	Acetochlor	34256-82-1	12.709		C14H20NO2	234.148855	234.149404
	Acetochlor	34256-82-1	12.709		C12H14NOCl	223.075843	223.076392
	Acetochlor	34256-82-1	12.709		C11H12NO	174.091340	174.091889
	Acetochlor	34256-82-1	12.709		C10H12NO	162.091340	162.091889
	Acetochlor	34256-82-1	12.709		C10H12N	146.096426	146.096974
	Acetochlor	34256-82-1	12.709		C9H10N	132.080776	132.081324
*	Acibenzolar-S-Methyl 2849	135158-54-2	12.954	209.99220	C8H6N2OS2		
*	Acibenzolar-S-Methyl 2849	135158-54-2	12.954		C8H6OS2	181.985458	181.986006
*	Acibenzolar-S-Methyl 2849	135158-54-2	12.954		C8H5OS2	180.977633	180.978181
*	Acibenzolar-S-Methyl 2849	135158-54-2	12.954		C7H3OS2	166.961983	166.962531
*	Acibenzolar-S-Methyl 2849	135158-54-2	12.954		C7H5S2	152.982718	152.983267
*	Acibenzolar-S-Methyl 2849	135158-54-2	12.954		C6H3N2S	135.001145	135.001694

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
*	Acibenzolar-S-Methyl 2849	135158-54-2	12.954		C7H3OS	134.989912	134.990460
*	Acibenzolar-S-Methyl 2849	135158-54-2	12.954		C6H3S	106.994997	106.995546
**	Alachlor	15972-60-8	12.893	269.11826	C14H20ClNO2		
**	Alachlor	15972-60-8	12.893		C13H17ClNO	238.099318	238.099867
**	Alachlor	15972-60-8	12.893		C13H16ClNO	237.091493	237.092042
**	Alachlor	15972-60-8	12.893		C12H15ClNO	224.083668	224.084217
**	Alachlor	15972-60-8	12.893		C13H16NO	202.122641	202.123189
**	Alachlor	15972-60-8	12.893		C12H14NO	188.106990	188.107539
**	Alachlor	15972-60-8	12.893		C11H15N	161.119901	161.120449
**	Alachlor	15972-60-8	12.893		C11H14N	160.112076	160.112624
**	Alachlor	15972-60-8	12.893		C11H12N	158.096426	158.096974
**	Alachlor	15972-60-8	12.893		C10H12N	146.096426	146.096974
**	Alachlor	15972-60-8	12.893		C10H10N	144.080776	144.081324
**	Alachlor	15972-60-8	12.893		C9H10N	132.080776	132.081324
**	Alachlor	15972-60-8	12.893		C8H8N	118.065126	118.065674
**	Allethrin	584-79-2	11.200	302.18819	C19H26O3		
**	Allethrin	584-79-2	11.200		C9H10O	134.072616	134.073165
**	Allethrin	584-79-2	11.200		C9H15	123.116827	123.117375
**	Allethrin	584-79-2	11.200		C8H7O	119.049141	119.049690
**	Allethrin	584-79-2	11.200		C8H9	105.069877	105.070425
**	Allethrin	584-79-2	11.200		C7H7	91.054227	91.054775
**	Allethrin	584-79-2	11.200		C6H7	79.054227	79.054775
	Allethrin	584-79-2	15.357	302.18820	C19H26O3		
	Allethrin	584-79-2	15.357		C9H12O	136.088266	136.088815
	Allethrin	584-79-2	15.357		C9H10O	134.072616	134.073165
	Allethrin	584-79-2	15.357		C9H15	123.116827	123.117375
	Allethrin	584-79-2	15.357		C8H7O	119.049141	119.049690
	Allethrin	584-79-2	15.357		C8H11	107.085527	107.086075
	Allethrin	584-79-2	15.357		C8H9	105.069877	105.070425
*	Anilofos	64249-01-0	21.730	367.02320	C13H19NO3PS2Cl		
*	Anilofos	64249-01-0	21.730		C11H13NSCl	226.045174	226.045723
*	Anilofos	64249-01-0	21.730		C11H14NOCl	211.075843	211.076392
*	Anilofos	64249-01-0	21.730		C8H7NSCl	183.998224	183.998773
*	Anilofos	64249-01-0	21.730		C3H8O2PS2	170.969784	170.970332
*	Anilofos	64249-01-0	21.730		C8H9NCl	154.041803	154.042352
*	Anilofos	64249-01-0	21.730		C2H6O2PS	124.982063	124.982612
**	Anthraquinone	84-65-1	13.872	208.05243	C14H8O2		
**	Anthraquinone	84-65-1	13.872		C14H8O2	208.051881	208.052429
**	Anthraquinone	84-65-1	13.872		C13H8O	180.056966	180.057515

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
**	Anthraquinone	84-65-1	13.872		C12H8	152.062052	152.062600
**	Anthraquinone	84-65-1	13.872		C12H7	151.054227	151.054775
	Aspon	3244-90-4	13.969	378.08530	C12H28O5P2S2		
	Aspon	3244-90-4	13.969		C9H22O5P2S2	336.037840	336.038388
	Aspon	3244-90-4	13.969		C6H17O5P2S2	294.998714	294.999263
	Aspon	3244-90-4	13.969		C3H11O5P2S2	252.951764	252.952313
	Aspon	3244-90-4	13.969		H5O5P2S2	210.904814	210.905363
	Aspon	3244-90-4	13.969		H4O5P2S2	209.896989	209.897538
	Aspon	3244-90-4	13.969		H3O4P2S2	192.894249	192.894798
	Aspon	3244-90-4	13.969		H4O3PS	114.961328	114.961876
*	Atraton	1610-17-9	10.620	211.14330	C9H17N5O		
*	Atraton	1610-17-9	10.620		C8H14N5O	196.119287	196.119835
*	Atraton	1610-17-9	10.620		C6H11N5O	169.095811	169.096360
*	Atraton	1610-17-9	10.620		C5H8N5O	154.072336	154.072885
*	Azaconazole Peak 1	60207-31-0	17.327	299.02280	C12H11N3O2Cl2		
*	Azaconazole Peak 1	60207-31-0	17.327		C9H7O2Cl2	216.981761	216.982310
*	Azaconazole Peak 1	60207-31-0	17.327		C7H3OCl2	172.955547	172.956095
	Aziprotryne	4658-28-0	11.610	225.07970	C7H11N7S		
	Aziprotryne	4658-28-0	11.610		C6H8N7S	210.055640	210.056189
	Aziprotryne	4658-28-0	11.610		C7H11N5S	197.072967	197.073516
	Aziprotryne	4658-28-0	11.610		C7H10N5S	196.065142	196.065691
	Aziprotryne	4658-28-0	11.610		C6H8N5S	182.049492	182.050041
	Aziprotryne	4658-28-0	11.610		C5H5N5S	167.026017	167.026566
	Aziprotryne	4658-28-0	11.610		C6H8N5	150.077422	150.077970
	Aziprotryne	4658-28-0	11.610		C6H11N4	139.097823	139.098371
	Barban (endo) (isomerA)	101-27-9	16.832	257.00100	C11H9NO2Cl2		
	Barban (endo) (isomerA)	101-27-9	16.832		C11H9NO2Cl	222.031633	222.032181
	Barban (endo) (isomerA)	101-27-9	16.832		C7H4NOCl	152.997593	152.998141
	Barban (endo) (isomerA)	101-27-9	16.832		C10H9N	143.072951	143.073499
	Barban (endo) (isomerA)	101-27-9	16.832		C6H6NCl	127.018328	127.018877
	Barban (endo) (isomerA)	101-27-9	16.832		C6H4NCl	125.002678	125.003227
	Benfluralin	1861-40-1	10.153	335.10930	C13H16N3O4F3		
	Benfluralin	1861-40-1	10.153		C10H9N3O4F3	292.053967	292.054515
	Benfluralin	1861-40-1	10.153		C10H9N3O3F3	276.059052	276.059601
	Benfluralin	1861-40-1	10.153		C8H5N3O4F3	264.022667	264.023215
*	Benoxacor	98730-04-2	12.218	259.01670	C11H11NO2Cl2		
*	Benoxacor	98730-04-2	12.218		C11H11NO2	189.078430	189.078979
*	Benoxacor	98730-04-2	12.218		C10H10NO2	176.070605	176.071154
*	Benoxacor	98730-04-2	12.218		C9H8NO	146.060040	146.060589

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
*	Benoxacor	98730-04-2	12.218		C8H8NO	134.060040	134.060589
*	Benoxacor	98730-04-2	12.218		C7H6NO	120.044390	120.044939
	Bensulide	741-58-2	12.218	397.06050	C14H24NO4PS3		
	Bensulide	741-58-2	12.218		C7H8NO2S	170.027026	170.027574
	Bensulide	741-58-2	12.218		C6H5O2S	141.000476	141.001025
	Bensulide	741-58-2	12.218		C6H5	77.038577	77.039125
	Benzoylprop-ethyl	22212-55-1	20.827	365.05850	C18H17NO3Cl2		
	Benzoylprop-ethyl	22212-55-1	20.827		C15H12NOCl2	292.029046	292.029594
	Benzoylprop-ethyl	22212-55-1	20.827		C6C(13)H5O	106.036846	106.037395
	Benzoylprop-ethyl	22212-55-1	20.827		C7H5O	105.033491	105.034040
	Benzoylprop-ethyl	22212-55-1	20.827		C6H5	77.038577	77.039125
**	Bifenox	42576-02-3	21.688	340.98578	C14H9Cl2NO5		
**	Bifenox	42576-02-3	21.688		C14H9Cl(37Cl)NO5	342.982279	342.982828
**	Bifenox	42576-02-3	21.688		C14H9Cl2NO5	340.985229	340.985778
**	Bifenox	42576-02-3	21.688		C13H6Cl(37Cl)NO4	311.963889	311.964438
**	Bifenox	42576-02-3	21.688		C14H9Cl2O4	310.987241	310.987789
**	Bifenox	42576-02-3	21.688		C13H6Cl2NO4	309.966839	309.967388
**	Bifenox	42576-02-3	21.688		C11H6Cl	173.015254	173.015803
**	Bixafen	581809-46-3	27.035	413.03095	C18H12Cl2F3N3O		
**	Bixafen	581809-46-3	27.035		C18H12Cl(37Cl)F3N3O	415.027453	415.028002
**	Bixafen	581809-46-3	27.035		C18H12Cl2F3N3O	413.030403	413.030952
**	Bixafen	581809-46-3	27.035		C6H5F2N2O	159.036446	159.036994
**	Bromacil	314-40-9	13.538	260.01604	C9H13BrN2O2		
**	Bromacil	314-40-9	13.538		C5H6(81Br)N2O2	206.958669	206.959218
**	Bromacil	314-40-9	13.538		C5H6BrN2O2	204.960716	204.961265
**	Bromacil	314-40-9	13.538		C5H3BrNO2	187.934167	187.934715
**	Bromacil	314-40-9	13.538		C4H5(81Br)NO	163.952856	163.953404
**	Bromacil	314-40-9	13.538		C4H5BrNO	161.954902	161.955451
	Butachlor	23184-66-9	16.283	311.16520	C17H26NO2Cl		
	Butachlor	23184-66-9	16.283		C17H26NO2	276.195805	276.196354
	Butachlor	23184-66-9	16.283		C13H16NOCl	237.091493	237.092042
	Butachlor	23184-66-9	16.283		C13H16NO	202.122641	202.123189
	Butachlor	23184-66-9	16.283		C12H14NO	188.106990	188.107539
	Butachlor	23184-66-9	16.283		C11H14NO	176.106990	176.107539
	Butachlor	23184-66-9	16.283		C11H14N	160.112076	160.112624
	Butachlor	23184-66-9	16.283		C10H12N	146.096426	146.096974
*	Butafenacil	134605-64-4	25.383	474.08050	C20H18N2O6ClF3		
*	Butafenacil	134605-64-4	25.383		C13H7N2O3ClF3	331.009181	331.009729
*	Butafenacil	134605-64-4	25.383		C8H3NO2Cl	179.984682	179.985231

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
	Butamifos	36335-67-8	16.552	332.09600	C13H21N2O4PS		
	Butamifos	36335-67-8	16.552		C13H21NO2PS	286.102513	286.103061
	Butamifos	36335-67-8	16.552		C11H17NO2PS	258.071212	258.071761
	Butamifos	36335-67-8	16.552		C7H7NO4PS	231.982791	231.983340
	Butamifos	36335-67-8	16.552		C7H7NO4P	200.010721	200.011269
**	Butralin	33629-47-9	14.506	295.15321	C14H21N3O4		
**	Butralin	33629-47-9	14.506		C14H19N3O3	277.142093	277.142641
**	Butralin	33629-47-9	14.506		C12H16N3O4	266.113532	266.114081
**	Butralin	33629-47-9	14.506		C11H14N3O3	236.102968	236.103516
**	Butralin	33629-47-9	14.506		C9H10N3O4	224.066582	224.067131
**	Butralin	33629-47-9	14.506		C11H14N3O2	220.108053	220.108602
**	Buturon	3766-60-7	6.445	236.07164	C12H13CIN2O		
**	Buturon	3766-60-7	6.445		C7H4(37Cl)NO	154.994643	154.995191
**	Buturon	3766-60-7	6.445		C7H4CINO	152.997593	152.998141
**	Buturon	3766-60-7	6.445		C6H4CIN	125.002678	125.003227
	Butylate (Sutan)	2008-41-5	8.137	217.15000	C11H23NOS		
	Butylate (Sutan)	2008-41-5	8.137		C8H16NOS	174.094711	174.095260
	Butylate (Sutan)	2008-41-5	8.137		C9H18NO	156.138291	156.138839
	Butylate (Sutan)	2008-41-5	8.137		C7H16NS	146.099797	146.100345
**	Captafol	2425-6-1		346.91081	C10H9Cl4NO2S		
**	Captafol	2425-6-1			C2HCl2(37Cl)	131.910884	131.911433
**	Captafol	2425-6-1			C2HCl3	129.913834	129.914383
**	Captafol	2425-6-1			C2HCl2	94.944982	94.945530
**	Captafol	2425-6-1			C2ClS	90.940375	90.940924
**	Captafol	2425-6-1			C6H7	79.054227	79.054775
	Carbetamide	16118-49-3	14.158	236.11610	C12H16N2O3		
	Carbetamide	16118-49-3	14.158		C6C(13)H5NO	120.039920	120.040469
	Carbetamide	16118-49-3	14.158		C7H5NO	119.036565	119.037114
	Carbetamide	16118-49-3	14.158		C6H5N	91.041651	91.042199
	Carbetamide	16118-49-3	14.158		C3H6NO	72.044390	72.044939
**	Carfentrazone-ethyl	128639-02-1	19.195	411.03643	C15H14Cl2F3N3O3		
**	Carfentrazone-ethyl	128639-02-1	19.195		C15H13F3N3O3	340.090352	340.090901
**	Carfentrazone-ethyl	128639-02-1	19.195		C13H8ClF3N3O2	330.025165	330.025714
**	Carfentrazone-ethyl	128639-02-1	19.195		C13H9F3N3O3	312.059052	312.059601
**	Carfentrazone-ethyl	128639-02-1	19.195		C13H7ClF2N3O2	310.018937	310.019486
**	Carfentrazone-ethyl	128639-02-1	19.195		C11H8ClF3N3O	290.030251	290.030799
	Chinomethionate	196869	15.760	233.99220	C10H6N2OS2		
	Chinomethionate	196869	15.760		C9H6N2S2	205.996691	205.997240
	Chinomethionate	196869	15.760		C9H6N2S	174.024620	174.025169



	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
	Chinomethionate	196869	15.760		C9H5N2S	173.016795	173.017344
	Chinomethionate	196869	15.760		C8H6NS	148.021546	148.022095
	Chinomethionate	196869	15.760		C8H6N	116.049476	116.050024
**	Chlorbromuron	13360-45-7	7.970	291.96142	C9H10BrCIN2O2		
**	Chlorbromuron	13360-45-7	7.970		C7H3(81Br)(37Cl)NO	234.903108	234.903657
**	Chlorbromuron	13360-45-7	7.970		C7H3(81Br)CINO	232.906058	232.906607
**	Chlorbromuron	13360-45-7	7.970		C7H3BrCINO	230.908105	230.908654
**	Chlorbromuron	13360-45-7	7.970		C6H3CIN	123.994853	123.995402
**	Chlorbufam	1967-16-4	10.803	223.04001	C11H10CINO2		
**	Chlorbufam	1967-16-4	10.803		C7H4(37Cl)NO	154.994643	154.995191
**	Chlorbufam	1967-16-4	10.803		C7H4CINO	152.997593	152.998141
**	Chlorbufam	1967-16-4	10.803		C6H6CIN	127.018328	127.018877
**	Chlorbufam	1967-16-4	10.803		C6H4CIN	125.002678	125.003227
*	Chloroneb	2675-77-6	8.660	205.99010	C8H8O2Cl2		
*	Chloroneb	2675-77-6	8.660		C7H5O2Cl2	190.966111	190.966660
*	Chloroneb	2675-77-6	8.660		C6H2O2Cl	140.973783	140.974332
	Chlorthiamid	1918-13-4	12.521	204.95200	C7H5NSCl2		
	Chlorthiamid	1918-13-4	12.521		C7H3NCl2	170.963706	170.964255
	Chlorthiamid	1918-13-4	12.521		C7H2N	100.018175	100.018724
**	Coumaphos	56-72-4	24.815	362.01446	C14H16ClO5PS		
**	Coumaphos	56-72-4	24.815		C14H16(37Cl)O5PS	364.010960	364.011509
**	Coumaphos	56-72-4	24.815		C14H16ClO5PS	362.013910	362.014459
**	Coumaphos	56-72-4	24.815		C10H7(37Cl)O2S	227.982029	227.982578
**	Coumaphos	56-72-4	24.815		C10H7ClO2S	225.984980	225.985528
**	Coumaphos	56-72-4	24.815		C10H7ClO3	210.007823	210.008372
**	Coumaphos	56-72-4	24.815		C2H6O3P	109.004907	109.005456
**	Coumaphos	56-72-4	24.815		H2O2PS	96.950763	96.951312
	Crimidine	535-89-7	8.822	171.05630	C7H10N3Cl		
	Crimidine	535-89-7	8.822		C6H7N3Cl	156.032301	156.032850
	Crimidine	535-89-7	8.822		C6H7N2Cl	142.029227	142.029776
	Crimidine	535-89-7	8.822		C5H4N2Cl	127.005752	127.006301
	Crimidine	535-89-7	8.822		C6H6N3	120.055624	120.056172
	Crotoxyphos (Ciodrin)	7700-17-6	16.280	314.09190	C14H19O6P		
	Crotoxyphos (Ciodrin)	7700-17-6	16.280		C6H10O5P	193.026036	193.026585
	Crotoxyphos (Ciodrin)	7700-17-6	16.280		C2H8O4P	127.015472	127.016020
	Crotoxyphos (Ciodrin)	7700-17-6	16.280		C8H9	105.069877	105.070425
	Crotoxyphos (Ciodrin)	7700-17-6	16.280		C8H8	104.062052	104.062600
	Crotoxyphos (Ciodrin)	7700-17-6	16.280		C8H7	103.054227	103.054775
**	Cyanophos	2636-26-2	11.243	243.01190	C9H10NO3PS		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
**	Cyanophos	2636-26-2	11.243		C9H10NO3PS	243.011352	243.011901
**	Cyanophos	2636-26-2	11.243		C2H6O2PS	124.982063	124.982612
**	Cyanophos	2636-26-2	11.243		C2H6O3P	109.004907	109.005456
**	Cyanophos	2636-26-2	11.243		CH4O2P	78.994342	78.994891
**	Cycluron	2163-69-1	11.203	198.17321	C11H22N2O		
**	Cycluron	2163-69-1	11.203		C3H9N2O	89.070939	89.071488
**	Cycluron	2163-69-1	11.203		C6H10	82.077702	82.078250
**	Cycluron	2163-69-1	11.203		C3H6NO	72.044390	72.044939
**	Cycluron	2163-69-1	11.203		C5H9	69.069877	69.070425
**	Cyflufenamid	180409-60-3	17.654	412.12102	C20H17F5N2O2		
**	Cyflufenamid	180409-60-3	17.654		C8H2F4N	188.011788	188.012337
**	Cyflufenamid	180409-60-3	17.654		C7H2F3N	157.013385	157.013934
**	Cyflufenamid	180409-60-3	17.654		C8H5F4NO2	223.025093	223.025641
**	Cyflufenamid	180409-60-3	17.654		C16H4N2O	240.031814	240.032363
	Cythioate	115-93-5	19.955	296.98950	C8H12NO5PS2		
	Cythioate	115-93-5	19.955		C8H9O3PS	216.000453	216.001001
	Cythioate	115-93-5	19.955		C2H8O4P	127.015472	127.016020
	Cythioate	115-93-5	19.955		C2H6O2PS	124.982063	124.982612
	Cythioate	115-93-5	19.955		C2H6O3P	109.004907	109.005456
**	Dazomet	533-74-4	10.700	162.02854	C5H10N2S2		
**	Dazomet	533-74-4	10.700		C5H10N2S2	162.027992	162.028540
**	Dazomet	533-74-4	10.700		C3H7NS	89.029372	89.029920
**	Dazomet	533-74-4	10.700		CS2	75.943593	75.944142
**	Dazomet	533-74-4	10.700		C2H3NS	72.998072	72.998620
**	Dazomet	533-74-4	10.700		C2H2NS	71.990246	71.990795
**	Demeton-S	126-75-0	10.647	258.05132	C8H19O3PS2		
**	Demeton-S	126-75-0	10.647		H4O3PS	114.961328	114.961877
**	Demeton-S	126-75-0	10.647		H3O3PS	113.953503	113.954052
**	Demeton-S	126-75-0	10.647		C4H9S	89.041948	89.042496
**	Demeton-S	126-75-0	10.647		C4H8S	88.034123	88.034671
	Desethylatrazine	6190-65-4	10.014	187.06250	C6H10N5Cl		
	Desethylatrazine	6190-65-4	10.014		C5H7N5Cl	172.038449	172.038998
	Desethylatrazine	6190-65-4	10.014		C3H4N5Cl	145.014974	145.015523
**	Desmetryn	1014-69-3	12.766	213.10482	C8H15N5S		
**	Desmetryn	1014-69-3	12.766		C8H15N5S	213.104268	213.104817
**	Desmetryn	1014-69-3	12.766		C7H12N5S	198.080793	198.081341
**	Desmetryn	1014-69-3	12.766		C5H9N5S	171.057318	171.057866
**	Desmetryn	1014-69-3	12.766		C4H6N5S	156.033843	156.034391
	DiazinonO-analog	962-58-3	12.766	288.12390	C12H21N2O4P		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
	DiazinonO-analog	962-58-3	12.766		C11H18N2O4P	273.099870	273.100419
	DiazinonO-analog	962-58-3	12.766		C10H17N2O4P	260.092045	260.092594
	DiazinonO-analog	962-58-3	12.766		C9H14N2O4P	245.068570	245.069118
	DiazinonO-analog	962-58-3	12.766		C8H12N2O	152.094414	152.094963
	DiazinonO-analog	962-58-3	12.766		C8H11N2O	151.086589	151.087138
	DiazinonO-analog	962-58-3	12.766		C7H9N2O	137.070939	137.071488
	DiazinonO-analog	962-58-3	12.766		C8H10N2	134.083850	134.084398
	Dibutylchloredate	1770-80-5	22.550	497.94930	C17H20O4Cl6		
	Dibutylchloredate	1770-80-5	22.550		C9H4O4Cl6	385.823526	385.824075
	Dibutylchloredate	1770-80-5	22.550		C9H3O3Cl6	368.820787	368.821335
	Dibutylchloredate	1770-80-5	22.550		C9H3O4Cl4	314.877996	314.878544
	Dibutylchloredate	1770-80-5	22.550		C7H2Cl5	260.859365	260.859914
	Dibutylchloredate	1770-80-5	22.550		C5Cl5	234.843715	234.844264
	Dicapthon	2463-84-5	14.252	296.96280	C8H9NO5PSCI		
	Dicapthon	2463-84-5	14.252		C7C(13)H9NO5PS	262.996711	262.997259
	Dicapthon	2463-84-5	14.252		C8H9NO5PS	261.993356	261.993905
	Dicapthon	2463-84-5	14.252		C8H9O3PS	216.000453	216.001001
	Dicapthon	2463-84-5	14.252		C2H6O2PS	124.982063	124.982612
**	Dichlobenil	1194-65-6	7.641	170.96425	C7H3Cl2N		
**	Dichlobenil	1194-65-6	7.641		C7H3Cl(37Cl)N	172.960756	172.961304
**	Dichlobenil	1194-65-6	7.641		C7H3Cl2N	170.963706	170.964254
**	Dichlobenil	1194-65-6	7.641		C7H2N	100.018175	100.018724
**	Dichlofenthion	97-17-6	12.450	313.97001	C10H13Cl2O3PS		
**	Dichlofenthion	97-17-6	12.450		C10H13ClO3PS	279.000606	279.001155
**	Dichlofenthion	97-17-6	12.450		C2ClN5O4S	224.935404	224.935952
**	Dichlofenthion	97-17-6	12.450		C6H5ClO3PS	222.938006	222.938554
**	Dichlofenthion	97-17-6	12.450		C6H4Cl(37Cl)O	163.960421	163.960970
**	Dichlofenthion	97-17-6	12.450		C6H4Cl2O	161.963372	161.963920
**	Dichlofenthion	97-17-6	12.450		H2O2PS	96.950763	96.951312
*	Dichlone	117-80-6	11.704	225.95880	C10H4O2Cl2		
*	Dichlone	117-80-6	11.704		C10H4O2Cl	190.989433	190.989982
*	Dichlone	117-80-6	11.704		C9H4OCl	162.994519	162.995067
*	Dichlone	117-80-6	11.704		C8H4Cl	134.999604	135.000153
	Dichlormid	37764-25-3	7.705	207.02180	C8H11NOCl2		
	Dichlormid	37764-25-3	7.705		C8H11NOCl	172.052368	172.052917
	Dichlormid	37764-25-3	7.705		C5H6NOCl2	165.982096	165.982644
	Dichlormid	37764-25-3	7.705		C8H10NO	136.075690	136.076239
	Dichlormid	37764-25-3	7.705		C7H10NO	124.075690	124.076239
	Dichlorophen	97-23-4	8.270	268.00580	C13H10O2Cl2		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
	Dichlorophen	97-23-4	8.270		C13H10O2Cl	233.036384	233.036932
	Dichlorophen	97-23-4	8.270		C13H8OCl	215.025819	215.026368
	Dichlorophen	97-23-4	8.270		C7H6OCl	141.010169	141.010718
	Dichlorophen	97-23-4	8.270		C6H5OCl	128.002344	128.002892
	Dichlorprop-methyl (Ester)	57153-17-0	9.588	248.00070	C10H10O3Cl2		
	Dichlorprop-methyl (Ester)	57153-17-0	9.588		C8H7OCl2	188.986847	188.987395
	Dichlorprop-methyl (Ester)	57153-17-0	9.588		C6H4OCl2	161.963372	161.963920
*	Diclobutrazol	75736-33-3	17.170	327.09050	C15H19N3OCl2		
*	Diclobutrazol	75736-33-3	17.170		C11H10N3OCl2	270.019544	270.020092
*	Diclobutrazol	75736-33-3	17.170		C7H5Cl2	158.976282	158.976831
*	Diclofop-methyl	51338-27-3	20.069	340.02690	C16H14O4Cl2		
*	Diclofop-methyl	51338-27-3	20.069		C14H11O2Cl2	281.013061	281.013610
*	Diclofop-methyl	51338-27-3	20.069		C12H8O2Cl2	253.989586	253.990135
*	Diclofop-methyl	51338-27-3	20.069		C12H7O2Cl2	252.981761	252.982310
**	Difenoxuron	14214-32-5	13.868	286.13174	C16H18N2O3		
**	Difenoxuron	14214-32-5	13.868		C14H11NO3	241.073345	241.073893
**	Difenoxuron	14214-32-5	13.868		C13H8NO3	226.049870	226.050418
**	Difenoxuron	14214-32-5	13.868		C12H8NO2	198.054955	198.055504
**	Dimefuron	34205-21-5	15.084	338.11457	C15H19ClN4O3		
**	Dimefuron	34205-21-5	15.084		C13H12ClN3O3	293.056170	293.056719
**	Dimefuron	34205-21-5	15.084		C12H12ClN3O	249.066341	249.066890
**	Dimefuron	34205-21-5	15.084		C7H3(37Cl)N2O	167.989892	167.990440
**	Dimefuron	34205-21-5	15.084		C7H3ClN2O	165.992842	165.993390
**	Dimefuron	34205-21-5	15.084		C7H3N2O	131.023989	131.024538
**	Dimethachlor	50563-36-5	12.480	255.10261	C13H18ClNO2		
**	Dimethachlor	50563-36-5	12.480		C10H12ClNO	197.060193	197.060742
**	Dimethachlor	50563-36-5	12.480		C9H12N	134.096426	134.096974
**	Dimethachlor	50563-36-5	12.480		C9H10N	132.080776	132.081324
**	Dimethachlor	50563-36-5	12.480		C9H10NO	148.075690	148.076239
	Dimethenamid	87674-68-8	12.591	275.07470	C12H18NO2SCl		
	Dimethenamid	87674-68-8	12.591		C10H13NOSCl	230.040089	230.040637
	Dimethenamid	87674-68-8	12.591		C8H10NOSCl	203.016614	203.017162
	Dimethenamid	87674-68-8	12.591		C8H12NS	154.068496	154.069045
**	Dinoseb	88-85-7	11.655	240.07462	C10H12N2O5		
**	Dinoseb	88-85-7	11.655		C8H7N2O5	211.034948	211.035496
**	Dinoseb	88-85-7	11.655		C8H5NO3	163.026394	163.026943
**	Dinoseb	88-85-7	11.655		C8H5NO2	147.031480	147.032028
**	Dioxacarb	6988-21-2	12.343	223.08446	C11H13NO4		
**	Dioxacarb	6988-21-2	12.343		C9H10O3	166.062446	166.062994

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
**	Dioxacarb	6988-21-2	12.343		C9H9O3	165.054621	165.055169
**	Dioxacarb	6988-21-2	12.343		C7H6O2	122.036231	122.036779
**	Dioxacarb	6988-21-2	12.343		C7H5O2	121.028406	121.028954
*	Diphenamid	957-51-7	14.510	239.13100	C16H17NO		
*	Diphenamid	957-51-7	14.510		C13H11	167.085527	167.086075
*	Diphenamid	957-51-7	14.510		C13H9	165.069877	165.070425
*	Diphenamid	957-51-7	14.510		C12H8	152.062052	152.062600
*	Diphenamid	957-51-7	14.510		C3H6NO	72.044390	72.044939
	Dithiopyr	97886-45-8	13.400	401.05430	C15H16NO2S2F5		
	Dithiopyr	97886-45-8	13.400		C14H13NO2SF5	354.058167	354.058715
	Dithiopyr	97886-45-8	13.400		C13H9NO2F5	306.054796	306.055345
	Dithiopyr	97886-45-8	13.400		C13H8NO2F4	286.048568	286.049116
*	Dodemorph	1593-77-7	14.410	281.27190	C18H35NO		
*	Dodemorph	1593-77-7	14.410		C15H28NO	238.216541	238.217090
*	Dodemorph	1593-77-7	14.410		C9H16NO	154.122641	154.123189
*	Dodemorph	1593-77-7	14.410		C8H15NO	141.114816	141.115364
**	Edifenphos	17109-49-8	19.191	310.02511	C14H15O2PS2		
**	Edifenphos	17109-49-8	19.191		C6H6O2PS	172.982063	172.982612
**	Edifenphos	17109-49-8	19.191		C8H10S	138.049773	138.050321
**	Edifenphos	17109-49-8	19.191		C6H6S	110.018473	110.019021
**	Edifenphos	17109-49-8	19.191		C6H5S	109.010648	109.011196
**	Esprocarb	85785-20-2	13.537	265.15004	C15H23NOS		
**	Esprocarb	85785-20-2	13.537		C12H16NOS	222.094712	222.095260
**	Esprocarb	85785-20-2	13.537		C11H16N	162.127726	162.128275
**	Esprocarb	85785-20-2	13.537		C7H7	91.054227	91.054775
*	Etaconazole Peak 1	60207-93-4	18.177	327.05410	C14H15N3O2Cl2		
*	Etaconazole Peak 1	60207-93-4	18.177		C11H11O2Cl2	245.013061	245.013610
*	Etaconazole Peak 1	60207-93-4	18.177		C7H5O2Cl2	190.966111	190.966660
*	Etaconazole Peak 1	60207-93-4	18.177		C7H3OCl2	172.955547	172.956095
**	Ethalfuralin	55283-68-6	9.895	333.09364	C13H14F3N3O4		
**	Ethalfuralin	55283-68-6	9.895		C13H13F3N3O3	316.090352	316.090901
**	Ethalfuralin	55283-68-6	9.895		C10H9F3N3O4	292.053967	292.054515
**	Ethalfuralin	55283-68-6	9.895		C10H9F3N3O3	276.059052	276.059601
**	Ethalfuralin	55283-68-6	9.895		C8H5F3N3O4	264.022667	264.023215
**	Etoxazole	153233-91-1	21.549	359.16969	C21H23F2NO2		
**	Etoxazole	153233-91-1	21.549		C19H18F2NO2	330.130012	330.130560
**	Etoxazole	153233-91-1	21.549		C18H16F2NO	300.119447	300.119996
**	Etoxazole	153233-91-1	21.549		C13H18NO	204.138291	204.138839
**	Etoxazole	153233-91-1	21.549		C13H15O	187.111742	187.112290

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
**	Etoazole	153233-91-1	21.549		C7H3F2O	141.014648	141.015196
	Fenobucarb (Baycarb)	3766-81-2	9.529	207.12590	C12H17NO2		
	Fenobucarb (Baycarb)	3766-81-2	9.529		C10H14O	150.103916	150.104465
	Fenobucarb (Baycarb)	3766-81-2	9.529		C8H9O	121.064791	121.065340
	Fenoprop-methylester	4841-20-7	11.069	281.96170	C10H9O3Cl3		
	Fenoprop-methylester	4841-20-7	11.069		C8H6OCl3	222.947874	222.948423
	Fenoprop-methylester	4841-20-7	11.069		C6H3OCl3	195.924399	195.924948
**	Fenothiocarb	62850-32-2	15.916	253.11365	C13H19NO2S		
**	Fenothiocarb	62850-32-2	15.916		C7H14NOS	160.079061	160.079610
**	Fenothiocarb	62850-32-2	15.916		C6H6O	94.041316	94.041865
**	Fenothiocarb	62850-32-2	15.916		C4H8S	88.034123	88.034671
**	Fenothiocarb	62850-32-2	15.916		C3H6NO	72.044390	72.044939
**	Fenoxaprop-ethyl	66441-23-4	23.896	361.07170	C18H16ClNO5		
**	Fenoxaprop-ethyl	66441-23-4	23.896		C18H16ClNO5	361.071152	361.071700
**	Fenoxaprop-ethyl	66441-23-4	23.896		C15H11(37Cl)NO3	290.039247	290.039796
**	Fenoxaprop-ethyl	66441-23-4	23.896		C15H11ClNO3	288.042197	288.042746
**	Fenoxaprop-ethyl	66441-23-4	23.896		C13H8ClNO3	261.018722	261.019271
**	Fenpiclonil	74738-17-3	20.707	235.99080	C11H6Cl2N2		
**	Fenpiclonil	74738-17-3	20.707		C11H6Cl(37Cl)N2	237.987305	237.987853
**	Fenpiclonil	74738-17-3	20.707		C11H6Cl2N2	235.990255	235.990804
**	Fenpiclonil	74738-17-3	20.707		C11H6ClN2	201.021402	201.021951
**	Fenpiclonil	74738-17-3	20.707		C10H5ClN	174.010503	174.011052
*	Fensulfothion	115-90-2	18.030	308.03060	C11H17O4PS2		
*	Fensulfothion	115-90-2	18.030		C10H14O4PS2	293.006563	293.007112
*	Fensulfothion	115-90-2	18.030		C11H17O3PS2	292.035124	292.035672
*	Fensulfothion	115-90-2	18.030		C9H13O3PS2	264.003824	264.004372
*	Fensulfothion	115-90-2	18.030		C7H9O3PS2	235.972523	235.973072
*	Fensulfothion	115-90-2	18.030		C7H8S2	156.006193	156.006742
*	Fensulfothion	115-90-2	18.030		C6H5O2S	141.000476	141.001025
*	Fensulfothion	115-90-2	18.030		C3H9O2PS	140.005538	140.006087
*	Fensulfothion-sulfon	14255-72-2	18.655	324.02550	C11H17O5PS2		
*	Fensulfothion-sulfon	14255-72-2	18.655		C7H8O4PS	218.987542	218.988091
*	Fensulfothion-sulfon	14255-72-2	18.655		C7H8O2S2	187.996022	187.996571
*	Fensulfothion-sulfon	14255-72-2	18.655		C6H5O3S	156.995391	156.995940
**	Fonicamid	158062-67-0	9.351	229.04630	C9H6F3N3O		
**	Fonicamid	158062-67-0	9.351		C7H3F3NO	174.016125	174.016673
**	Fonicamid	158062-67-0	9.351		C7H3F3N2	172.024284	172.024833
**	Fonicamid	158062-67-0	9.351		C6H3F3N	146.021210	146.021759
	Fluchloralin	33245-39-5	11.608	355.05470	C12H13N3O4ClF3		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
	Fluchloralin	33245-39-5	11.608		C10H8N3O4CIF3	326.014995	326.015543
	Fluchloralin	33245-39-5	11.608		C11H11N3O4F3	306.069617	306.070166
	Fluchloralin	33245-39-5	11.608		C8H5N3O4F3	264.022667	264.023215
**	Flumioxazin	103361-09-7	27.936	354.10159	C19H15FN2O4		
**	Flumioxazin	103361-09-7	27.936		C9H15F2N7O6	355.104639	355.105188
**	Flumioxazin	103361-09-7	27.936		C19H15FN2O4	354.101037	354.101585
**	Flumioxazin	103361-09-7	27.936		C18H15FN2O3	326.106122	326.106671
**	Flumioxazin	103361-09-7	27.936		C15H12FN2O3	287.082647	287.083195
**	Flumioxazin	103361-09-7	27.936		C13H8FN2O3	259.051347	259.051895
**	Flumioxazin	103361-09-7	27.936		C13H6N	176.049476	176.050024
**	Fluometuron	2164-17-2	9.681	232.08235	C10H11F3N2O		
**	Fluometuron	2164-17-2	9.681		C10H11F3N2O	232.081799	232.082348
**	Fluometuron	2164-17-2	9.681		C8H4F3NO	187.023950	187.024498
**	Fluometuron	2164-17-2	9.681		C7H4F3N	159.029035	159.029584
**	Fluometuron	2164-17-2	9.681		C3H6NO	72.044390	72.044939
	Fluoroglycofen-ethyl	77501-90-7	23.716	447.03330	C18H13NO7CIF3		
	Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7NO4CIF3	345.001021	345.001570
	Fluoroglycofen-ethyl	77501-90-7	23.716		C14H6NO4CIF3	343.993196	343.993745
	Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7O3CIF3	315.003033	315.003581
	Fluoroglycofen-ethyl	77501-90-7	23.716		C13H7NO2CIF3	301.011192	301.011741
	Fluoroglycofen-ethyl	77501-90-7	23.716		C8H3O2CIF3	222.976818	222.977367
	Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7O2	207.044056	207.044604
	Fluridone	59756-60-4	27.432	329.10270	C19H14NOF3		
	Fluridone	59756-60-4	27.432		C19H13NOF3	328.094375	328.094924
	Flurprimidol	56425-91-3	12.430	312.10860	C15H15N2O2F3		
	Flurprimidol	56425-91-3	12.430		C12H8N2O2F3	269.053239	269.053787
	Flurprimidol	56425-91-3	12.430		C8H4O2F3	189.015790	189.016339
	Flurprimidol	56425-91-3	12.430		C5H3N2O	107.023989	107.024538
**	Furalaxyl	57646-30-7	15.448	301.13141	C17H19NO4		
**	Furalaxyl	57646-30-7	15.448		C15H16NO2	242.117555	242.118104
**	Furalaxyl	57646-30-7	15.448		C8H10NO2	152.070605	152.071154
**	Furalaxyl	57646-30-7	15.448		C5H3O2	95.012756	95.013304
**	Furathiocarb	65907-30-4	22.199	382.15624	C18H26N2O5S		
**	Furathiocarb	65907-30-4	22.199		C10H10O2S	194.039602	194.040151
**	Furathiocarb	65907-30-4	22.199		C10H12O2	164.083181	164.083730
**	Furathiocarb	65907-30-4	22.199		C10H11O2	163.075356	163.075905
**	Furathiocarb	65907-30-4	22.199		C9H11O	135.080441	135.080990
**	Furathiocarb	65907-30-4	22.199		C7OH7	107.049141	107.049690
**	Furilazole	121776-33-8	10.800	277.02725	C11H13Cl2NO3		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
**	Furilazole	121776-33-8	10.800		C10H10Cl2NO3	262.003225	262.003774
**	Furilazole	121776-33-8	10.800		C8H8Cl(37Cl)NO2	221.989710	221.990259
**	Furilazole	121776-33-8	10.800		C8H8Cl2NO2	219.992660	219.993209
**	Furilazole	121776-33-8	10.800		C6H9ClNO	146.036718	146.037267
**	Hexaflumuron	86479-06-3	8.172	459.98162	C16H8Cl2F6N2O3		
**	Hexaflumuron	86479-06-3	8.172		C9H3Cl(37Cl)F4NO2	304.944198	304.944746
**	Hexaflumuron	86479-06-3	8.172		C9H3Cl2F4NO2	302.947148	302.947697
**	Hexaflumuron	86479-06-3	8.172		C7H2Cl(37Cl)NO2	203.942760	203.943309
**	Hexaflumuron	86479-06-3	8.172		C7H2Cl2NO2	201.945710	201.946259
**	Hexaflumuron	86479-06-3	8.172		C6H2Cl(37Cl)NO	175.947845	175.948394
**	Hexaflumuron	86479-06-3	8.172		C6H2Cl2NO	173.950795	173.951344
	Imibenconazole	86598-92-7	30.864	409.99270	C17H13N4SCl3		
	Imibenconazole	86598-92-7	30.864		C17H13N4SCl2	375.023249	375.023798
	Imibenconazole	86598-92-7	30.864		C10H7N4Cl2	253.004228	253.004777
	Imibenconazole	86598-92-7	30.864		C7H3NCl2	170.963706	170.964255
	Imibenconazole	86598-92-7	30.864		C7H6Cl	125.015254	125.015803
*	Iprobenfos	26087-47-8	11.990	288.09490	C13H21O3PS		
*	Iprobenfos	26087-47-8	11.990		C7H9O3PS	204.000453	204.001001
*	Iprobenfos	26087-47-8	11.990		C7H7	91.054227	91.054775
*	Isazofos (Miral)	42509-80-8	11.770	313.04170	C9H17N3O3PSCI		
*	Isazofos (Miral)	42509-80-8	11.770		C7H13N3O3PSCI	285.009828	285.010376
*	Isazofos (Miral)	42509-80-8	11.770		C5H9N3O3PSCI	256.978527	256.979076
*	Isazofos (Miral)	42509-80-8	11.770		C5H9N3OCl	162.042866	162.043415
*	Isazofos (Miral)	42509-80-8	11.770		C5H8N3OCl	161.035041	161.035590
*	Isazofos (Miral)	42509-80-8	11.770		C2H2N3OCl	118.988091	118.988639
*	isocarbamid (Azolamide)	30979-48-7	11.173	185.11640	C8H15N3O2		
*	isocarbamid (Azolamide)	30979-48-7	11.173		C5H8N3O2	142.061103	142.061652
*	isocarbamid (Azolamide)	30979-48-7	11.173		C4H8N3O2	130.061103	130.061652
*	isocarbamid (Azolamide)	30979-48-7	11.173		C5H8NO	98.060040	98.060589
*	Isocarbophos (Isocarbofos)	24353-61-5	14.305	289.05380	C11H16NO4PS		
*	Isocarbophos (Isocarbofos)	24353-61-5	14.305		C8H9NO3PS	230.003527	230.004075
*	Isocarbophos (Isocarbofos)	24353-61-5	14.305		C7H4OS	135.997737	135.998285
*	Isocarbophos (Isocarbofos)	24353-61-5	14.305		C7H5O2	121.028406	121.028954
*	Isocarbophos (Isocarbofos)	24353-61-5	14.305		C7H4O2	120.020581	120.021129
**	Isodrin	465-73-6	14.700	361.87572	C12H8Cl6		
**	Isodrin	465-73-6	14.700		C7H2Cl3(37Cl)2	264.853465	264.854013
**	Isodrin	465-73-6	14.700		C7H2Cl4(37Cl)	262.856415	262.856963
**	Isodrin	465-73-6	14.700		C7H2Cl5	260.859365	260.859913
**	Isodrin	465-73-6	14.700		C7H4Cl(37Cl)2	196.931409	196.931958



	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
**	Isodrin	465-73-6	14.700		C7H4Cl2(37Cl)	194.934359	194.934908
**	Isodrin	465-73-6	14.700		C7H4Cl3	192.937310	192.937858
**	Isoxaben	82558-50-7	23.698	332.17361	C18H24N2O4		
**	Isoxaben	82558-50-7	23.698		C9H9O3	165.054621	165.055169
**	Isoxaben	82558-50-7	23.698		C8O3H6	150.031145	150.031694
**	Isoxaben	82558-50-7	23.698		C6O2H3	107.012756	107.013304
**	Isoxathion	18854-01-8	17.501	313.05377	C13H16NO4PS		
**	Isoxathion	18854-01-8	17.501		C9H7NOS	177.024286	177.024835
**	Isoxathion	18854-01-8	17.501		C8H4NO	130.028740	130.029289
**	Isoxathion	18854-01-8	17.501		C7H5O	105.033491	105.034040
**	Lenacil	2164-8-1	19.295	234.13683	C13H18N2O2		
**	Lenacil	2164-8-1	19.295		C7H9N2O2	153.065854	153.066403
**	Lenacil	2164-8-1	19.295		C7NO2H6	136.039305	136.039853
**	Leptophos	21609-90-5	22.387	409.86996	C13H10BrCl2O2PS		
**	Leptophos	21609-90-5	22.387		C13H10(81Br)(37Cl)O2PS	378.895557	378.896105
**	Leptophos	21609-90-5	22.387		C13H10(81Br)ClO2PS	376.898507	376.899055
**	Leptophos	21609-90-5	22.387		C13H10BrClO2PS	374.900553	374.901102
**	Leptophos	21609-90-5	22.387		CH8CIP5S	241.871783	241.872332
**	Leptophos	21609-90-5	22.387		C7H8OPS	171.002799	171.003348
**	Leptophos	21609-90-5	22.387		C7H8O2P	155.025643	155.026191
	Lethane 384	112-56-1	8.822	203.09800	C9H17NO2S		
	Lethane 384	112-56-1	8.822		C5H8NOS	130.032111	130.032660
	Lethane 384	112-56-1	8.822		C5H9O2	101.059706	101.060255
	Lethane 384	112-56-1	8.822		C3H4NS	86.005896	86.006445
	Lethane 384	112-56-1	8.822		C2H4S	60.002822	60.003371
	Lethane 384	112-56-1	8.822		C4H9	57.069877	57.070425
*	Mefenpyr-diethyl	135590-91-9	20.590	372.06440	C16H18N2O4Cl2		
*	Mefenpyr-diethyl	135590-91-9	20.590		C13H13N2O2Cl2	299.034859	299.035408
*	Mefenpyr-diethyl	135590-91-9	20.590		C11H7N2OCl2	252.992995	252.993543
*	Mefenpyr-diethyl	135590-91-9	20.590		C10H9N2Cl2	227.013730	227.014279
	Mefluidide	53780-34-0	20.590	310.05990	C11H13N2O3SF3		
	Mefluidide	53780-34-0	20.590		C9H11N2O2SF3	268.048784	268.049333
	Mefluidide	53780-34-0	20.590		C10H13N2O	177.102239	177.102788
	Mefluidide	53780-34-0	20.590		C8H11N2	135.091675	135.092223
**	Mepronil	55814-41-0	18.630	269.14158	C17H19NO2		
**	Mepronil	55814-41-0	18.630		C17H19NO2	269.141030	269.141579
**	Mepronil	55814-41-0	18.630		C14H10O2	210.067531	210.068080
**	Mepronil	55814-41-0	18.630		C8H7O	119.049141	119.049690
**	Mepronil	55814-41-0	18.630		C7H7	91.054227	91.054775

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
	Methabenzthiazuron	18691-97-9	10.080	221.06230	C10H11N3OS		
	Methabenzthiazuron	18691-97-9	10.080		C8H8N2S	164.040270	164.040819
	Methabenzthiazuron	18691-97-9	10.080		C8H7N2S	163.032445	163.032994
	Methabenzthiazuron	18691-97-9	10.080		C7H6NS	136.021546	136.022095
	Methabenzthiazuron	18691-97-9	10.080		C7H5NS	135.013721	135.014270
	Methabenzthiazuron	18691-97-9	10.080		C6H4S	108.002822	108.003371
**	Methoprene	40596-69-8	15.490	310.25079	C19H34O3		
**	Methoprene	40596-69-8	15.490		C6H7O2	111.044056	111.044604
**	Methoprene	40596-69-8	15.490		C8H13	109.101177	109.101725
**	Methoprene	40596-69-8	15.490		C8H11	107.085527	107.086075
**	Methoprene	40596-69-8	15.490		C7H7	91.054227	91.054775
**	Methoprene	40596-69-8	15.490		C6H9	81.069877	81.070425
**	Methoprene	40596-69-8	15.490		C4H9O	73.064791	73.065340
**	Metolachlor	51218-45-2	13.912	283.13391	C15H22ClNO2		
**	Metolachlor	51218-45-2	13.912		C13H17ClNO	238.099318	238.099867
**	Metolachlor	51218-45-2	13.912		C11H16N	162.127726	162.128275
**	Metolachlor	51218-45-2	13.912		C10NH12	146.096426	146.096974
**	Monuron	150-68-5	6.443	198.05599	C9H11ClN2O		
**	Monuron	150-68-5	6.443		C7H4(37Cl)NO	154.994643	154.995191
**	Monuron	150-68-5	6.443		C7H4ClNO	152.997593	152.998141
**	Monuron	150-68-5	6.443		C6H4ClN	125.002678	125.003227
**	Monuron	150-68-5	6.443		C6H4N	90.033826	90.034374
**	Nicotine	54-11-5	7.641	162.11570	C10H14N2		
**	Nicotine	54-11-5	7.641		C10H13N2	161.107325	161.107873
**	Nicotine	54-11-5	7.641		C8H9N2	133.076025	133.076573
**	Nicotine	54-11-5	7.641		C5H10N	84.080776	84.081324
**	Nitrofen	1836-75-5	17.522	282.98030	C12H7Cl2NO3		
**	Nitrofen	1836-75-5	17.522		C12H7Cl(37Cl)NO3	284.976800	284.977348
**	Nitrofen	1836-75-5	17.522		C12H7Cl2NO3	282.979750	282.980298
**	Nitrofen	1836-75-5	17.522		C12H7Cl2O2	252.981761	252.982310
**	Nitrofen	1836-75-5	17.522		C12H7(37Cl)O	204.015044	204.015592
**	Nitrofen	1836-75-5	17.522		C12H7ClO	202.017994	202.018543
**	Nitrofen	1836-75-5	17.522		C10H7Cl	162.023079	162.023628
**	Nitrofen	1836-75-5	17.522		C11H7	139.054227	139.054775
	Nitrothal-isopropyl	10552-74-6	14.330	295.10560	C14H17NO6		
	Nitrothal-isopropyl	10552-74-6	14.330		C11H12NO6	254.065914	254.066462
	Nitrothal-isopropyl	10552-74-6	14.330		C11H10NO5	236.055349	236.055897
	Nitrothal-isopropyl	10552-74-6	14.330		C8H6NO6	212.018963	212.019512
	Nitrothal-isopropyl	10552-74-6	14.330		C8H4NO5	194.008399	194.008947

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
**	Novaluron	116714-46-6	7.782	492.01231	C17H9CIF8N2O4		
**	Novaluron	116714-46-6	7.782		C6H6CIF8NO2	310.995383	310.995932
**	Novaluron	116714-46-6	7.782		C9H6CIF6NO2	308.998577	308.999125
**	Novaluron	116714-46-6	7.782		C6H5(37Cl)NO	144.002468	144.003016
**	Novaluron	116714-46-6	7.782		C6H5CINO	142.005418	142.005966
**	Novaluron	116714-46-6	7.782		C5H5CIN	114.010503	114.011052
	O.O.O-Triethylphosphorothioate	126-68-1	6.596	198.04800	C6H15O3PS		
	O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H8O3PS	142.992628	142.993176
	O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H7O2PS	125.989888	125.990437
	O.O.O-Triethylphosphorothioate	126-68-1	6.596		C4H10O2P	121.041292	121.041841
	O.O.O-Triethylphosphorothioate	126-68-1	6.596		H4O3PS	114.961328	114.961876
	O.O.O-Triethylphosphorothioate	126-68-1	6.596		H3O3PS	113.953503	113.954051
	O.O.O-Triethylphosphorothioate	126-68-1	6.596		H2O2PS	96.950763	96.951312
	O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H6O2P	93.009992	93.010541
	Oryzalin	19044-88-3	13.910	346.09470	C12H18N4O6S		
	Oryzalin	19044-88-3	13.910		C10H13N4O6S	317.055031	317.055580
	Oryzalin	19044-88-3	13.910		C10H13N4O5S	301.060117	301.060665
	Oryzalin	19044-88-3	13.910		C7H7N4O6S	275.008081	275.008630
	Oryzalin	19044-88-3	13.910		C7H4N3O6S	257.981532	257.982081
	Pentanochlor (Sloan)	2307-68-8	13.560	239.10770	C13H18NOCl		
	Pentanochlor (Sloan)	2307-68-8	13.560		C10H12NOCl	197.060193	197.060742
	Pentanochlor (Sloan)	2307-68-8	13.560		C7H8NCl	141.033978	141.034527
	Pethoxamid	106700-29-2	15.540	295.13390	C16H22NO2Cl		
	Pethoxamid	106700-29-2	15.540		C15H19NO2Cl	280.109883	280.110432
	Pethoxamid	106700-29-2	15.540		C16H22NO2	260.164505	260.165054
	Pethoxamid	106700-29-2	15.540		C13H15NOCl	236.083668	236.084217
	Pethoxamid	106700-29-2	15.540		C13H14NO2	216.101905	216.102454
	Pethoxamid	106700-29-2	15.540		C10H11	131.085527	131.086075
	Plifenate (Penfenate)	21757-82-4	12.769	333.88890	C10H7O2Cl5		
	Plifenate (Penfenate)	21757-82-4	12.769		C8H4Cl4	239.906162	239.906711
	Plifenate (Penfenate)	21757-82-4	12.769		C9H7O2Cl2	216.981761	216.982310
	Plifenate (Penfenate)	21757-82-4	12.769		C7H3OCl2	172.955547	172.956095
	Plifenate (Penfenate)	21757-82-4	12.769		C8H4Cl2	169.968457	169.969006
*	Pretilachlor	51218-49-6	16.810	311.16520	C17H26NO2Cl		
*	Pretilachlor	51218-49-6	16.810		C16H24NO2	262.180155	262.180704
*	Pretilachlor	51218-49-6	16.810		C13H17NOCl	238.099318	238.099867
*	Pretilachlor	51218-49-6	16.810		C12H16NOCl	225.091493	225.092042
*	Pretilachlor	51218-49-6	16.810		C13H16NO	202.122641	202.123189
*	Pretilachlor	51218-49-6	16.810		C11H14NO	176.106990	176.107539

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
*	Pretilachlor	51218-49-6	16.810		C11H16N	162.127726	162.128275
	Profluralin	26399-36-0	11.305	347.10930	C14H16N3O4F3		
	Profluralin	26399-36-0	11.305		C14H15N3O3F3	330.106002	330.106551
	Profluralin	26399-36-0	11.305		C12H11N3O4F3	318.069617	318.070166
	Propachlor	1918-16-7	9.609	211.07640	C11H14NOCl		
	Propachlor	1918-16-7	9.609		C11H14NO	176.106990	176.107539
	Propachlor	1918-16-7	9.609		C8H8NOCl	169.028893	169.029442
	Propachlor	1918-16-7	9.609		C8H10N	120.080776	120.081324
	Propachlor	1918-16-7	9.609		C7H6NO	120.044390	120.044939
*	Propaphos	7292-16-2	15.740	304.08980	C13H21O4PS		
*	Propaphos	7292-16-2	15.740		C10H15O4PS	262.042318	262.042866
*	Propaphos	7292-16-2	15.740		C7H9O4PS	219.995367	219.995916
*	Propaphos	7292-16-2	15.740		C7H7O3PS	201.984803	201.985351
*	Propaphos	7292-16-2	15.740		C7H8OS	140.029037	140.029586
*	Rabenzazole	40341-04-6	14.168	212.10620	C12H12N4		
*	Rabenzazole	40341-04-6	14.168		C12H9N3	195.079099	195.079647
*	Rabenzazole	40341-04-6	14.168		C10H8N3	170.071274	170.071822
*	Rabenzazole	40341-04-6	14.168		C7H6N2	118.052550	118.053098
	Resmethrin	10453-86-8	20.208	338.18820	C22H26O3		
	Resmethrin	10453-86-8	20.208		C12H11O	171.080441	171.080990
	Resmethrin	10453-86-8	20.208		C11H11	143.085527	143.086075
	Resmethrin	10453-86-8	20.208		C10H8	128.062052	128.062600
	Resmethrin	10453-86-8	20.208		C9H15	123.116827	123.117375
*	Schradan	152-16-9	10.886	286.13240	C8H24N4O3P2		
*	Schradan	152-16-9	10.886		C6H19N3O3P2	243.089616	243.090165
*	Schradan	152-16-9	10.886		C4H13N2O3P2	199.039592	199.040140
*	Schradan	152-16-9	10.886		C4H14N2O2P	153.078741	153.079289
*	Schradan	152-16-9	10.886		C4H12N2OP	135.068176	135.068725
*	Tebupirimphos (Tebupirimfos)	96182-53-5	12.047	318.11670	C13H23N2O3PS		
*	Tebupirimphos (Tebupirimfos)	96182-53-5	12.047		C10H17N2O3PS	276.069201	276.069750
*	Tebupirimphos (Tebupirimfos)	96182-53-5	12.047		C9H14N2O3PS	261.045726	261.046275
*	Tebupirimphos (Tebupirimfos)	96182-53-5	12.047		C7H11N2O3PS	234.022251	234.022799
*	Tebupirimphos (Tebupirimfos)	96182-53-5	12.047		C8H12N2O	152.094414	152.094963
*	Tebupirimphos (Tebupirimfos)	96182-53-5	12.047		C7H9N2O	137.070939	137.071488
*	Terbufos	13071-79-9	11.310	288.04410	C9H21O2PS3		
*	Terbufos	13071-79-9	11.310		C5H12O2PS3	230.973155	230.973703
*	Terbufos	13071-79-9	11.310		C4H10O2PS	153.013363	153.013912
*	Terbufos	13071-79-9	11.310		H2O2PS	96.950763	96.951312
	Thenylchlor	96491-05-3	19.961	323.07470	C16H18NO2SCI		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
	Thenylchlor	96491-05-3	19.961		C16H18NO2S	288.105276	288.105825
	Thenylchlor	96491-05-3	19.961		C7H6NO2S	168.011376	168.011924
	Thenylchlor	96491-05-3	19.961		C7H9OS	141.036862	141.037411
	Thenylchlor	96491-05-3	19.961		C9H10N	132.080776	132.081324
	Thenylchlor	96491-05-3	19.961		C6H7OS	127.021212	127.021761
	Tiocarbazil (Drepamon)	36756-79-3	14.252	279.16570	C16H25NOS		
	Tiocarbazil (Drepamon)	36756-79-3	14.252		C9H18NO	156.138291	156.138839
	Tiocarbazil (Drepamon)	36756-79-3	14.252		C5H10NO	100.075690	100.076239
	Tiocarbazil (Drepamon)	36756-79-3	14.252		C7H7	91.054227	91.054775
*	Tribufos	78-48-8	16.820	314.09620	C12H27OPS3		
*	Tribufos	78-48-8	16.820		C8H19OPS3	258.033015	258.033564
*	Tribufos	78-48-8	16.820		C8H19OPS2	226.060945	226.061493
*	Tribufos	78-48-8	16.820		C4H11OPS3	201.970415	201.970964
*	Tribufos	78-48-8	16.820		C4H10OPS2	168.990519	168.991068
*	Tribufos	78-48-8	16.820		H4OPS3	146.915640	146.916188
	Triclopyr-methylester (methyl)	60825-26-5	11.300	268.94130	C8H6NO3Cl3		
	Triclopyr-methylester (methyl)	60825-26-5	11.300		C6H3NOCl3	209.927473	209.928022
	Triclopyr-methylester (methyl)	60825-26-5	11.300		C5HNCl3	179.916909	179.917457
	XMC / 3,5-Xylyl methylcarbamate	2655-14-3	6.668	179.09460	C10H13NO2		
	XMC / 3,5-Xylyl methylcarbamate	2655-14-3	6.668		C8H10O	122.072616	122.073165
	XMC / 3,5-Xylyl methylcarbamate	2655-14-3	6.668		C7H7O	107.049141	107.049690