

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

Exact Mass Pesticide Database for use by GC-HRMS

Report 5

Elena Hakme

Mette Erecius Poulsen

January 2020

CONTENT:

<i>1. Introduction</i>	3
<i>2. Analytical conditions for GC-HRMS</i>	3
<i>3. Exact mass database of 233 pesticides for use by GC-HRMS</i>	5

1. Introduction

This report describes an exact mass database of 233 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 2019 with exact mass fragments of 30 pesticides and together with the pesticides included in the database in 2014, 2015 and 2017, 2018, the total number of pesticides with exact mass fragments is now 233. The analysis done till 2018 were performed on GC-ToF-MS. The 30 new compounds added in 2019 were injected on GC-Orbitrap-MS.

The intention is to use the database in conjunction with Agilent MassHunter software using ToF-MS. 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 233 pesticides and used that in an analysis of a pesticide mixture and for pesticide screening.

Moreover, this database was transposed into the GC-Orbitrap Database for pesticide screening on GC-Orbitrap-MS using the Thermo Trace Finder Software.

Using two different HRMS systems with different oven temperature programs, result in compounds eluting at different retention time (maximum of ± 1 min difference). Therefore, the retention time of the 30 new compounds analysed on GC-Orbitrap-MS are slightly adjusted before their addition to the PCDL. Same for the 230 compounds transposed from ToF-MS to the Orbitrap-MS. Mixtures of standards were injected on the Orbitrap-MS and retention times were collected/adjusted. Retention time parameter is one of the main important criteria for identification in screening, whether working on Agilent MassHunter software or on Thermo Trace Finder software for target screening.

2. Analytical conditions for GC-HRMS

GC-ToF-MS

GC conditions

Inlet: PTV

Inlet temperature: 60 °C

Injection volume: 5 μ l

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 μ m x 0.25 μ m

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 and held for 12 min. Total run time 31.8 min.

Mass Spectrometer conditions

Ion source temperature: 230 °C

Transfer line temperature: 300 °C

Ionization: electron impact

Electron energy: 70 eV

Sampling rate: 4 GHz

Full Scan Mass range: 50 - 500 AMU

GC-Orbitrap-MS

GC conditions

Inlet: PTV

Inlet temperature: 70 °C

Injection volume: 1 μ l

Carrier gas: Helium

Carrier flow: 1.2 ml/min

Columns: TG-5SILMS 30mx0.25mmx0.25 μ m

Oven temperature program: 60 °C in 1.5 min., 25 °C/min. to 90 °C, hold in 1.5 min, 25 °C/min. to 180 °C, 5 °C/min. to 280 °C, and up to 300°C at a rate of 10°C/min, Total runtime 32 min.

Mass Spectrometer conditions

Ion source temperature: 280 °C

Transfer line temperature: 280 °C

Ionization: electron impact

Electron energy: 70 eV

Resolution: 60 000

AGC target: 1e6

Full Scan Mass range: 50 - 500 AMU

3. Exact mass database of 233 pesticides for use by GC-HRMS

53 compounds in 2014, 28 compounds added in 2015, 52 compounds added in 2017, 70 compounds added in 2018, and 30 compounds added in 2019.

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2018	1-Naphthylacetamide	86-86-2	13.2	185.084064	C12H11NO		
2018	1-Naphthylacetamide	86-86-2	13.2		C12H11NO	185.0835154	185.084064
2018	1-Naphthylacetamide	86-86-2	13.2		C9H7	115.0542264	115.054775
2018	1-Naphthylacetamide	86-86-2	13.2		C11H10	142.0777014	142.07825
2018	1-Naphthylacetic_acid	86-87-3	13.3	186.06808	C12H10O2		
2018	1-Naphthylacetic_acid	86-87-3	13.3		C11H9	141.0698764	141.070425
2018	1-Naphthylacetic_acid	86-87-3	13.3		C9H7	115.0542264	115.054775
2018	1-Naphthylacetic_acid	86-87-3	13.3		C11H7	139.0542264	139.054775
2019	2-3-4-6-Tetrachlorophenol	58-90-2	10	229.885977	C6H2Cl4O		
2019	2-3-4-6-Tetrachlorophenol	58-90-2	10		C6H2Cl4O	229.8854284	229.885977
2019	2-3-4-6-Tetrachlorophenol	58-90-2	10		C6H2Cl2(37Cl)2O	233.8795284	233.880077
2019	2-3-4-6-Tetrachlorophenol	58-90-2	10		C6H2Cl3(37Cl)O	231.8824784	231.883027
2019	2-3-4-6-Tetrachlorophenol	58-90-2	10		C6HCl3O	193.9087504	193.909299
2019	2-4-6-Trichlorophenol	88-06-2	8.44	195.924949	C6H3Cl3O		
2019	2-4-6-Trichlorophenol	88-06-2	8.44		C6H3Cl3O	195.9244004	195.924949
2019	2-4-6-Trichlorophenol	88-06-2	8.44		C6H2Cl2O	159.9477224	159.948271
2019	2-4-6-Trichlorophenol	88-06-2	8.44		C5H2Cl2	131.9528064	131.953355
2014	2,4-D Butyl ester	94-80-4	12.607	276.032	C12H14O3Cl2		
2014	2,4-D Butyl ester	94-80-4	12.607		C8H6O3Cl2	219.968851	219.969399
2014	2,4-D Butyl ester	94-80-4	12.607		C8H6O3Cl	184.999998	185.000547
2014	2,4-D Butyl ester	94-80-4	12.607		C7H5OCl2	174.971197	174.971745
2014	2,4-D Butyl ester	94-80-4	12.607		C6H4OCl2	161.963372	161.96392
2014	2,4-D Butyl ester	94-80-4	12.607		C6H3Cl2	144.960632	144.961181
2014	2,4,5-T-methylester	1928-37-6	11.387	267.9461	C9H7O3Cl3		
2014	2,4,5-T-methylester	1928-37-6	11.387		C9H7O3Cl2	232.976676	232.977225
2014	2,4,5-T-methylester	1928-37-6	11.387		C7H4OCl3	208.932224	208.932773
2014	2,4-DB-methylester	18625-12-2	12.196	262.0164	C11H12O3Cl2		
2014	2,4-DB-methylester	18625-12-2	12.196		C10H9O2Cl2	230.997411	230.99796
2014	2,4-DB-methylester	18625-12-2	12.196		C6H4OCl2	161.963372	161.96392
2014	2,4-DB-methylester	18625-12-2	12.196		C5H9O2	101.059706	101.060255
2015	2,4-D-methylester	1928-38-7	9.776	233.985	C9H8O3Cl2		
2015	2,4-D-methylester	1928-38-7	9.776		C9H8O3Cl	199.015648	199.016197
2015	2,4-D-methylester	1928-38-7	9.776		C7H5OCl2	174.971197	174.971745

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2015	2,4-D-methylester	1928-38-7	9.776		C6H3OCI2	160.955547	160.956095
2019	3-trifluoromethylaniline	98-16-8	6.35	161.045233	C7H6F3N		
2019	3-trifluoromethylaniline	98-16-8	6.35		C7H6F3N	161.0446844	161.045233
2019	3-trifluoromethylaniline	98-16-8	6.35		C7H6F2N	142.0462814	142.04683
2019	3-trifluoromethylaniline	98-16-8	6.35		C6H4F2	114.0275574	114.028106
2019	4-nonylphenol	104-40-5	13.18	220.182715	C15H24O		
2019	4-nonylphenol	104-40-5	13.18		C7H7O	107.0491414	107.04969
2019	4-nonylphenol	104-40-5	13.18		C15H24O	220.1821664	220.182715
2019	4-nonylphenol	104-40-5	13.18		C6H5	77.03857642	77.039125
2019	4-nonylphenol	104-40-5	13.18		C6(C13)H7O	107.0491414	107.04969
2014	4,4'-Dichlorobenzophenone	90-98-2	14.183	249.9952	C13H8OCI2		
2014	4,4'-Dichlorobenzophenone	90-98-2	14.183		C13H8OCI	215.025819	215.026368
2014	4,4'-Dichlorobenzophenone	90-98-2	14.183		C7H4OCI	138.994519	138.995067
2014	4,4'-Dichlorobenzophenone	90-98-2	14.183		C6H4Cl	110.999604	111.000153
2018	8-Hydroxyquinoline	148-24-3	7.7	145.052764	C9H7NO		
2018	8-Hydroxyquinoline	148-24-3	7.7		C9H7NO	145.0522154	145.052764
2018	8-Hydroxyquinoline	148-24-3	7.7		C8H7N	117.0573004	117.057849
2018	8-Hydroxyquinoline	148-24-3	7.7		C7H6	90.04640142	90.04695
2014	Acetochlor	34256-82-1	12.709	269.1183	C14H20NO2Cl		
2014	Acetochlor	34256-82-1	12.709		C14H20NO2	234.148855	234.149404
2014	Acetochlor	34256-82-1	12.709		C12H14NOCl	223.075843	223.076392
2014	Acetochlor	34256-82-1	12.709		C11H12NO	174.09134	174.091889
2014	Acetochlor	34256-82-1	12.709		C10H12NO	162.09134	162.091889
2014	Acetochlor	34256-82-1	12.709		C10H12N	146.096426	146.096974
2014	Acetochlor	34256-82-1	12.709		C9H10N	132.080776	132.081324
2015	Acibenzolar-S-Methyl	135158-54-2	12.954	209.9922	C8H6N2OS2		
2015	Acibenzolar-S-Methyl	135158-54-2	12.954		C8H6OS2	181.985458	181.986006
2015	Acibenzolar-S-Methyl	135158-54-2	12.954		C8H5OS2	180.977633	180.978181
2015	Acibenzolar-S-Methyl	135158-54-2	12.954		C7H3OS2	166.961983	166.962531
2015	Acibenzolar-S-Methyl	135158-54-2	12.954		C7H5S2	152.982718	152.983267
2015	Acibenzolar-S-Methyl	135158-54-2	12.954		C6H3N2S	135.001145	135.001694
2015	Acibenzolar-S-Methyl	135158-54-2	12.954		C7H3OS	134.989912	134.99046
2015	Acibenzolar-S-Methyl	135158-54-2	12.954		C6H3S	106.994997	106.995546
2017	Alachlor	15972-60-8	12.893	269.11826	C14H20ClNO2		
2017	Alachlor	15972-60-8	12.893		C13H17ClNO	238.099318	238.099867
2017	Alachlor	15972-60-8	12.893		C13H16ClNO	237.091493	237.092042
2017	Alachlor	15972-60-8	12.893		C12H15ClNO	224.083668	224.084217
2017	Alachlor	15972-60-8	12.893		C13H16NO	202.122641	202.123189
2017	Alachlor	15972-60-8	12.893		C12H14NO	188.10699	188.107539

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2017	Alachlor	15972-60-8	12.893		C11H15N	161.119901	161.120449
2017	Alachlor	15972-60-8	12.893		C11H14N	160.112076	160.112624
2017	Alachlor	15972-60-8	12.893		C11H12N	158.096426	158.096974
2017	Alachlor	15972-60-8	12.893		C10H12N	146.096426	146.096974
2017	Alachlor	15972-60-8	12.893		C10H10N	144.080776	144.081324
2017	Alachlor	15972-60-8	12.893		C9H10N	132.080776	132.081324
2017	Alachlor	15972-60-8	12.893		C8H8N	118.065126	118.065674
2017	Allethrin	584-79-2	11.2	302.18819	C19H26O3		
2017	Allethrin	584-79-2	11.2		C9H10O	134.072616	134.073165
2017	Allethrin	584-79-2	11.2		C9H15	123.116827	123.117375
2017	Allethrin	584-79-2	11.2		C8H7O	119.049141	119.04969
2017	Allethrin	584-79-2	11.2		C8H9	105.069877	105.070425
2017	Allethrin	584-79-2	11.2		C7H7	91.054227	91.054775
2017	Allethrin	584-79-2	11.2		C6H7	79.054227	79.054775
2014	Allethrin	584-79-2	15.357	302.1882	C19H26O3		
2014	Allethrin	584-79-2	15.357		C9H12O	136.088266	136.088815
2014	Allethrin	584-79-2	15.357		C9H10O	134.072616	134.073165
2014	Allethrin	584-79-2	15.357		C9H15	123.116827	123.117375
2014	Allethrin	584-79-2	15.357		C8H7O	119.049141	119.04969
2014	Allethrin	584-79-2	15.357		C8H11	107.085527	107.086075
2014	Allethrin	584-79-2	15.357		C8H9	105.069877	105.070425
2018	Ametoctradin	865318-97-4	23.7	275.210995	C15H25N5		
2018	Ametoctradin	865318-97-4	23.7		C8H10N5	176.0930714	176.09362
2018	Ametoctradin	865318-97-4	23.7		C9H12N5	190.1087214	190.10927
2018	Ametoctradin	865318-97-4	23.7		C8H11N5	177.1008964	177.101445
2018	Amidosulfuron	120923-37-7	27.7	369.041294	C9H15N5O7S2		
2018	Amidosulfuron	120923-37-7	27.7		C4H5N4O4S2	236.9746764	236.975225
2018	Amidosulfuron	120923-37-7	27.7		C5H11N4S	159.0698944	159.070443
2018	Amidosulfuron	120923-37-7	27.7		C4H5N4O4(34S)S	238.9704724	238.971021
2015	Anilofos	64249-01-0	21.73	367.0232	C13H19NO3PS2Cl		
2015	Anilofos	64249-01-0	21.73		C11H13NSCl	226.045174	226.045723
2015	Anilofos	64249-01-0	21.73		C11H14NOCl	211.075843	211.076392
2015	Anilofos	64249-01-0	21.73		C8H7NSCl	183.998224	183.998773
2015	Anilofos	64249-01-0	21.73		C3H8O2PS2	170.969784	170.970332
2015	Anilofos	64249-01-0	21.73		C8H9NCl	154.041803	154.042352
2015	Anilofos	64249-01-0	21.73		C2H6O2PS	124.982063	124.982612
2017	Anthraquinone	84-65-1	13.872	208.05243	C14H8O2		
2017	Anthraquinone	84-65-1	13.872		C14H8O2	208.051881	208.052429
2017	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
2017	Anthraquinone	84-65-1	13.872		C12H8	152.062052	152.0626
2017	Anthraquinone	84-65-1	13.872		C12H7	151.054227	151.054775
2019	Aramite	140-57-8	17.95/ 18.23	334.10056	C15H23ClO4S		
2019	Aramite	140-57-8	17.95/ 18.23		C5H10ClO3S	185.0033714	185.00392
2019	Aramite	140-57-8	17.95/ 18.23		C12H15O	175.1117414	175.11229
2019	Aramite	140-57-8	17.95/ 18.23		C9H11O	135.0804404	135.080989
2019	Aramite	140-57-8	17.95/ 18.23		C14H20ClO4S	319.0765364	319.077085
2014	Aspon	3244-90-4	13.969	378.0853	C12H28O5P2S2		
2014	Aspon	3244-90-4	13.969		C9H22O5P2S2	336.03784	336.038388
2014	Aspon	3244-90-4	13.969		C6H17O5P2S2	294.998714	294.999263
2014	Aspon	3244-90-4	13.969		C3H11O5P2S2	252.951764	252.952313
2014	Aspon	3244-90-4	13.969		H5O5P2S2	210.904814	210.905363
2014	Aspon	3244-90-4	13.969		H4O5P2S2	209.896989	209.897538
2014	Aspon	3244-90-4	13.969		H3O4P2S2	192.894249	192.894798
2014	Aspon	3244-90-4	13.969		H4O3PS	114.961328	114.961876
2015	Atraton	1610-17-9	10.62	211.1433	C9H17N5O		
2015	Atraton	1610-17-9	10.62		C8H14N5O	196.119287	196.119835
2015	Atraton	1610-17-9	10.62		C6H11N5O	169.095811	169.09636
2015	Atraton	1610-17-9	10.62		C5H8N5O	154.072336	154.072885
2015	Azaconazole	60207-31-0	17.327	299.0228	C12H11N3O2Cl2		
2015	Azaconazole	60207-31-0	17.327		C9H7O2Cl2	216.981761	216.98231
2015	Azaconazole	60207-31-0	17.327		C7H3OCl2	172.955547	172.956095
2018	Azinphos-ethyl	2642-71-9	24.17	345.037073	C12H16N3O3PS2		
2018	Azinphos-ethyl	2642-71-9	24.17		C8H6N3O	160.050539	160.051087
2018	Azinphos-ethyl	2642-71-9	24.17		C8H6NO	132.044391	132.044939
2018	Azinphos-ethyl	2642-71-9	24.17		C4H10O2P	121.041295	121.041843
2018	Azinphos-ethyl	2642-71-9	24.17		C7H6N	104.049476	104.050024
2018	Azinphos-ethyl	2642-71-9	24.17		C6H5	77.038577	77.039125
2018	Azinphos-ethyl	2642-71-9	24.17		H2O2PS	96.950767	96.951315
2018	Azinphos-methyl	86-50-0	23.04	317.005774	C10H12N3O3PS2		
2018	Azinphos-methyl	86-50-0	23.04		C8H6N3O	160.050539	160.051087
2018	Azinphos-methyl	86-50-0	23.04		C8H6NO	132.044391	132.044939
2018	Azinphos-methyl	86-50-0	23.04		C2H6O2PS	124.982067	124.982615
2018	Azinphos-methyl	86-50-0	23.04		C7H6N	104.049476	104.050024
2018	Azinphos-methyl	86-50-0	23.04		C2H6O2P	93.009995	93.010543
2018	Azinphos-methyl	86-50-0	23.04		C6H5	77.038577	77.039125
2014	Aziprotryne	4658-28-0	11.61	225.0797	C7H11N7S		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2014	Aziprotryne	4658-28-0	11.61		C6H8N7S	210.05564	210.056189
2014	Aziprotryne	4658-28-0	11.61		C7H11N5S	197.072967	197.073516
2014	Aziprotryne	4658-28-0	11.61		C7H10N5S	196.065142	196.065691
2014	Aziprotryne	4658-28-0	11.61		C6H8N5S	182.049492	182.050041
2014	Aziprotryne	4658-28-0	11.61		C5H5N5S	167.026017	167.026566
2014	Aziprotryne	4658-28-0	11.61		C6H8N5	150.077422	150.07797
2014	Aziprotryne	4658-28-0	11.61		C6H11N4	139.097823	139.098371
2014	Barban	101-27-9	16.832	257.001	C11H9NO2Cl2		
2014	Barban	101-27-9	16.832		C11H9NO2Cl	222.031633	222.032181
2014	Barban	101-27-9	16.832		C7H4NOCl	152.997593	152.998141
2014	Barban	101-27-9	16.832		C10H9N	143.072951	143.073499
2014	Barban	101-27-9	16.832		C6H6NCl	127.018328	127.018877
2014	Barban	101-27-9	16.832		C6H4NCl	125.002678	125.003227
2014	Benfluralin	1861-40-1	10.153	335.1093	C13H16N3O4F3		
2014	Benfluralin	1861-40-1	10.153		C10H9N3O4F3	292.053967	292.054515
2014	Benfluralin	1861-40-1	10.153		C10H9N3O3F3	276.059052	276.059601
2014	Benfluralin	1861-40-1	10.153		C8H5N3O4F3	264.022667	264.023215
2015	Benoxacor	98730-04-2	12.218	259.0167	C11H11NO2Cl2		
2015	Benoxacor	98730-04-2	12.218		C11H11NO2	189.07843	189.078979
2015	Benoxacor	98730-04-2	12.218		C10H10NO2	176.070605	176.071154
2015	Benoxacor	98730-04-2	12.218		C9H8NO	146.06004	146.060589
2015	Benoxacor	98730-04-2	12.218		C8H8NO	134.06004	134.060589
2015	Benoxacor	98730-04-2	12.218		C7H6NO	120.04439	120.044939
2014	Bensulide	741-58-2	12.218	397.0605	C14H24NO4PS3		
2014	Bensulide	741-58-2	12.218		C7H8NO2S	170.027026	170.027574
2014	Bensulide	741-58-2	12.218		C6H5O2S	141.000476	141.001025
2014	Bensulide	741-58-2	12.218		C6H5	77.038577	77.039125
2014	Benzoylprop-ethyl	22212-55-1	20.827	365.0585	C18H17NO3Cl2		
2014	Benzoylprop-ethyl	22212-55-1	20.827		C15H12NOCl2	292.029046	292.029594
2014	Benzoylprop-ethyl	22212-55-1	20.827		C6C(13)H5O	106.036846	106.037395
2014	Benzoylprop-ethyl	22212-55-1	20.827		C7H5O	105.033491	105.03404
2014	Benzoylprop-ethyl	22212-55-1	20.827		C6H5	77.038577	77.039125
2018	Bifenazate	149877-41-8	21.99	300.147392	C17H20N2O3		
2018	Bifenazate	149877-41-8	21.99		C17H20N2O3	300.146844	300.147392
2018	Bifenazate	149877-41-8	21.99		C14H14N2O3	258.099895	258.100443
2018	Bifenazate	149877-41-8	21.99		C13H14N2O	214.110065	214.110613
2018	Bifenazate	149877-41-8	21.99		C13H10NO	196.075691	196.076239
2018	Bifenazate	149877-41-8	21.99		C12H10NO	184.075691	184.076239
2018	Bifenazate	149877-41-8	21.99		C12H10O	170.072617	170.073165

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2018	Bifenazate	149877-41-8	21.99		C12H8	152.062052	152.0626
2017	Bifenox	42576-02-3	21.688	340.98578	C14H9Cl2NO5		
2017	Bifenox	42576-02-3	21.688		C14H9Cl(37Cl)NO5	342.982279	342.982828
2017	Bifenox	42576-02-3	21.688		C14H9Cl2NO5	340.985229	340.985778
2017	Bifenox	42576-02-3	21.688		C13H6Cl(37Cl)NO4	311.963889	311.964438
2017	Bifenox	42576-02-3	21.688		C14H9Cl2O4	310.987241	310.987789
2017	Bifenox	42576-02-3	21.688		C13H6Cl2NO4	309.966839	309.967388
2017	Bifenox	42576-02-3	21.688		C11H6Cl	173.015254	173.015803
2017	Bixafen	581809-46-3	27.035	413.03095	C18H12Cl2F3N3O		
2017	Bixafen	581809-46-3	27.035		C18H12Cl(37Cl)F3N3O	415.027453	415.028002
2017	Bixafen	581809-46-3	27.035		C18H12Cl2F3N3O	413.030403	413.030952
2017	Bixafen	581809-46-3	27.035		C6H5F2N2O	159.036446	159.036994
2017	Bromacil	314-40-9	13.538	260.01604	C9H13BrN2O2		
2017	Bromacil	314-40-9	13.538		C5H6(81Br)N2O2	206.958669	206.959218
2017	Bromacil	314-40-9	13.538		C5H6BrN2O2	204.960716	204.961265
2017	Bromacil	314-40-9	13.538		C5H3BrNO2	187.934167	187.934715
2017	Bromacil	314-40-9	13.538		C4H5(81Br)NO	163.952856	163.953404
2017	Bromacil	314-40-9	13.538		C4H5BrNO	161.954902	161.955451
2014	Butachlor	23184-66-9	16.283	311.1652	C17H26NO2Cl		
2014	Butachlor	23184-66-9	16.283		C17H26NO2	276.195805	276.196354
2014	Butachlor	23184-66-9	16.283		C13H16NOCl	237.091493	237.092042
2014	Butachlor	23184-66-9	16.283		C13H16NO	202.122641	202.123189
2014	Butachlor	23184-66-9	16.283		C12H14NO	188.10699	188.107539
2014	Butachlor	23184-66-9	16.283		C11H14NO	176.10699	176.107539
2014	Butachlor	23184-66-9	16.283		C11H14N	160.112076	160.112624
2014	Butachlor	23184-66-9	16.283		C10H12N	146.096426	146.096974
2015	Butafenacil	134605-64-4	25.383	474.0805	C20H18N2O6ClF3		
2015	Butafenacil	134605-64-4	25.383		C13H7N2O3ClF3	331.009181	331.009729
2015	Butafenacil	134605-64-4	25.383		C8H3NO2Cl	179.984682	179.985231
2014	Butamifos	36335-67-8	16.552	332.096	C13H21N2O4PS		
2014	Butamifos	36335-67-8	16.552		C13H21NO2PS	286.102513	286.103061
2014	Butamifos	36335-67-8	16.552		C11H17NO2PS	258.071212	258.071761
2014	Butamifos	36335-67-8	16.552		C7H7NO4PS	231.982791	231.98334
2014	Butamifos	36335-67-8	16.552		C7H7NO4P	200.010721	200.011269
2017	Butralin	33629-47-9	14.506	295.15321	C14H21N3O4		
2017	Butralin	33629-47-9	14.506		C14H19N3O3	277.142093	277.142641
2017	Butralin	33629-47-9	14.506		C12H16N3O4	266.113532	266.114081
2017	Butralin	33629-47-9	14.506		C11H14N3O3	236.102968	236.103516
2017	Butralin	33629-47-9	14.506		C9H10N3O4	224.066582	224.067131

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2017	Butralin	33629-47-9	14.506		C11H14N3O2	220.108053	220.108602
2017	Buturon	3766-60-7	6.445	236.07164	C12H13CIN2O		
2017	Buturon	3766-60-7	6.445		C7H4(37Cl)NO	154.994643	154.995191
2017	Buturon	3766-60-7	6.445		C7H4CINO	152.997593	152.998141
2017	Buturon	3766-60-7	6.445		C6H4CIN	125.002678	125.003227
2014	Butylate	2008-41-5	8.137	217.15	C11H23NOS		
2014	Butylate	2008-41-5	8.137		C8H16NOS	174.094711	174.09526
2014	Butylate	2008-41-5	8.137		C9H18NO	156.138291	156.138839
2014	Butylate	2008-41-5	8.137		C7H16NS	146.099797	146.100345
2017	Captafol	2425-06-1		346.91081	C10H9Cl4NO2S		
2017	Captafol	2425-06-1			C2HCl2(37Cl)	131.910884	131.911433
2017	Captafol	2425-06-1			C2HCl3	129.913834	129.914383
2017	Captafol	2425-06-1			C2HCl2	94.944982	94.94553
2017	Captafol	2425-06-1			C2ClS	90.940375	90.940924
2017	Captafol	2425-06-1			C6H7	79.054227	79.054775
2014	Carbetamide	16118-49-3	14.158	236.1161	C12H16N2O3		
2014	Carbetamide	16118-49-3	14.158		C6C(13)H5NO	120.03992	120.040469
2014	Carbetamide	16118-49-3	14.158		C7H5NO	119.036565	119.037114
2014	Carbetamide	16118-49-3	14.158		C6H5N	91.041651	91.042199
2014	Carbetamide	16118-49-3	14.158		C3H6NO	72.04439	72.044939
2017	Carfentrazone-ethyl	128639-02-1	19.195	411.03643	C15H14Cl2F3N3O3		
2017	Carfentrazone-ethyl	128639-02-1	19.195		C15H13F3N3O3	340.090352	340.090901
2017	Carfentrazone-ethyl	128639-02-1	19.195		C13H8ClF3N3O2	330.025165	330.025714
2017	Carfentrazone-ethyl	128639-02-1	19.195		C13H9F3N3O3	312.059052	312.059601
2017	Carfentrazone-ethyl	128639-02-1	19.195		C13H7ClF2N3O2	310.018937	310.019486
2017	Carfentrazone-ethyl	128639-02-1	19.195		C11H8ClF3N3O	290.030251	290.030799
2018	Carvone	99-49-0	8.9	150.104465	C10H14O		
2018	Carvone	99-49-0	8.9		C7H7	91.05422642	91.054775
2018	Carvone	99-49-0	8.9		C7H9	93.06987642	93.070425
2018	Carvone	99-49-0	8.9		C6H7	79.05422642	79.054775
2019	Chlorthiamid	1918-13-4	13.28	204.951977	C7H5Cl2NS		
2019	Chlorthiamid	1918-13-4	13.28		C7H5ClNS	169.9825754	169.983124
2019	Chlorthiamid	1918-13-4	13.28		C7H5(37Cl)NS	171.9796254	171.980174
2019	Chlorthiamid	1918-13-4	13.28		C7H5Cl2NS	204.9514284	204.951977
2019	Chlorthiamid	1918-13-4	13.28		C7H5Cl(37Cl)NS	206.9484784	206.949027
2014	Chinomethionate	2439-01-2	15.76	233.9922	C10H6N2OS2		
2014	Chinomethionate	2439-01-2	15.76		C9H6N2S2	205.996691	205.99724
2014	Chinomethionate	2439-01-2	15.76		C9H6N2S	174.02462	174.025169
2014	Chinomethionate	2439-01-2	15.76		C9H5N2S	173.016795	173.017344

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2014	Chinomethionate	2439-01-2	15.76		C8H6NS	148.021546	148.022095
2014	Chinomethionate	2439-01-2	15.76		C8H6N	116.049476	116.050024
2018	Chlorantraniliprole	500008-45-7	21.5	480.970792	C18H14BrCl2N5O2		
2018	Chlorantraniliprole	500008-45-7	21.5		C13H8Cl2N2O	278.0008204	278.001369
2018	Chlorantraniliprole	500008-45-7	21.5		C9H14BrClN2O	279.9972534	279.997802
2018	Chlorantraniliprole	500008-45-7	21.5		C13H8ClN2O	243.0319674	243.032516
2019	Chlorbenside	103-17-3	16.54	267.988028	C13H10Cl2S		
2019	Chlorbenside	103-17-3	16.54		C7H6Cl	125.0152544	125.015803
2019	Chlorbenside	103-17-3	16.54		C7H6(37Cl)	127.0123044	127.012853
2019	Chlorbenside	103-17-3	16.54		C7H5	89.03857642	89.039125
2019	Chlorbenside	103-17-3	16.54		C13H10Cl2S	267.9874794	267.988028
2017	Chlorbromuron	13360-45-7	7.97	291.96142	C9H10BrClN2O2		
2017	Chlorbromuron	13360-45-7	7.97		C7H3(81Br)(37Cl)NO	234.903108	234.903657
2017	Chlorbromuron	13360-45-7	7.97		C7H3(81Br)ClNO	232.906058	232.906607
2017	Chlorbromuron	13360-45-7	7.97		C7H3BrClNO	230.908105	230.908654
2017	Chlorbromuron	13360-45-7	7.97		C6H3ClN	123.994853	123.995402
2017	Chlorbufam	1967-16-4	10.803	223.04001	C11H10ClNO2		
2017	Chlorbufam	1967-16-4	10.803		C7H4(37Cl)NO	154.994643	154.995191
2017	Chlorbufam	1967-16-4	10.803		C7H4ClNO	152.997593	152.998141
2017	Chlorbufam	1967-16-4	10.803		C6H6ClN	127.018328	127.018877
2017	Chlorbufam	1967-16-4	10.803		C6H4ClN	125.002678	125.003227
2019	Chlorfenprop-methyl	14437-17-3	10.19	232.005786	C10H10Cl2O2		
2019	Chlorfenprop-methyl	14437-17-3	10.19		C9H6ClO	165.0101694	165.010718
2019	Chlorfenprop-methyl	14437-17-3	10.19		C7H6Cl	125.0152544	125.015803
2019	Chlorfenprop-methyl	14437-17-3	10.19		C10H9ClO2	196.0285594	196.029108
2019	Chlorfenprop-methyl	14437-17-3	10.19		C9H6(37Cl)O	199.9790224	199.979571
2018	Chloridazon	1698-60-8	19.4	221.03559	C10H8ClN3O		
2018	Chloridazon	1698-60-8	19.4		C10H8ClN3O	221.0350414	221.03559
2018	Chloridazon	1698-60-8	19.4		C10H8(37Cl)N3O	223.0320914	223.03264
2018	Chloridazon	1698-60-8	19.4		C6H5	77.03857642	77.039125
2015	Chloroneb	2675-77-6	8.66	205.9901	C8H8O2Cl2		
2015	Chloroneb	2675-77-6	8.66		C7H5O2Cl2	190.966111	190.96666
2015	Chloroneb	2675-77-6	8.66		C6H2O2Cl	140.973783	140.974332
2018	Chlorpropylate	5836-10-2	17.9	338.047651	C17H16Cl2O3		
2018	Chlorpropylate	5836-10-2	17.9		C7H4ClO	138.9945194	138.995068
2018	Chlorpropylate	5836-10-2	17.9		C13H9Cl2O	251.0024974	251.003046
2018	Chlorpropylate	5836-10-2	17.9		C6H4Cl	110.9996044	111.000153
2014	Chlorthiamid	1918-13-4	12.521	204.952	C7H5NSCl2		
2014	Chlorthiamid	1918-13-4	12.521		C7H3NCl2	170.963706	170.964255

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2014	Chlorthiamid	1918-13-4	12.521		C7H2N	100.018175	100.018724
2018	Cinidon-ethyl	142891-20-1	31.2	393.053465	C19H17Cl2NO4		
2018	Cinidon-ethyl	142891-20-1	31.2		C17H13ClNO4	330.0527634	330.053312
2018	Cinidon-ethyl	142891-20-1	31.2		C19H17ClNO4	358.0840634	358.084612
2018	Cinidon-ethyl	142891-20-1	31.2		C15H9ClNO4	302.0214634	302.022012
2018	Clodinafop-propargyl	105512-06-9	19.5	349.051715	C17H13ClFNO4		
2018	Clodinafop-propargyl	105512-06-9	19.5		C11H6ClFNO2	238.0065614	238.00711
2018	Clodinafop-propargyl	105512-06-9	19.5		C13H10ClFNO2	266.0378614	266.03841
2018	Clodinafop-propargyl	105512-06-9	19.5		C17H13ClFNO4	349.0511664	349.051715
2019	Clopyralid	1702-17-6	6.23	190.954085	C5H3Cl2N	146.9637064	146.964255
2019	Clopyralid	1702-17-6	6.23		C5H2N	76.01817442	76.018723
2019	Clopyralid	1702-17-6	6.23		C4H2Cl	84.98395442	84.984503
2019	Clopyralid	1702-17-6	6.23		C5H3ClN	111.9948534	111.995402
2017	Coumaphos	56-72-4	24.815	362.01446	C14H16ClO5PS		
2017	Coumaphos	56-72-4	24.815		C14H16(37Cl)O5PS	364.01096	364.011509
2017	Coumaphos	56-72-4	24.815		C14H16ClO5PS	362.01391	362.014459
2017	Coumaphos	56-72-4	24.815		C10H7(37Cl)O2S	227.982029	227.982578
2017	Coumaphos	56-72-4	24.815		C10H7ClO2S	225.98498	225.985528
2017	Coumaphos	56-72-4	24.815		C10H7ClO3	210.007823	210.008372
2017	Coumaphos	56-72-4	24.815		C2H6O3P	109.004907	109.005456
2017	Coumaphos	56-72-4	24.815		H2O2PS	96.950763	96.951312
2014	Crimidine	535-89-7	8.822	171.0563	C7H10N3Cl		
2014	Crimidine	535-89-7	8.822		C6H7N3Cl	156.032301	156.03285
2014	Crimidine	535-89-7	8.822		C6H7N2Cl	142.029227	142.029776
2014	Crimidine	535-89-7	8.822		C5H4N2Cl	127.005752	127.006301
2014	Crimidine	535-89-7	8.822		C6H6N3	120.055624	120.056172
2014	Crotoxypfos	7700-17-6	16.28	314.0919	C14H19O6P		
2014	Crotoxypfos	7700-17-6	16.28		C6H10O5P	193.026036	193.026585
2014	Crotoxypfos	7700-17-6	16.28		C2H8O4P	127.015472	127.01602
2014	Crotoxypfos	7700-17-6	16.28		C8H9	105.069877	105.070425
2014	Crotoxypfos	7700-17-6	16.28		C8H8	104.062052	104.0626
2014	Crotoxypfos	7700-17-6	16.28		C8H7	103.054227	103.054775
2019	Cyanazine	21725-46-2	14.66	240.089022	C9H13ClN6		
2019	Cyanazine	21725-46-2	14.66		C8H10ClN6	225.0649984	225.065547
2019	Cyanazine	21725-46-2	14.66		C7H9ClN5	198.0540994	198.054648
2019	Cyanazine	21725-46-2	14.66		C7H9ClN6	212.0571734	212.057722
2019	Cyanazine	21725-46-2	14.66		C9H13ClN6	240.0884734	240.089022
2018	Cyanofenphos	13067-93-1	19.84	303.048289	C15H14NO2PS		
2018	Cyanofenphos	13067-93-1	19.84		C8H10OPS	185.018452	185.019

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2018	Cyanofenphos	13067-93-1	19.84		C8H10O2P	169.041295	169.041843
2018	Cyanofenphos	13067-93-1	19.84		C6H6OPS	156.987152	156.9877
2018	Cyanofenphos	13067-93-1	19.84		C6H6O2P	141.009994	141.010542
2017	Cyanophos	2636-26-2	11.243	243.0119	C9H10NO3PS		
2017	Cyanophos	2636-26-2	11.243		C9H10NO3PS	243.011352	243.011901
2017	Cyanophos	2636-26-2	11.243		C2H6O2PS	124.982063	124.982612
2017	Cyanophos	2636-26-2	11.243		C2H6O3P	109.004907	109.005456
2017	Cyanophos	2636-26-2	11.243		CH4O2P	78.994342	78.994891
2018	Cycloxydim	101205-02-1	24	325.171165	C17H27NO3S		
2018	Cycloxydim	101205-02-1	24		C10H12NO2	178.0862554	178.086804
2018	Cycloxydim	101205-02-1	24		C6H6NO	108.0443904	108.044939
2018	Cycloxydim	101205-02-1	24		C5H9S	101.0419484	101.042497
2017	Cycluron	2163-69-1	11.203	198.17321	C11H22N2O		
2017	Cycluron	2163-69-1	11.203		C3H9N2O	89.070939	89.071488
2017	Cycluron	2163-69-1	11.203		C6H10	82.077702	82.07825
2017	Cycluron	2163-69-1	11.203		C3H6NO	72.04439	72.044939
2017	Cycluron	2163-69-1	11.203		C5H9	69.069877	69.070425
2017	Cyflufenamid	180409-60-3	17.654	412.12102	C20H17F5N2O2		
2017	Cyflufenamid	180409-60-3	17.654		C8H2F4N	188.011788	188.012337
2017	Cyflufenamid	180409-60-3	17.654		C7H2F3N	157.013385	157.013934
2017	Cyflufenamid	180409-60-3	17.654		C8H5F4NO2	223.025093	223.025641
2017	Cyflufenamid	180409-60-3	17.654		C16H4N2O	240.031814	240.032363
2018	Cyprazin	22936-86-3	13.22	227.093773	C9H14CIN5		
2018	Cyprazin	22936-86-3	13.22		C9H13CIN5	226.0854	226.085948
2018	Cyprazin	22936-86-3	13.22		C8H11CIN5	212.06975	212.070298
2018	Cyprazin	22936-86-3	13.22		C6H7CIN5	184.03845	184.038998
2018	Cyprazin	22936-86-3	13.22		C5H5CIN5	170.0228	170.023348
2018	Cyprazin	22936-86-3	13.22		C5H4N5	134.046122	134.04667
2018	Cyromazine	66215-27-8	11.2	166.096694	C6H10N6		
2018	Cyromazine	66215-27-8	11.2		C5H7N6	151.0726704	151.073219
2018	Cyromazine	66215-27-8	11.2		C6H9N6	165.0883204	165.088869
2018	Cyromazine	66215-27-8	11.2		C4H5N4	109.0508724	109.051421
2014	Cythioate	115-93-5	19.955	296.9895	C8H12NO5PS2		
2014	Cythioate	115-93-5	19.955		C8H9O3PS	216.000453	216.001001
2014	Cythioate	115-93-5	19.955		C2H8O4P	127.015472	127.01602
2014	Cythioate	115-93-5	19.955		C2H6O2PS	124.982063	124.982612
2014	Cythioate	115-93-5	19.955		C2H6O3P	109.004907	109.005456
2017	Dazomet	533-74-4	10.7	162.02854	C5H10N2S2		
2017	Dazomet	533-74-4	10.7		C5H10N2S2	162.027992	162.02854

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2017	Dazomet	533-74-4	10.7		C3H7NS	89.029372	89.02992
2017	Dazomet	533-74-4	10.7		CS2	75.943593	75.944142
2017	Dazomet	533-74-4	10.7		C2H3NS	72.998072	72.99862
2017	Dazomet	533-74-4	10.7		C2H2NS	71.990246	71.990795
2019	DCPA	1861-32-1	14.74	329.902022	C10H6Cl4O4		
2019	DCPA	1861-32-1	14.74		C9H3Cl4O3	298.8830834	298.883632
2019	DCPA	1861-32-1	14.74		C9H3Cl3(37Cl)O3	333.8519364	333.852485
2019	DCPA	1861-32-1	14.74		C9H3Cl2(37Cl)2O3	368.8207894	368.821338
2019	DCPA	1861-32-1	14.74		C10H6Cl4O4	329.9014734	329.902022
2019	DCPA	1861-32-1	14.74		C10H6Cl3(37Cl)O4	364.8703264	364.870875
2017	Demeton-S	126-75-0	10.647	258.05132	C8H19O3PS2		
2017	Demeton-S	126-75-0	10.647		H4O3PS	114.961328	114.961877
2017	Demeton-S	126-75-0	10.647		H3O3PS	113.953503	113.954052
2017	Demeton-S	126-75-0	10.647		C4H9S	89.041948	89.042496
2017	Demeton-S	126-75-0	10.647		C4H8S	88.034123	88.034671
2014	Desethylatrazine	6190-65-4	10.014	187.0625	C6H10N5Cl		
2014	Desethylatrazine	6190-65-4	10.014		C5H7N5Cl	172.038449	172.038998
2014	Desethylatrazine	6190-65-4	10.014		C3H4N5Cl	145.014974	145.015523
2017	Desmetryn	1014-69-3	12.766	213.10482	C8H15N5S		
2017	Desmetryn	1014-69-3	12.766		C8H15N5S	213.104268	213.104817
2017	Desmetryn	1014-69-3	12.766		C7H12N5S	198.080793	198.081341
2017	Desmetryn	1014-69-3	12.766		C5H9N5S	171.057318	171.057866
2017	Desmetryn	1014-69-3	12.766		C4H6N5S	156.033843	156.034391
2019	Diafenthiuron	67-45-8	18.59	384.223534	C23H32N2OS		
2019	Diafenthiuron	67-45-8	18.59		C19H21NOS	311.1338374	311.134386
2019	Diafenthiuron	67-45-8	18.59		C15H12NOS	254.0634124	254.063961
2019	Diafenthiuron	67-45-8	18.59		C18H18NOS	296.1103624	296.110911
2019	Diafenthiuron	67-45-8	18.59		C18H16NO	262.1226404	262.123189
2019	Diafenthiuron	67-45-8	18.59		C19H20NO	278.1539404	278.154489
2018	Dialifos	10311-84-9	23.7	393.002519	C14H17ClNO4PS2		
2018	Dialifos	10311-84-9	23.7		C10H7ClNO2	208.0159834	208.016532
2018	Dialifos	10311-84-9	23.7		C7H4O	104.0256664	104.026215
2018	Dialifos	10311-84-9	23.7		C10H7(37Cl)NO2	210.0130334	210.013582
2018	Diallate	2303-16-4	11.16	269.040792	C10H17Cl2NOS		
2018	Diallate	2303-16-4	11.16		C10H17(37Cl)NO(S34)	234.071391	234.071939
2018	Diallate	2303-16-4	11.16		C10H17ClNOS	234.071391	234.071939
2018	Diallate	2303-16-4	11.16		C7H11ClNOS	192.024441	192.024989
2018	Diallate	2303-16-4	11.16		C7H14NO	128.106991	128.107539
2018	Diallate	2303-16-4	11.16		C3H3Cl2	108.960633	108.961181

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2018	Diallate	2303-16-4	11.16		C4H8NO	86.060041	86.060589
2014	DiazinonO-analog	962-58-3	12.766	288.1239	C12H21N2O4P		
2014	DiazinonO-analog	962-58-3	12.766		C11H18N2O4P	273.09987	273.100419
2014	DiazinonO-analog	962-58-3	12.766		C10H17N2O4P	260.092045	260.092594
2014	DiazinonO-analog	962-58-3	12.766		C9H14N2O4P	245.06857	245.069118
2014	DiazinonO-analog	962-58-3	12.766		C8H12N2O	152.094414	152.094963
2014	DiazinonO-analog	962-58-3	12.766		C8H11N2O	151.086589	151.087138
2014	DiazinonO-analog	962-58-3	12.766		C7H9N2O	137.070939	137.071488
2014	DiazinonO-analog	962-58-3	12.766		C8H10N2	134.08385	134.084398
2014	Dibutylchloredate	1770-80-5	22.55	497.9493	C17H20O4Cl6		
2014	Dibutylchloredate	1770-80-5	22.55		C9H4O4Cl6	385.823526	385.824075
2014	Dibutylchloredate	1770-80-5	22.55		C9H3O3Cl6	368.820787	368.821335
2014	Dibutylchloredate	1770-80-5	22.55		C9H3O4Cl4	314.877996	314.878544
2014	Dibutylchloredate	1770-80-5	22.55		C7H2Cl5	260.859365	260.859914
2014	Dibutylchloredate	1770-80-5	22.55		C5Cl5	234.843715	234.844264
2019	Dicamba-methyester	6597-78-0	9.59	233.985051	C9H8Cl2O3		
2019	Dicamba-methyester	6597-78-0	9.59		C8H5Cl2O2	202.9661124	202.966661
2019	Dicamba-methyester	6597-78-0	9.59		C7H2Cl2O2	187.9426374	187.943186
2019	Dicamba-methyester	6597-78-0	9.59		C6H2Cl2O	159.9477224	159.948271
2019	Dicamba-methyester	6597-78-0	9.59		C5H2Cl	96.98395442	96.984503
2019	Dicamba-methyester	6597-78-0	9.59		C9H8Cl2O3	233.9845024	233.985051
2014	Dicapthon	2463-84-5	14.252	296.9628	C8H9NO5PSCI		
2014	Dicapthon	2463-84-5	14.252		C7C(13)H9NO5PS	262.996711	262.997259
2014	Dicapthon	2463-84-5	14.252		C8H9NO5PS	261.993356	261.993905
2014	Dicapthon	2463-84-5	14.252		C8H9O3PS	216.000453	216.001001
2014	Dicapthon	2463-84-5	14.252		C2H6O2PS	124.982063	124.982612
2017	Dichlobenil	1194-65-6	7.641	170.96425	C7H3Cl2N		
2017	Dichlobenil	1194-65-6	7.641		C7H3Cl(37Cl)N	172.960756	172.961304
2017	Dichlobenil	1194-65-6	7.641		C7H3Cl2N	170.963706	170.964254
2017	Dichlobenil	1194-65-6	7.641		C7H2N	100.018175	100.018724
2017	Dichlofenthion	97-17-6	12.45	313.97001	C10H13Cl2O3PS		
2017	Dichlofenthion	97-17-6	12.45		C10H13ClO3PS	279.000606	279.001155
2017	Dichlofenthion	97-17-6	12.45		C2ClN5O4S	224.935404	224.935952
2017	Dichlofenthion	97-17-6	12.45		C6H5ClO3PS	222.938006	222.938554
2017	Dichlofenthion	97-17-6	12.45		C6H4Cl(37Cl)O	163.960421	163.96097
2017	Dichlofenthion	97-17-6	12.45		C6H4Cl2O	161.963372	161.96392
2017	Dichlofenthion	97-17-6	12.45		H2O2PS	96.950763	96.951312
2015	Dichlone	117-80-6	11.704	225.9588	C10H4O2Cl2		
2015	Dichlone	117-80-6	11.704		C10H4O2Cl	190.989433	190.989982

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2015	Dichlone	117-80-6	11.704		C9H4OCl	162.994519	162.995067
2015	Dichlone	117-80-6	11.704		C8H4Cl	134.999604	135.000153
2014	Dichlormid	37764-25-3	7.705	207.0218	C8H11NOCl ₂		
2014	Dichlormid	37764-25-3	7.705		C8H11NOCl	172.052368	172.052917
2014	Dichlormid	37764-25-3	7.705		C5H6NOCl ₂	165.982096	165.982644
2014	Dichlormid	37764-25-3	7.705		C8H10NO	136.07569	136.076239
2014	Dichlormid	37764-25-3	7.705		C7H10NO	124.07569	124.076239
2014	Dichlorophen	97-23-4	8.27	268.0058	C13H10O2Cl ₂		
2014	Dichlorophen	97-23-4	8.27		C13H10O2Cl	233.036384	233.036932
2014	Dichlorophen	97-23-4	8.27		C13H8OCl	215.025819	215.026368
2014	Dichlorophen	97-23-4	8.27		C7H6OCl	141.010169	141.010718
2014	Dichlorophen	97-23-4	8.27		C6H5OCl	128.002344	128.002892
2014	Dichlorprop-methylester	57153-17-0	9.588	248.0007	C10H10O3Cl ₂		
2014	Dichlorprop-methylester	57153-17-0	9.588		C8H7OCl ₂	188.986847	188.987395
2014	Dichlorprop-methylester	57153-17-0	9.588		C6H4OCl ₂	161.963372	161.96392
2015	Diclobutrazol	75736-33-3	17.17	327.0905	C15H19N3OCl ₂		
2015	Diclobutrazol	75736-33-3	17.17		C11H10N3OCl ₂	270.019544	270.020092
2015	Diclobutrazol	75736-33-3	17.17		C7H5Cl ₂	158.976282	158.976831
2015	Diclofop-methyl	51338-27-3	20.069	340.0269	C16H14O4Cl ₂		
2015	Diclofop-methyl	51338-27-3	20.069		C14H11O2Cl ₂	281.013061	281.01361
2015	Diclofop-methyl	51338-27-3	20.069		C12H8O2Cl ₂	253.989586	253.990135
2015	Diclofop-methyl	51338-27-3	20.069		C12H7O2Cl ₂	252.981761	252.98231
2018	Dicrotophos	141-66-2	10	237.076612	C8H16NO5P		
2018	Dicrotophos	141-66-2	10		C2H6O3P	109.0049094	109.005458
2018	Dicrotophos	141-66-2	10		C3H6NO	72.04439042	72.044939
2018	Dicrotophos	141-66-2	10		C6H10O5P	193.0260394	193.026588
2017	Difenoxuron	14214-32-5	13.868	286.13174	C16H18N2O3		
2017	Difenoxuron	14214-32-5	13.868		C14H11NO3	241.073345	241.073893
2017	Difenoxuron	14214-32-5	13.868		C13H8NO3	226.04987	226.050418
2017	Difenoxuron	14214-32-5	13.868		C12H8NO2	198.054955	198.055504
2018	Diflufenican	83164-33-4	20.1	394.074068	C19H11F5N2O2		
2018	Diflufenican	83164-33-4	20.1		C13H7F3NO2	266.0423394	266.042888
2018	Diflufenican	83164-33-4	20.1		C19H11F5N2O2	394.0735194	394.074068
2018	Diflufenican	83164-33-4	20.1		C13H6F2N2O	246.0361104	246.036659
2017	Dimefuron	34205-21-5	15.084	338.11457	C15H19ClN4O3		
2017	Dimefuron	34205-21-5	15.084		C13H12ClN3O3	293.05617	293.056719
2017	Dimefuron	34205-21-5	15.084		C12H12ClN3O	249.066341	249.06689
2017	Dimefuron	34205-21-5	15.084		C7H3(37Cl)N2O	167.989892	167.99044
2017	Dimefuron	34205-21-5	15.084		C7H3ClN2O	165.992842	165.99339

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2017	Dimefuron	34205-21-5	15.084		C7H3N2O	131.023989	131.024538
2017	Dimethachlor	50563-36-5	12.48	255.10261	C13H18ClNO2		
2017	Dimethachlor	50563-36-5	12.48		C10H12ClNO	197.060193	197.060742
2017	Dimethachlor	50563-36-5	12.48		C9H12N	134.096426	134.096974
2017	Dimethachlor	50563-36-5	12.48		C9H10N	132.080776	132.081324
2017	Dimethachlor	50563-36-5	12.48		C9H10NO	148.07569	148.076239
2014	Dimethenamid	87674-68-8	12.591	275.0747	C12H18NO2SCI		
2014	Dimethenamid	87674-68-8	12.591		C10H13NOSCI	230.040089	230.040637
2014	Dimethenamid	87674-68-8	12.591		C8H10NOSCI	203.016614	203.017162
2014	Dimethenamid	87674-68-8	12.591		C8H12NS	154.068496	154.069045
2018	Dimethirimol	5221-53-4	12.33	209.152811	C11H19N3O		
2018	Dimethirimol	5221-53-4	12.33		C11H19N3O	209.152263	209.152811
2018	Dimethirimol	5221-53-4	12.33		C8H12N3O	166.097489	166.098037
2018	Dimethirimol	5221-53-4	12.33		C5H6NO	96.044391	96.044939
2018	Dimethomorph	110488-70-5	30.153 0.64	387.123737	C21H22ClNO4		
2018	Dimethomorph	110488-70-5	30.153 0.65		C21H22ClNO4	387.123189	387.123737
2018	Dimethomorph	110488-70-5	30.153 0.66		C16H5(37Cl)O2	301.0626	301.063148
2018	Dimethomorph	110488-70-5	30.153 0.67		C17H14ClO3	301.0626	301.063148
2018	Dimethomorph	110488-70-5	30.153 0.68		C16H5ClO2	274.07551	274.076058
2018	Dimethomorph	110488-70-5	30.153 0.69		C9H9O3	165.054622	165.05517
2018	Dimoxystrobin	149961-52-4	21.1	326.163043	C19H22N2O3		
2018	Dimoxystrobin	149961-52-4	21.1		C8H6N	116.0494754	116.050024
2018	Dimoxystrobin	149961-52-4	21.1		C7H5	89.03857642	89.039125
2018	Dimoxystrobin	149961-52-4	21.1		C11H13N2O2	205.0971544	205.097703
2018	Diniconazole	83657-24-3	18.1	325.074868	C15H17Cl2N3O		
2018	Diniconazole	83657-24-3	18.1		C11H8Cl2N3O	268.0038944	268.004443
2018	Diniconazole	83657-24-3	18.1		C11H7ClN3O	232.0272164	232.027765
2018	Diniconazole	83657-24-3	18.1		C8H5Cl	136.0074294	136.007978
2017	Dinoseb	88-85-7	11.655	240.07462	C10H12N2O5		
2017	Dinoseb	88-85-7	11.655		C8H7N2O5	211.034948	211.035496
2017	Dinoseb	88-85-7	11.655		C8H5NO3	163.026394	163.026943
2017	Dinoseb	88-85-7	11.655		C8H5NO2	147.03148	147.032028
2018	Dinoterb	1420-07-1	12.22	240.074623	C10H12N2O5		
2018	Dinoterb	1420-07-1	12.22		C10H12N2O5	240.074075	240.074623
2018	Dinoterb	1420-07-1	12.22		C9H9N2O5	225.0506	225.051148
2018	Dinoterb	1420-07-1	12.22		C9H7N3O	173.058364	173.058912
2018	Dinoterb	1420-07-1	12.22		C9H7O	131.049142	131.04969
2018	Dinoterb	1420-07-1	12.22		C9H7NO2	161.047131	161.047679
2018	Dinoterb	1420-07-1	12.22		C8H7	103.054227	103.054775

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2017	Dioxacarb	6988-21-2	12.343	223.08446	C11H13NO4		
2017	Dioxacarb	6988-21-2	12.343		C9H10O3	166.062446	166.062994
2017	Dioxacarb	6988-21-2	12.343		C9H9O3	165.054621	165.055169
2017	Dioxacarb	6988-21-2	12.343		C7H6O2	122.036231	122.036779
2017	Dioxacarb	6988-21-2	12.343		C7H5O2	121.028406	121.028954
2018	Dioxathion	78-34-2	25.1	456.008753	C12H26O6P2S4		
2018	Dioxathion	78-34-2	25.1		C8H16O4PS2	271.0222184	271.022767
2018	Dioxathion	78-34-2	25.1		C4H10O2PS2	184.9854384	184.985987
2018	Dioxathion	78-34-2	25.1		C4H10O2PS	153.0133664	153.013915
2015	Diphenamid	957-51-7	14.51	239.131	C16H17NO		
2015	Diphenamid	957-51-7	14.51		C13H11	167.085527	167.086075
2015	Diphenamid	957-51-7	14.51		C13H9	165.069877	165.070425
2015	Diphenamid	957-51-7	14.51		C12H8	152.062052	152.0626
2015	Diphenamid	957-51-7	14.51		C3H6NO	72.04439	72.044939
2014	Dithiopyr	97886-45-8	13.4	401.0543	C15H16NO2S2F5		
2014	Dithiopyr	97886-45-8	13.4		C14H13NO2SF5	354.058167	354.058715
2014	Dithiopyr	97886-45-8	13.4		C13H9NO2F5	306.054796	306.055345
2014	Dithiopyr	97886-45-8	13.4		C13H8NO2F4	286.048568	286.049116
2015	Dodemorph	1593-77-7	14.41	281.2719	C18H35NO		
2015	Dodemorph	1593-77-7	14.41		C15H28NO	238.216541	238.21709
2015	Dodemorph	1593-77-7	14.41		C9H16NO	154.122641	154.123189
2015	Dodemorph	1593-77-7	14.41		C8H15NO	141.114816	141.115364
2017	Edifenphos	17109-49-8	19.191	310.02511	C14H15O2PS2		
2017	Edifenphos	17109-49-8	19.191		C6H6O2PS	172.982063	172.982612
2017	Edifenphos	17109-49-8	19.191		C8H10S	138.049773	138.050321
2017	Edifenphos	17109-49-8	19.191		C6H6S	110.018473	110.019021
2017	Edifenphos	17109-49-8	19.191		C6H5S	109.010648	109.011196
2018	EPTC	759-94-4	8.36	189.118736	C9H19NOS		
2018	EPTC	759-94-4	8.36		C7H14NOS	160.079063	160.079611
2018	EPTC	759-94-4	8.36		C6H14NS	132.084148	132.084696
2018	EPTC	759-94-4	8.36		C7H14NO	128.106991	128.107539
2018	EPTC	759-94-4	8.36		C4H8NO	86.060041	86.060589
2017	Esprocarb	85785-20-2	13.537	265.15004	C15H23NOS		
2017	Esprocarb	85785-20-2	13.537		C12H16NOS	222.094712	222.09526
2017	Esprocarb	85785-20-2	13.537		C11H16N	162.127726	162.128275
2017	Esprocarb	85785-20-2	13.537		C7H7	91.054227	91.054775
2015	Etaconazole	60207-93-4	18.177	327.0541	C14H15N3O2Cl2		
2015	Etaconazole	60207-93-4	18.177		C11H11O2Cl2	245.013061	245.01361
2015	Etaconazole	60207-93-4	18.177		C7H5O2Cl2	190.966111	190.96666

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2015	Etaconazole	60207-93-4	18.177		C7H3OCI2	172.955547	172.956095
2017	Ethalfuralin	55283-68-6	9.895	333.09364	C13H14F3N3O4		
2017	Ethalfuralin	55283-68-6	9.895		C13H13F3N3O3	316.090352	316.090901
2017	Ethalfuralin	55283-68-6	9.895		C10H9F3N3O4	292.053967	292.054515
2017	Ethalfuralin	55283-68-6	9.895		C10H9F3N3O3	276.059052	276.059601
2017	Ethalfuralin	55283-68-6	9.895		C8H5F3N3O4	264.022667	264.023215
2017	Etoazole	153233-91-1	21.549	359.16969	C21H23F2NO2		
2017	Etoazole	153233-91-1	21.549		C19H18F2NO2	330.130012	330.13056
2017	Etoazole	153233-91-1	21.549		C18H16F2NO	300.119447	300.119996
2017	Etoazole	153233-91-1	21.549		C13H18NO	204.138291	204.138839
2017	Etoazole	153233-91-1	21.549		C13H15O	187.111742	187.11229
2017	Etoazole	153233-91-1	21.549		C7H3F2O	141.014648	141.015196
2018	Etridiazole	2593-15-9	8.3	245.918819	C5H5Cl3N2OS		
2018	Etridiazole	2593-15-9	8.3		C3HCl2N2OS	182.9181174	182.918666
2018	Etridiazole	2593-15-9	8.3		C5H5Cl2N2OS	210.9494174	210.949966
2018	Etridiazole	2593-15-9	8.3		C5H5(35Cl)ClN2OS	212.9464674	212.947016
2018	Etrimfos	38260-54-7	11.8	292.064668	C10H17N2O4PS		
2018	Etrimfos	38260-54-7	11.8		C9H13N2O2	181.0971544	181.097703
2018	Etrimfos	38260-54-7	11.8		C10H17N2O4PS	292.0641194	292.064668
2018	Etrimfos	38260-54-7	11.8		C7H9N2O2	153.0658534	153.066402
2018	Famoxadone	131807-57-3	29.8	374.126658	C22H18N2O4		
2018	Famoxadone	131807-57-3	29.8		C21H18N2O2	330.1362794	330.136828
2018	Famoxadone	131807-57-3	29.8		C15H12O2	224.0831814	224.08373
2018	Famoxadone	131807-57-3	29.8		C14H12O	196.0882664	196.088815
2018	Fenamiphos	22224-92-6	17.08	303.105804	C13H22NO3PS		
2018	Fenamiphos	22224-92-6	17.08		C13H22NO3PS	303.105256	303.105804
2018	Fenamiphos	22224-92-6	17.08		C12H19NO3PS	288.081781	288.082329
2018	Fenamiphos	22224-92-6	17.08		C10H15NO3PS	260.05048	260.051028
2018	Fenamiphos	22224-92-6	17.08		C10H12O3PS	243.023932	243.02448
2018	Fenamiphos	22224-92-6	17.08		C8H10O3PS	217.008282	217.00883
2018	Fenamiphos	22224-92-6	17.08		C8H10OS	154.044689	154.045237
2014	Fenobucarb	3766-81-2	9.529	207.1259	C12H17NO2		
2014	Fenobucarb	3766-81-2	9.529		C10H14O	150.103916	150.104465
2014	Fenobucarb	3766-81-2	9.529		C8H9O	121.064791	121.06534
2014	Fenoprop-methylester	4841-20-7	11.069	281.9617	C10H9O3Cl3		
2014	Fenoprop-methylester	4841-20-7	11.069		C8H6OCl3	222.947874	222.948423
2014	Fenoprop-methylester	4841-20-7	11.069		C6H3OCl3	195.924399	195.924948
2017	Fenothiocarb	62850-32-2	15.916	253.11365	C13H19NO2S		
2017	Fenothiocarb	62850-32-2	15.916		C7H14NOS	160.079061	160.07961

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2017	Fenothiocarb	62850-32-2	15.916		C6H6O	94.041316	94.041865
2017	Fenothiocarb	62850-32-2	15.916		C4H8S	88.034123	88.034671
2017	Fenothiocarb	62850-32-2	15.916		C3H6NO	72.04439	72.044939
2017	Fenoxaprop-ethyl	66441-23-4	23.896	361.0717	C18H16ClNO5		
2017	Fenoxaprop-ethyl	66441-23-4	23.896		C18H16ClNO5	361.071152	361.0717
2017	Fenoxaprop-ethyl	66441-23-4	23.896		C15H11(37Cl)NO3	290.039247	290.039796
2017	Fenoxaprop-ethyl	66441-23-4	23.896		C15H11ClNO3	288.042197	288.042746
2017	Fenoxaprop-ethyl	66441-23-4	23.896		C13H8ClNO3	261.018722	261.019271
2018	Fenoxaprop-p-ethyl	71283-80-2	23.9	361.071702	C18H16ClNO5		
2018	Fenoxaprop-p-ethyl	71283-80-2	23.9		C15H11ClNO3	288.0421984	288.042747
2018	Fenoxaprop-p-ethyl	71283-80-2	23.9		C18H16ClNO5	361.0711524	361.071701
2018	Fenoxaprop-p-ethyl	71283-80-2	23.9		C13H8ClNO3	261.0187234	261.019272
2017	Fenpiclonil	74738-17-3	20.707	235.9908	C11H6Cl2N2		
2017	Fenpiclonil	74738-17-3	20.707		C11H6Cl(37Cl)N2	237.987305	237.987853
2017	Fenpiclonil	74738-17-3	20.707		C11H6Cl2N2	235.990255	235.990804
2017	Fenpiclonil	74738-17-3	20.707		C11H6ClN2	201.021402	201.021951
2017	Fenpiclonil	74738-17-3	20.707		C10H5ClN	174.010503	174.011052
2018	Fenson	80-38-6	15.17	267.996094	C12H9ClO3S		
2018	Fenson	80-38-6	15.17		C12H9ClO3S	267.995546	267.996094
2018	Fenson	80-38-6	15.17		C6H5O2S	141.000479	141.001027
2018	Fenson	80-38-6	15.17		C6H4ClO	126.99452	126.995068
2018	Fenson	80-38-6	15.17		C5H4Cl	98.999605	99.000153
2018	Fenson	80-38-6	15.17		C6H5	77.038577	77.039125
2015	Fensulfothion	115-90-2	18.03	308.0306	C11H17O4PS2		
2015	Fensulfothion	115-90-2	18.03		C10H14O4PS2	293.006563	293.007112
2015	Fensulfothion	115-90-2	18.03		C11H17O3PS2	292.035124	292.035672
2015	Fensulfothion	115-90-2	18.03		C9H13O3PS2	264.003824	264.004372
2015	Fensulfothion	115-90-2	18.03		C7H9O3PS2	235.972523	235.973072
2015	Fensulfothion	115-90-2	18.03		C7H8S2	156.006193	156.006742
2015	Fensulfothion	115-90-2	18.03		C6H5O2S	141.000476	141.001025
2015	Fensulfothion	115-90-2	18.03		C3H9O2PS	140.005538	140.006087
2015	Fensulfothion-sulfon	14255-72-2	18.655	324.0255	C11H17O5PS2		
2015	Fensulfothion-sulfon	14255-72-2	18.655		C7H8O4PS	218.987542	218.988091
2015	Fensulfothion-sulfon	14255-72-2	18.655		C7H8O2S2	187.996022	187.996571
2015	Fensulfothion-sulfon	14255-72-2	18.655		C6H5O3S	156.995391	156.99594
2017	Flonicamid	158062-67-0	9.351	229.0463	C9H6F3N3O		
2017	Flonicamid	158062-67-0	9.351		C7H3F3NO	174.016125	174.016673
2017	Flonicamid	158062-67-0	9.351		C7H3F3N2	172.024284	172.024833
2017	Flonicamid	158062-67-0	9.351		C6H3F3N	146.02121	146.021759

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2018	Fluazinam	79622-59-6	15.1	463.95138	C13H4Cl2F6N4O4		
2018	Fluazinam	79622-59-6	15.1		C13H4Cl2F6N3O2	417.9579274	417.958476
2018	Fluazinam	79622-59-6	15.1		C13H4Cl2F6N2	371.9650234	371.965572
2018	Fluazinam	79622-59-6	15.1		C13H4(37Cl)ClF6N3O2	419.9549774	419.955526
2014	Fluchloralin	33245-39-5	11.608	355.0547	C12H13N3O4ClF3		
2014	Fluchloralin	33245-39-5	11.608		C10H8N3O4ClF3	326.014995	326.015543
2014	Fluchloralin	33245-39-5	11.608		C11H11N3O4F3	306.069617	306.070166
2014	Fluchloralin	33245-39-5	11.608		C8H5N3O4F3	264.022667	264.023215
2018	Flufenacet	142459-58-3	14.1	363.066461	C14H13F4N3O2S		
2018	Flufenacet	142459-58-3	14.1		C9H10FN	151.0791784	151.079727
2018	Flufenacet	142459-58-3	14.1		C5H2F3N2O2S	210.9783604	210.978909
2018	Flufenacet	142459-58-3	14.1		C8H7FN	136.0557034	136.056252
2018	Flumetralin	62924-70-3	16.2	421.045247	C16H12ClF4N3O4		
2018	Flumetralin	62924-70-3	16.2		C7H5ClF	143.0058324	143.006381
2018	Flumetralin	62924-70-3	16.2		C7H5(37Cl)F	145.0028824	145.003431
2018	Flumetralin	62924-70-3	16.2		C16H11ClF4N3O3	404.0419584	404.042507
2017	Flumioxazin	103361-09-7	27.936	354.10159	C19H15FN2O4		
2017	Flumioxazin	103361-09-7	27.936		C9H15F2N7O6	355.104639	355.105188
2017	Flumioxazin	103361-09-7	27.936		C19H15FN2O4	354.101037	354.101585
2017	Flumioxazin	103361-09-7	27.936		C18H15FN2O3	326.106122	326.106671
2017	Flumioxazin	103361-09-7	27.936		C15H12FN2O3	287.082647	287.083195
2017	Flumioxazin	103361-09-7	27.936		C13H8FN2O3	259.051347	259.051895
2017	Flumioxazin	103361-09-7	27.936		C13H6N	176.049476	176.050024
2017	Fluometuron	2164-17-2	9.681	232.08235	C10H11F3N2O		
2017	Fluometuron	2164-17-2	9.681		C10H11F3N2O	232.081799	232.082348
2017	Fluometuron	2164-17-2	9.681		C8H4F3NO	187.02395	187.024498
2017	Fluometuron	2164-17-2	9.681		C7H4F3N	159.029035	159.029584
2017	Fluometuron	2164-17-2	9.681		C3H6NO	72.04439	72.044939
2014	Fluoroglycofen-ethyl	77501-90-7	23.716	447.0333	C18H13NO7ClF3		
2014	Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7NO4ClF3	345.001021	345.00157
2014	Fluoroglycofen-ethyl	77501-90-7	23.716		C14H6NO4ClF3	343.993196	343.993745
2014	Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7O3ClF3	315.003033	315.003581
2014	Fluoroglycofen-ethyl	77501-90-7	23.716		C13H7NO2ClF3	301.011192	301.011741
2014	Fluoroglycofen-ethyl	77501-90-7	23.716		C8H3O2ClF3	222.976818	222.977367
2014	Fluoroglycofen-ethyl	77501-90-7	23.716		C14H7O2	207.044056	207.044604
2014	Fluridone	59756-60-4	27.432	329.1027	C19H14NOF3		
2014	Fluridone	59756-60-4	27.432		C19H13NOF3	328.094375	328.094924
2018	Flurochloridone	61213-25-0	14.3	311.009153	C12H10Cl2F3NO		
2018	Flurochloridone	61213-25-0	14.3		C8H4F3NO	187.0239494	187.024498

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2018	Flurochloridone	61213-25-0	14.3		C8H7F3N	174.0525094	174.053058
2018	Flurochloridone	61213-25-0	14.3		C12H10Cl2F3NO	311.0086054	311.009154
2014	Flurprimidol	56425-91-3	12.43	312.1086	C15H15N2O2F3		
2014	Flurprimidol	56425-91-3	12.43		C12H8N2O2F3	269.053239	269.053787
2014	Flurprimidol	56425-91-3	12.43		C8H4O2F3	189.01579	189.016339
2014	Flurprimidol	56425-91-3	12.43		C5H3N2O	107.023989	107.024538
2018	Flurtamone	96525-23-4	22.2	333.097663	C18H14F3NO2		
2018	Flurtamone	96525-23-4	22.2		C8H10N	120.0807754	120.081324
2018	Flurtamone	96525-23-4	22.2		C18H14F3NO2	333.0971144	333.097663
2018	Flurtamone	96525-23-4	22.2		C10H8F3N	199.0603344	199.060883
2019	Flutianil	958647-10-4	28.28	426.048369	C19H14F4N2OS2		
2019	Flutianil	958647-10-4	28.28		C19H14F4N2OS2	426.0478204	426.048369
2019	Flutianil	958647-10-4	28.28		C18H14F4NOS	368.0726744	368.073223
2019	Flutianil	958647-10-4	28.28		C12H11N2OS	231.0586614	231.05921
2018	Fluxapyroxad	907204-31-3	21.3	381.090052	C18H12F5N3O		
2018	Fluxapyroxad	907204-31-3	21.3		C6H5F2N2O	159.0364454	159.036994
2018	Fluxapyroxad	907204-31-3	21.3		C18H12F5N3O	381.0895034	381.090052
2018	Fluxapyroxad	907204-31-3	21.3		C12H6F3N	221.0446844	221.045233
2018	Fuberidazole	3878-19-1	12.7	184.063663	C11H8N2O		
2018	Fuberidazole	3878-19-1	12.7		C11H8N2O	184.0631144	184.063663
2018	Fuberidazole	3878-19-1	12.7		C10H8N2	156.0681994	156.068748
2018	Fuberidazole	3878-19-1	12.7		C10H7N2	155.0603744	155.060923
2017	Furalaxyl	57646-30-7	15.448	301.13141	C17H19NO4		
2017	Furalaxyl	57646-30-7	15.448		C15H16NO2	242.117555	242.118104
2017	Furalaxyl	57646-30-7	15.448		C8H10NO2	152.070605	152.071154
2017	Furalaxyl	57646-30-7	15.448		C5H3O2	95.012756	95.013304
2017	Furathiocarb	65907-30-4	22.199	382.15624	C18H26N2O5S		
2017	Furathiocarb	65907-30-4	22.199		C10H10O2S	194.039602	194.040151
2017	Furathiocarb	65907-30-4	22.199		C10H12O2	164.083181	164.08373
2017	Furathiocarb	65907-30-4	22.199		C10H11O2	163.075356	163.075905
2017	Furathiocarb	65907-30-4	22.199		C9H11O	135.080441	135.08099
2017	Furathiocarb	65907-30-4	22.199		C7OH7	107.049141	107.04969
2017	Furilazole	121776-33-8	10.8	277.02725	C11H13Cl2NO3		
2017	Furilazole	121776-33-8	10.8		C10H10Cl2NO3	262.003225	262.003774
2017	Furilazole	121776-33-8	10.8		C8H8Cl(37Cl)NO2	221.98971	221.990259
2017	Furilazole	121776-33-8	10.8		C8H8Cl2NO2	219.99266	219.993209
2017	Furilazole	121776-33-8	10.8		C6H9ClNO	146.036718	146.037267
2017	Hexaflumuron	86479-06-3	8.172	459.98162	C16H8Cl2F6N2O3		
2017	Hexaflumuron	86479-06-3	8.172		C9H3Cl(37Cl)F4NO2	304.944198	304.944746

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2017	Hexaflumuron	86479-06-3	8.172		C9H3Cl2F4NO2	302.947148	302.947697
2017	Hexaflumuron	86479-06-3	8.172		C7H2Cl(37Cl)NO2	203.94276	203.943309
2017	Hexaflumuron	86479-06-3	8.172		C7H2Cl2NO2	201.94571	201.946259
2017	Hexaflumuron	86479-06-3	8.172		C6H2Cl(37Cl)NO	175.947845	175.948394
2017	Hexaflumuron	86479-06-3	8.172		C6H2Cl2NO	173.950795	173.951344
2014	Imibenconazole	86598-92-7	30.864	409.9927	C17H13N4SCl3		
2014	Imibenconazole	86598-92-7	30.864		C17H13N4SCl2	375.023249	375.023798
2014	Imibenconazole	86598-92-7	30.864		C10H7N4Cl2	253.004228	253.004777
2014	Imibenconazole	86598-92-7	30.864		C7H3NCl2	170.963706	170.964255
2014	Imibenconazole	86598-92-7	30.864		C7H6Cl	125.015254	125.015803
2015	Iprobenfos	26087-47-8	11.99	288.0949	C13H21O3PS		
2015	Iprobenfos	26087-47-8	11.99		C7H9O3PS	204.000453	204.001001
2015	Iprobenfos	26087-47-8	11.99		C7H7	91.054227	91.054775
2015	Isazofos (Miral)	42509-80-8	11.77	313.0417	C9H17N3O3PSCI		
2015	Isazofos (Miral)	42509-80-8	11.77		C7H13N3O3PSCI	285.009828	285.010376
2015	Isazofos (Miral)	42509-80-8	11.77		C5H9N3O3PSCI	256.978527	256.979076
2015	Isazofos (Miral)	42509-80-8	11.77		C5H9N3OCI	162.042866	162.043415
2015	Isazofos (Miral)	42509-80-8	11.77		C5H8N3OCI	161.035041	161.03559
2015	Isazofos (Miral)	42509-80-8	11.77		C2H2N3OCI	118.988091	118.988639
2015	isocarbamid (Azolamide)	30979-48-7	11.173	185.1164	C8H15N3O2		
2015	isocarbamid (Azolamide)	30979-48-7	11.173		C5H8N3O2	142.061103	142.061652
2015	isocarbamid (Azolamide)	30979-48-7	11.173		C4H8N3O2	130.061103	130.061652
2015	isocarbamid (Azolamide)	30979-48-7	11.173		C5H8NO	98.06004	98.060589
2015	Isocarbophos (Isocarbofos)	24353-61-5	14.305	289.0538	C11H16NO4PS		
2015	Isocarbophos (Isocarbofos)	24353-61-5	14.305		C8H9NO3PS	230.003527	230.004075
2015	Isocarbophos (Isocarbofos)	24353-61-5	14.305		C7H4OS	135.997737	135.998285
2015	Isocarbophos (Isocarbofos)	24353-61-5	14.305		C7H5O2	121.028406	121.028954
2015	Isocarbophos (Isocarbofos)	24353-61-5	14.305		C7H4O2	120.020581	120.021129
2017	Isodrin	465-73-6	14.7	361.87572	C12H8Cl6		
2017	Isodrin	465-73-6	14.7		C7H2Cl3(37Cl)2	264.853465	264.854013
2017	Isodrin	465-73-6	14.7		C7H2Cl4(37Cl)	262.856415	262.856963
2017	Isodrin	465-73-6	14.7		C7H2Cl5	260.859365	260.859913
2017	Isodrin	465-73-6	14.7		C7H4Cl(37Cl)2	196.931409	196.931958
2017	Isodrin	465-73-6	14.7		C7H4Cl2(37Cl)	194.934359	194.934908
2017	Isodrin	465-73-6	14.7		C7H4Cl3	192.93731	192.937858
2018	Isofenphos	25311-71-1	15.2	345.116369	C15H24NO4PS		
2018	Isofenphos	25311-71-1	15.2		C7H5O2	121.0284064	121.028955
2018	Isofenphos	25311-71-1	15.2		C9H10O4P	213.0311244	213.031673
2018	Isofenphos	25311-71-1	15.2		C7H6O4P	184.9998244	185.000373

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2018	Isoprocarb	2631-40-5	8.9	193.110279	C11H15NO2		
2018	Isoprocarb	2631-40-5	8.9		C8H9O	121.0647904	121.065339
2018	Isoprocarb	2631-40-5	8.9		C9H12O	136.0882664	136.088815
2018	Isoprocarb	2631-40-5	8.9		C8H7	103.0542264	103.054775
2017	Isoxaben	82558-50-7	23.698	332.17361	C18H24N2O4		
2017	Isoxaben	82558-50-7	23.698		C9H9O3	165.054621	165.055169
2017	Isoxaben	82558-50-7	23.698		C8O3H6	150.031145	150.031694
2017	Isoxaben	82558-50-7	23.698		C6O2H3	107.012756	107.013304
2018	Isoxaflutole	141112-29-0	14.4	359.043914	C15H12F3NO4S		
2018	Isoxaflutole	141112-29-0	14.4		C14H8F3NO2	279.0501644	279.050713
2018	Isoxaflutole	141112-29-0	14.4		C7H3F3O	160.0130504	160.013599
2018	Isoxaflutole	141112-29-0	14.4		C13H7F3O2	252.0392654	252.039814
2017	Isoxathion	18854-01-8	17.501	313.05377	C13H16NO4PS		
2017	Isoxathion	18854-01-8	17.501		C9H7NOS	177.024286	177.024835
2017	Isoxathion	18854-01-8	17.501		C8H4NO	130.02874	130.029289
2017	Isoxathion	18854-01-8	17.501		C7H5O	105.033491	105.03404
2017	Lenacil	2164-08-1	19.295	234.13683	C13H18N2O2		
2017	Lenacil	2164-08-1	19.295		C7H9N2O2	153.065854	153.066403
2017	Lenacil	2164-08-1	19.295		C7NO2H6	136.039305	136.039853
2017	Leptophos	21609-90-5	22.387	409.86996	C13H10BrClO2PS		
2017	Leptophos	21609-90-5	22.387		C13H10(81Br)(37Cl)O2PS	378.895557	378.896105
2017	Leptophos	21609-90-5	22.387		C13H10(81Br)ClO2PS	376.898507	376.899055
2017	Leptophos	21609-90-5	22.387		C13H10BrClO2PS	374.900553	374.901102
2017	Leptophos	21609-90-5	22.387		CH8CIP5S	241.871783	241.872332
2017	Leptophos	21609-90-5	22.387		C7H8OPS	171.002799	171.003348
2017	Leptophos	21609-90-5	22.387		C7H8O2P	155.025643	155.026191
2014	Lethane 384	112-56-1	8.822	203.098	C9H17NO2S		
2014	Lethane 384	112-56-1	8.822		C5H8NOS	130.032111	130.03266
2014	Lethane 384	112-56-1	8.822		C5H9O2	101.059706	101.060255
2014	Lethane 384	112-56-1	8.822		C3H4NS	86.005896	86.006445
2014	Lethane 384	112-56-1	8.822		C2H4S	60.002822	60.003371
2014	Lethane 384	112-56-1	8.822		C4H9	57.069877	57.070425
2015	Mefenpyr-diethyl	135590-91-9	20.59	372.0644	C16H18N2O4Cl2		
2015	Mefenpyr-diethyl	135590-91-9	20.59		C13H13N2O2Cl2	299.034859	299.035408
2015	Mefenpyr-diethyl	135590-91-9	20.59		C11H7N2OCl2	252.992995	252.993543
2015	Mefenpyr-diethyl	135590-91-9	20.59		C10H9N2Cl2	227.01373	227.014279
2014	Mefluidide	53780-34-0	20.59	310.0599	C11H13N2O3SF3		
2014	Mefluidide	53780-34-0	20.59		C9H11N2O2SF3	268.048784	268.049333
2014	Mefluidide	53780-34-0	20.59		C10H13N2O	177.102239	177.102788

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2014	Mefluidide	53780-34-0	20.59		C8H11N2	135.091675	135.092223
2017	Mepronil	55814-41-0	18.63	269.14158	C17H19NO2		
2017	Mepronil	55814-41-0	18.63		C17H19NO2	269.14103	269.141579
2017	Mepronil	55814-41-0	18.63		C14H10O2	210.067531	210.06808
2017	Mepronil	55814-41-0	18.63		C8H7O	119.049141	119.04969
2017	Mepronil	55814-41-0	18.63		C7H7	91.054227	91.054775
2014	Methabenzthiazuron	18691-97-9	10.08	221.0623	C10H11N3OS		
2014	Methabenzthiazuron	18691-97-9	10.08		C8H8N2S	164.04027	164.040819
2014	Methabenzthiazuron	18691-97-9	10.08		C8H7N2S	163.032445	163.032994
2014	Methabenzthiazuron	18691-97-9	10.08		C7H6NS	136.021546	136.022095
2014	Methabenzthiazuron	18691-97-9	10.08		C7H5NS	135.013721	135.01427
2014	Methabenzthiazuron	18691-97-9	10.08		C6H4S	108.002822	108.003371
2017	Methoprene	40596-69-8	15.49	310.25079	C19H34O3		
2017	Methoprene	40596-69-8	15.49		C6H7O2	111.044056	111.044604
2017	Methoprene	40596-69-8	15.49		C8H13	109.101177	109.101725
2017	Methoprene	40596-69-8	15.49		C8H11	107.085527	107.086075
2017	Methoprene	40596-69-8	15.49		C7H7	91.054227	91.054775
2017	Methoprene	40596-69-8	15.49		C6H9	81.069877	81.070425
2017	Methoprene	40596-69-8	15.49		C4H9O	73.064791	73.06534
2018	Metobromuron	3060-89-7	7	258.000389	C9H11BrN2O2		
2018	Metobromuron	3060-89-7	7		C7H4BrNO	196.9470764	196.947625
2018	Metobromuron	3060-89-7	7		C6H4BrN	168.9521614	168.95271
2018	Metobromuron	3060-89-7	7		C6H4N	90.03382542	90.034374
2017	Metolachlor	51218-45-2	13.912	283.13391	C15H22ClNO2		
2017	Metolachlor	51218-45-2	13.912		C13H17ClNO	238.099318	238.099867
2017	Metolachlor	51218-45-2	13.912		C11H16N	162.127726	162.128275
2017	Metolachlor	51218-45-2	13.912		C10NH12	146.096426	146.096974
2018	Metrafenone	220899-03-6	23.8	408.057236	C19H21BrO5		
2018	Metrafenone	220899-03-6	23.8		C18H18BrO5	393.0332124	393.033761
2018	Metrafenone	220899-03-6	23.8		C18H18BrO4	377.0382974	377.038846
2018	Metrafenone	220899-03-6	23.8		C11H13O4	209.0808364	209.081385
2019	Mexacarbate	315-18-4	12.56	222.136828	C12H18N2O2		
2019	Mexacarbate	315-18-4	12.56		C10H15NO	165.1148154	165.115364
2019	Mexacarbate	315-18-4	12.56		C10H14NO	164.1069904	164.107539
2019	Mexacarbate	315-18-4	12.56		C9H12NO	150.0913404	150.091889
2019	Mexacarbate	315-18-4	12.56		C12H18N2O2	222.1362794	222.136828
2019	MGK-264	113-48-4	15.25	275.188529	C17H25NO2		
2019	MGK-264	113-48-4	15.25		C9H10NO2	164.0706054	164.071154

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2019	MGK-264	113-48-4	15.25		C8H9O	121.0647904	121.065339
2019	MGK-264	113-48-4	15.25		C5H5NO2	111.0314804	111.032029
2019	MGK-264	113-48-4	15.25		C4H4NO2	98.02365542	98.024204
2017	Monuron	150-68-5	6.443	198.05599	C9H11ClN2O		
2017	Monuron	150-68-5	6.443		C7H4(37Cl)NO	154.994643	154.995191
2017	Monuron	150-68-5	6.443		C7H4ClNO	152.997593	152.998141
2017	Monuron	150-68-5	6.443		C6H4ClN	125.002678	125.003227
2017	Monuron	150-68-5	6.443		C6H4N	90.033826	90.034374
2019	Naled	300-76-5	10.79	377.782576	C4H7Br2Cl2O4P		
2019	Naled	300-76-5	10.79		C2H7ClO3P	144.9815874	144.982136
2019	Naled	300-76-5	10.79		C4H7ClO4P	184.9765024	184.977051
2019	Naled	300-76-5	10.79		C2H6O3P	109.0049094	109.005458
2019	Naled	300-76-5	10.79		CH4O2P	78.99434442	78.994893
2017	Nicotine	54-11-5	7.641	162.1157	C10H14N2		
2017	Nicotine	54-11-5	7.641		C10H13N2	161.107325	161.107873
2017	Nicotine	54-11-5	7.641		C8H9N2	133.076025	133.076573
2017	Nicotine	54-11-5	7.641		C5H10N	84.080776	84.081324
2017	Nitrofen	1836-75-5	17.522	282.9803	C12H7Cl2NO3		
2017	Nitrofen	1836-75-5	17.522		C12H7Cl(37Cl)NO3	284.9768	284.977348
2017	Nitrofen	1836-75-5	17.522		C12H7Cl2NO3	282.97975	282.980298
2017	Nitrofen	1836-75-5	17.522		C12H7Cl2O2	252.981761	252.98231
2017	Nitrofen	1836-75-5	17.522		C12H7(37Cl)O	204.015044	204.015592
2017	Nitrofen	1836-75-5	17.522		C12H7ClO	202.017994	202.018543
2017	Nitrofen	1836-75-5	17.522		C10H7Cl	162.023079	162.023628
2017	Nitrofen	1836-75-5	17.522		C11H7	139.054227	139.054775
2014	Nitrothal-isopropyl	10552-74-6	14.33	295.1056	C14H17NO6		
2014	Nitrothal-isopropyl	10552-74-6	14.33		C11H12NO6	254.065914	254.066462
2014	Nitrothal-isopropyl	10552-74-6	14.33		C11H10NO5	236.055349	236.055897
2014	Nitrothal-isopropyl	10552-74-6	14.33		C8H6NO6	212.018963	212.019512
2014	Nitrothal-isopropyl	10552-74-6	14.33		C8H4NO5	194.008399	194.008947
2017	Novaluron	116714-46-6	7.782	492.01231	C17H9ClF8N2O4		
2017	Novaluron	116714-46-6	7.782		C6H6ClF8NO2	310.995383	310.995932
2017	Novaluron	116714-46-6	7.782		C9H6ClF6NO2	308.998577	308.999125
2017	Novaluron	116714-46-6	7.782		C6H5(37Cl)NO	144.002468	144.003016
2017	Novaluron	116714-46-6	7.782		C6H5ClNO	142.005418	142.005966
2017	Novaluron	116714-46-6	7.782		C5H5ClN	114.010503	114.011052
2014	O.O.O-Triethylphosphorothioate	126-68-1	6.596	198.048	C6H15O3PS		
2014	O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H8O3PS	142.992628	142.993176
2014	O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H7O2PS	125.989888	125.990437

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2014	O.O.O-Triethylphosphorothioate	126-68-1	6.596		C4H10O2P	121.041292	121.041841
2014	O.O.O-Triethylphosphorothioate	126-68-1	6.596		H4O3PS	114.961328	114.961876
2014	O.O.O-Triethylphosphorothioate	126-68-1	6.596		H3O3PS	113.953503	113.954051
2014	O.O.O-Triethylphosphorothioate	126-68-1	6.596		H2O2PS	96.950763	96.951312
2014	O.O.O-Triethylphosphorothioate	126-68-1	6.596		C2H6O2P	93.009992	93.010541
2019	Orbencarb	34622-58-7	14.16	257.064114	C12H16CINOS		
2019	Orbencarb	34622-58-7	14.16		C12H16NOS	222.0947124	222.095261
2019	Orbencarb	34622-58-7	14.16		C7H6Cl	125.0152544	125.015803
2019	Orbencarb	34622-58-7	14.16		C5H10NO	100.0756904	100.076239
2014	Oryzalin	19044-88-3	13.91	346.0947	C12H18N4O6S		
2014	Oryzalin	19044-88-3	13.91		C10H13N4O6S	317.055031	317.05558
2014	Oryzalin	19044-88-3	13.91		C10H13N4O5S	301.060117	301.060665
2014	Oryzalin	19044-88-3	13.91		C7H7N4O6S	275.008081	275.00863
2014	Oryzalin	19044-88-3	13.91		C7H4N3O6S	257.981532	257.982081
2018	Oxadiargyl	39807-15-3	18.2	340.038149	C15H14Cl2N2O3		
2018	Oxadiargyl	39807-15-3	18.2		C8H5ClN	150.0105034	150.011052
2018	Oxadiargyl	39807-15-3	18.2		C9H5Cl2NO	212.9742714	212.97482
2018	Oxadiargyl	39807-15-3	18.2		C8H5Cl2N	184.9793564	184.979905
2018	Oxasulfuron	144651-06-9	12.5	406.094707	C17H18N4O6S		
2018	Oxasulfuron	144651-06-9	12.5		C8H12NS	154.0684974	154.069046
2018	Oxasulfuron	144651-06-9	12.5		C5H5N3O6	203.0172884	203.017837
2018	Oxasulfuron	144651-06-9	12.5		C6H7S	111.0262984	111.026847
2018	Oxyfluorfen	42874-03-3	17.2	361.032871	C15H11ClF3NO4		
2018	Oxyfluorfen	42874-03-3	17.2		C13H7F3O2	252.0392654	252.039814
2018	Oxyfluorfen	42874-03-3	17.2		C13H6ClF3NO2	300.0033674	300.003916
2018	Oxyfluorfen	42874-03-3	17.2		C15H11ClF3NO4	361.0323224	361.032871
2018	Penflufen	494793-67-8	18.7	317.19034	C18H24FN3O		
2018	Penflufen	494793-67-8	18.7		C6H6FN2O	141.0458674	141.046416
2018	Penflufen	494793-67-8	18.7		C15H17FN3O	274.1350164	274.135565
2018	Penflufen	494793-67-8	18.7		C18H24FN3O	317.1897914	317.19034
2014	Pentanochlor	2307-68-8	13.56	239.1077	C13H18NOCl		
2014	Pentanochlor	2307-68-8	13.56		C10H12NOCl	197.060193	197.060742
2014	Pentanochlor	2307-68-8	13.56		C7H8NCl	141.033978	141.034527
2018	Penthiopyrad	183675-82-3	18.4	359.127918	C16H20F3N3OS		
2018	Penthiopyrad	183675-82-3	18.4		C12H11F3N3OS	302.0569444	302.057493
2018	Penthiopyrad	183675-82-3	18.4		C16H20F3N3OS	359.1273694	359.127918
2018	Penthiopyrad	183675-82-3	18.4		C6H4F3N2O	177.0270234	177.027572
2014	Pethoxamid	106700-29-2	15.54	295.1339	C16H22NO2Cl		
2014	Pethoxamid	106700-29-2	15.54		C15H19NO2Cl	280.109883	280.110432

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2014	Pethoxamid	106700-29-2	15.54		C16H22NO2	260.164505	260.165054
2014	Pethoxamid	106700-29-2	15.54		C13H15NOCl	236.083668	236.084217
2014	Pethoxamid	106700-29-2	15.54		C13H14NO2	216.101905	216.102454
2014	Pethoxamid	106700-29-2	15.54		C10H11	131.085527	131.086075
2019	Pindone	83-26-1	12.46	230.094295	C14H14O3		
2019	Pindone	83-26-1	12.46		C10H5O3	173.0233214	173.02387
2019	Pindone	83-26-1	12.46		C9H6O2	146.0362314	146.03678
2019	Pindone	83-26-1	12.46		C7H5O	105.0334914	105.03404
2019	Pindone	83-26-1	12.46		C14H14O3	230.0937464	230.094295
2018	Piperonylbutoxide	51-03-6	20.2	338.209325	C19H30O5		
2018	Piperonylbutoxide	51-03-6	20.2		C11H12O2	176.0831814	176.08373
2018	Piperonylbutoxide	51-03-6	20.2		C9H9O2	149.0597054	149.060254
2018	Piperonylbutoxide	51-03-6	20.2		C9H11	119.0855264	119.086075
2018	Pirimiphos-ethyl	23505-41-1	14.7	333.127602	C13H24N3O3PS		
2018	Pirimiphos-ethyl	23505-41-1	14.7		C7H10N3S	168.0589954	168.059544
2018	Pirimiphos-ethyl	23505-41-1	14.7		C12H21N3O3PS	318.1035784	318.104127
2018	Pirimiphos-ethyl	23505-41-1	14.7		C11H19N3O3PS	304.0879284	304.088477
2014	Plifenate	21757-82-4	12.769	333.8889	C10H7O2Cl5		
2014	Plifenate	21757-82-4	12.769		C8H4Cl4	239.906162	239.906711
2014	Plifenate	21757-82-4	12.769		C9H7O2Cl2	216.981761	216.98231
2014	Plifenate	21757-82-4	12.769		C7H3OCl2	172.955547	172.956095
2014	Plifenate	21757-82-4	12.769		C8H4Cl2	169.968457	169.969006
2015	Pretilachlor	51218-49-6	16.81	311.1652	C17H26NO2Cl		
2015	Pretilachlor	51218-49-6	16.81		C16H24NO2	262.180155	262.180704
2015	Pretilachlor	51218-49-6	16.81		C13H17NOCl	238.099318	238.099867
2015	Pretilachlor	51218-49-6	16.81		C12H16NOCl	225.091493	225.092042
2015	Pretilachlor	51218-49-6	16.81		C13H16NO	202.122641	202.123189
2015	Pretilachlor	51218-49-6	16.81		C11H14NO	176.10699	176.107539
2015	Pretilachlor	51218-49-6	16.81		C11H16N	162.127726	162.128275
2014	Profluralin	26399-36-0	11.305	347.1093	C14H16N3O4F3		
2014	Profluralin	26399-36-0	11.305		C14H15N3O3F3	330.106002	330.106551
2014	Profluralin	26399-36-0	11.305		C12H11N3O4F3	318.069617	318.070166
2019	Promecarb	2631-37-0	11.07	207.125928	C12H17NO2		
2019	Promecarb	2631-37-0	11.07		C9H11O	135.0804404	135.080989
2019	Promecarb	2631-37-0	11.07		C7H7	91.05422642	91.054775
2019	Promecarb	2631-37-0	11.07		C8H11	107.0855264	107.086075
2019	Promecarb	2631-37-0	11.07		C10H14O	150.1039164	150.104465
2014	Propachlor	1918-16-7	9.609	211.0764	C11H14NOCl		
2014	Propachlor	1918-16-7	9.609		C11H14NO	176.10699	176.107539

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2014	Propachlor	1918-16-7	9.609		C8H8NOCl	169.028893	169.029442
2014	Propachlor	1918-16-7	9.609		C8H10N	120.080776	120.081324
2014	Propachlor	1918-16-7	9.609		C7H6NO	120.04439	120.044939
2018	Propanil	709-98-8	12.4	217.00612	C9H9Cl2NO		
2018	Propanil	709-98-8	12.4		C6H5Cl2N	160.9793564	160.979905
2018	Propanil	709-98-8	12.4		C6H5(37Cl)ClN	162.9764064	162.976955
2018	Propanil	709-98-8	12.4		C9H9Cl2NO	217.0055714	217.00612
2015	Propaphos	7292-16-2	15.74	304.0898	C13H21O4PS		
2015	Propaphos	7292-16-2	15.74		C10H15O4PS	262.042318	262.042866
2015	Propaphos	7292-16-2	15.74		C7H9O4PS	219.995367	219.995916
2015	Propaphos	7292-16-2	15.74		C7H7O3PS	201.984803	201.985351
2015	Propaphos	7292-16-2	15.74		C7H8OS	140.029037	140.029586
2019	Propetamphos	31218-83-4	11.95	281.085069	C10H20NO4PS		
2019	Propetamphos	31218-83-4	11.95		C3H9NOPS	138.0137004	138.014249
2019	Propetamphos	31218-83-4	11.95		C5H7O4PS	193.9797214	193.98027
2019	Propetamphos	31218-83-4	11.95		CH5NOPS	109.9824004	109.982949
2019	Propetamphos	31218-83-4	11.95		C7H13NO3PS	222.0348304	222.035379
2018	Proquinazid	189278-12-4	20	381.965431	C14H8Cl3F3N2O		
2018	Proquinazid	189278-12-4	20		C8H5IN2O2	287.9390314	287.93958
2018	Proquinazid	189278-12-4	20		C7H4INO	244.9332174	244.933766
2018	Proquinazid	189278-12-4	20		C8H3INO2	271.9203074	271.920856
2018	Pyraclufos	89784-60-1	23.7	360.046431	C14H18ClN2O3PS		
2018	Pyraclufos	89784-60-1	23.7		C9H7ClN2O	194.0241424	194.024691
2018	Pyraclufos	89784-60-1	23.7		H2O2PS	96.95076642	96.951315
2018	Pyraclufos	89784-60-1	23.7		C14H18ClN2O3PS	360.0458824	360.046431
2018	Pyridalyl	179101-81-6	26.8	488.96799	C18H14Cl4F3NO3		
2018	Pyridalyl	179101-81-6	26.8		C9H9F3NO	204.0630744	204.063623
2018	Pyridalyl	179101-81-6	26.8		C3H3Cl2	108.9606324	108.961181
2018	Pyridalyl	179101-81-6	26.8		C6H5F3NO	164.0317744	164.032323
2019	Pyroquilon	57369-32-1	12.25	173.084064	C11H11NO		
2019	Pyroquilon	57369-32-1	12.25		C11H11NO	173.0835154	173.084064
2019	Pyroquilon	57369-32-1	12.25		C9H8N	130.0651254	130.065674
2019	Pyroquilon	57369-32-1	12.25		C10H10N	144.0807754	144.081324
2019	Pyroquilon	57369-32-1	12.25		C11H10NO	172.0756904	172.076239
2019	Quinoclamine	2797-51-5	15.15	207.008707	C10H6ClNO2		
2019	Quinoclamine	2797-51-5	15.15		C10H6ClNO2	207.0081584	207.008707
2019	Quinoclamine	2797-51-5	15.15		C10H6NO2	172.0393054	172.039854
2019	Quinoclamine	2797-51-5	15.15		C9H6NO	144.0443904	144.044939
2015	Rabenzazole	40341-04-6	14.168	212.1062	C12H12N4		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2015	Rabenzazole	40341-04-6	14.168		C12H9N3	195.079099	195.079647
2015	Rabenzazole	40341-04-6	14.168		C10H8N3	170.071274	170.071822
2015	Rabenzazole	40341-04-6	14.168		C7H6N2	118.05255	118.053098
2014	Resmethrin	10453-86-8	20.208	338.1882	C22H26O3		
2014	Resmethrin	10453-86-8	20.208		C12H11O	171.080441	171.08099
2014	Resmethrin	10453-86-8	20.208		C11H11	143.085527	143.086075
2014	Resmethrin	10453-86-8	20.208		C10H8	128.062052	128.0626
2014	Resmethrin	10453-86-8	20.208		C9H15	123.116827	123.117375
2015	Schradan	152-16-9	10.886	286.1324	C8H24N4O3P2		
2015	Schradan	152-16-9	10.886		C6H19N3O3P2	243.089616	243.090165
2015	Schradan	152-16-9	10.886		C4H13N2O3P2	199.039592	199.04014
2015	Schradan	152-16-9	10.886		C4H14N2O2P	153.078741	153.079289
2015	Schradan	152-16-9	10.886		C4H12N2OP	135.068176	135.068725
2018	Sebuthylazine	7286-69-3	12.73	229.109423	C9H16CIN5		
2018	Sebuthylazine	7286-69-3	12.73		C9H16CIN5	229.108875	229.109423
2018	Sebuthylazine	7286-69-3	12.73		C8H3CIN5	204.00715	204.007698
2018	Sebuthylazine	7286-69-3	12.73		C7H11CIN5	200.06975	200.070298
2018	Sebuthylazine	7286-69-3	12.73		C7H11(37Cl)N5	200.06975	200.070298
2018	Sebuthylazine	7286-69-3	12.73		C5H7CIN5	172.03845	172.038998
2018	Sebuthylazine	7286-69-3	12.73		C5H8N5	138.077422	138.07797
2018	Silafluofen	105024-66-6	27	408.192086	C25H29FO2Si		
2018	Silafluofen	105024-66-6	27		C10H15OSi	179.0886694	179.089218
2018	Silafluofen	105024-66-6	27		C15H15FOSi	258.0870724	258.087621
2018	Silafluofen	105024-66-6	27		C17H19FOSi	286.1183724	286.118921
2018	Simazine	122-34-9	11.63	201.078123	C7H12CIN5		
2018	Simazine	122-34-9	11.63		C7H12CIN5	201.077575	201.078123
2018	Simazine	122-34-9	11.63		C6H9CIN5	186.0541	186.054648
2018	Simazine	122-34-9	11.63		C5H8CIN5	173.046275	173.046823
2018	Simazine	122-34-9	11.63		C4H7CIN5	160.03845	160.038998
2018	Simazine	122-34-9	11.63		C4H4CIN4	143.011901	143.012449
2018	Simazine	122-34-9	11.63		C5H8N5	138.077422	138.07797
2018	Simazine	122-34-9	11.63		C5H7N4	123.066523	123.067071
2018	Simetryn	1014-70-6	13.6	213.104817	C8H15N5S		
2018	Simetryn	1014-70-6	13.6		C8H15N5S	213.104269	213.104817
2018	Simetryn	1014-70-6	13.6		C7H12N5S	198.080794	198.081342
2018	Simetryn	1014-70-6	13.6		C6H11N5S	185.072968	185.073516
2018	Simetryn	1014-70-6	13.6		C5H8N5S	170.049494	170.050042
2018	Simetryn	1014-70-6	13.6		C5H7N4S	155.038595	155.039143
2019	Sulfallate	95-06-7	11.3	223.025621	C8H14CINS2		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2019	Sulfallate	95-06-7	11.3		C8H14NS2	188.0562194	188.056768
2019	Sulfallate	95-06-7	11.3		C3H6NS	88.02154742	88.022096
2019	Sulfallate	95-06-7	11.3		C4H10N	72.08077542	72.081324
2019	Sulfallate	95-06-7	11.3		CH2NS	59.99024742	59.990796
2019	SWEP	1918-18-9	11.82	218.985385	C8H7Cl2NO2		
2019	SWEP	1918-18-9	11.82		C7H3Cl2NO	186.9586214	186.95917
2019	SWEP	1918-18-9	11.82		C8H7Cl2NO2	218.9848364	218.985385
2019	SWEP	1918-18-9	11.82		C6H3ClN	123.9948534	123.995402
2019	SWEP	1918-18-9	11.82		C8H7Cl2NO2	218.9848364	218.985385
2019	SWEP	1918-18-9	11.82		C6H3ClN	123.9948534	123.995402
2015	Tebupirimfos	96182-53-5	12.047	318.1167	C13H23N2O3PS		
2015	Tebupirimfos	96182-53-5	12.047		C10H17N2O3PS	276.069201	276.06975
2015	Tebupirimfos	96182-53-5	12.047		C9H14N2O3PS	261.045726	261.046275
2015	Tebupirimfos	96182-53-5	12.047		C7H11N2O3PS	234.022251	234.022799
2015	Tebupirimfos	96182-53-5	12.047		C8H12N2O	152.094414	152.094963
2015	Tebupirimfos	96182-53-5	12.047		C7H9N2O	137.070939	137.071488
2018	Tebutam	35256-85-0	11.08	233.177964	C15H23NO		
2018	Tebutam	35256-85-0	11.08		C15H23NO	233.177416	233.177964
2018	Tebutam	35256-85-0	11.08		C12H16NO	190.122641	190.123189
2018	Tebutam	35256-85-0	11.08		C8H16NO	142.122641	142.123189
2018	Tebutam	35256-85-0	11.08		C7H7	91.054227	91.054775
2018	Tebutam	35256-85-0	11.08		C4H9	57.069877	57.070425
2019	Terbacil	5902-51-2	12.45	216.066556	C9H13ClN2O2		
2019	Terbacil	5902-51-2	12.45		C5H6ClN2O2	161.0112314	161.01178
2019	Terbacil	5902-51-2	12.45		C5H5ClN2O2	160.0034074	160.003956
2019	Terbacil	5902-51-2	12.45		C5H6(37Cl)N2O2	163.0082814	163.00883
2019	Terbacil	5902-51-2	12.45		C4H4ClNO	116.9975934	116.998142
2015	Terbufos	13071-79-9	11.31	288.0441	C9H21O2PS3		
2015	Terbufos	13071-79-9	11.31		C5H12O2PS3	230.973155	230.973703
2015	Terbufos	13071-79-9	11.31		C4H10O2PS	153.013363	153.013912
2015	Terbufos	13071-79-9	11.31		H2O2PS	96.950763	96.951312
2019	Tetrahydrophthalimide_cis-1-2-3-6	1469-48-3	9.41	151.063329	C8H9NO2		
2019	Tetrahydrophthalimide_cis-1-2-3-6	1469-48-3	9.41		C8H9NO2	151.0627804	151.063329
2019	Tetrahydrophthalimide_cis-1-2-3-6	1469-48-3	9.41		C7H9NO	123.0678654	123.068414
2019	Tetrahydrophthalimide_cis-1-2-3-6	1469-48-3	9.41		C7H8NO	122.0600404	122.060589
2018	Tetrasul	2227-13-6	18.5	321.894434	C12H6Cl4S		
2018	Tetrasul	2227-13-6	18.5		C12H6Cl2S	251.9561794	251.956728
2018	Tetrasul	2227-13-6	18.5		C12H6(37Cl)ClS	253.9532294	253.953778
2018	Tetrasul	2227-13-6	18.5		C12H6(37Cl)Cl3S	323.8909354	323.891484

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2014	Thenylchlor	96491-05-3	19.961	323.0747	C16H18NO2SCI		
2014	Thenylchlor	96491-05-3	19.961		C16H18NO2S	288.105276	288.105825
2014	Thenylchlor	96491-05-3	19.961		C7H6NO2S	168.011376	168.011924
2014	Thenylchlor	96491-05-3	19.961		C7H9OS	141.036862	141.037411
2014	Thenylchlor	96491-05-3	19.961		C9H10N	132.080776	132.081324
2014	Thenylchlor	96491-05-3	19.961		C6H7OS	127.021212	127.021761
2019	Thiocyclam-hydrogen-oxalate	31895-22-4	9.57	271.000675	C7H13NO4S3		
2019	Thiocyclam-hydrogen-oxalate	31895-22-4	9.57		C4H9NS2	135.0170944	135.017643
2019	Thiocyclam-hydrogen-oxalate	31895-22-4	9.57		C3H6N	56.04947542	56.050024
2019	Thiocyclam-hydrogen-oxalate	31895-22-4	9.57		C4H9N	71.07295042	71.073499
2014	Tiocarbazil	36756-79-3	14.25	279.1657	C16H25NOS		
2014	Tiocarbazil	36756-79-3	14.25		C9H18NO	156.138291	156.138839
2014	Tiocarbazil	36756-79-3	14.25		C5H10NO	100.07569	100.076239
2014	Tiocarbazil	36756-79-3	14.25		C7H7	91.054227	91.054775
2018	Tralkoxydim	87820-88-0	22.8	329.199094	C20H27NO3		
2018	Tralkoxydim	87820-88-0	22.8		C7H7NO2	137.0471304	137.047679
2018	Tralkoxydim	87820-88-0	22.8		C6H7NO	109.0522154	109.052764
2018	Tralkoxydim	87820-88-0	22.8		C18H21NO2	283.1566804	283.157229
2018	Tralomethrin	66841-25-6	29	660.809838	C22H19Br4NO3		
2018	Tralomethrin	66841-25-6	29		C13H9O	181.0647914	181.06534
2018	Tralomethrin	66841-25-6	29		C7H9Br2	250.9065484	250.907097
2018	Tralomethrin	66841-25-6	29		C6H9Br2O	254.9014624	254.902011
2018	Triadimenol	55219-65-3	16.35	295.108755	C14H18CIN3O2		
2018	Triadimenol	55219-65-3	16.35		C8H14N3O	168.113139	168.113687
2018	Triadimenol	55219-65-3	16.35		C8H12N3	150.102573	150.103121
2018	Triadimenol	55219-65-3	16.35		C6H5ClO	128.002345	128.002893
2018	Triadimenol	55219-65-3	16.35		C4H6N3O	112.050539	112.051087
2018	Triallate	2303-17-5	12.63	303.00182	C10H16Cl3NOS		
2018	Triallate	2303-17-5	12.63		C10H16(37Cl)2NOS	268.032419	268.032967
2018	Triallate	2303-17-5	12.63		C10H16Cl2NOS	268.032419	268.032967
2018	Triallate	2303-17-5	12.63		C3H2Cl3	142.921661	142.922209
2018	Triallate	2303-17-5	12.63		C7H14NO	128.106991	128.107539
2018	Triallate	2303-17-5	12.63		C4H8NO	86.060041	86.060589
2019	Trietazine	1912-26-1	12.04	229.109423	C9H16CIN5		
2019	Trietazine	1912-26-1	12.04		C7H11CIN5	200.0697494	200.070298
2019	Trietazine	1912-26-1	12.04		C6H9CIN5	186.0540994	186.054648
2019	Trietazine	1912-26-1	12.04		C8H13CIN5	214.0853994	214.085948
2019	Trietazine	1912-26-1	12.04		C9H16CIN5	229.1088744	229.109423
2015	Tribufos	78-48-8	16.82	314.0962	C12H27OPS3		

	Compound	CAS	Rt	Molecular weight	Formula	Fragment m/z -e	Fragment m/z neutral
2015	Tribufos	78-48-8	16.82		C8H19OPS3	258.033015	258.033564
2015	Tribufos	78-48-8	16.82		C8H19OPS2	226.060945	226.061493
2015	Tribufos	78-48-8	16.82		C4H11OPS3	201.970415	201.970964
2015	Tribufos	78-48-8	16.82		C4H10OPS2	168.990519	168.991068
2015	Tribufos	78-48-8	16.82		H4OPS3	146.91564	146.916188
2018	Trichloronate	327-98-0	14.4	331.936124	C10H12Cl3O2PS		
2018	Trichloronate	327-98-0	14.4		C2H6OPS	108.9871514	108.9877
2018	Trichloronate	327-98-0	14.4		C8H8Cl2O2PS	268.9354224	268.935971
2018	Trichloronate	327-98-0	14.4		C10H12Cl2O2PS	296.9667224	296.967271
2014	Triclopyr-methylester	60825-26-5	11.3	268.9413	C8H6NO3Cl3		
2014	Triclopyr-methylester	60825-26-5	11.3		C6H3NOCl3	209.927473	209.928022
2014	Triclopyr-methylester	60825-26-5	11.3		C5HNCl3	179.916909	179.917457
2018	Triflumizole	68694-11-1	15.6	345.085574	C15H15ClF3N3O		
2018	Triflumizole	68694-11-1	15.6		C8H4ClF3N	205.9978874	205.998436
2018	Triflumizole	68694-11-1	15.6		C7H3ClF3	178.9869884	178.987537
2018	Triflumizole	68694-11-1	15.6		C12H12ClF3NO	278.0554024	278.055951
2019	Vernolate	1929-77-7	9.01	203.134386	C10H21NOS		
2019	Vernolate	1929-77-7	9.01		C7H14NO	128.1069904	128.107539
2019	Vernolate	1929-77-7	9.01		C4H8NO	86.06004042	86.060589
2019	Vernolate	1929-77-7	9.01		C7H15NOS	161.0868874	161.087436
2019	Vernolate	1929-77-7	9.01		C7H16NS	146.0997974	146.100346
2014	XMC	2655-14-3	6.67	179.0946	C10H13NO2		
2014	XMC	2655-14-3	6.67		C8H10O	122.072616	122.073165
2014	XMC	2655-14-3	6.67		C7H7O	107.049141	107.04969