Accurate Mass Pesticide Database by LC-HRMS

1. Scope

This report shows a database of 188 pesticides by using liquid chromatography high resolution mass spectrometry (LC-HRMS).

2. Analytical conditions for the LC-HRMS

Settings for liquid chromatography:

- **Mobile phase A:** Water + 0.1 % Formic acid+ 5 mM Ammonium Formiate + 2 % MeOH
- **Mobile phase B:** MeOH + 0.1 % Formic acid+ 5 mM Ammonium Formiate + 2 % Water
- **Column:** C8 Zorbax Eclipse Plus 2.1x100mm, 1.8µm
- **Run Time:** 20 min
- **Injection volume:** 5 µL
- **Temperature of the column:** 35 °C
- **Gradient:**

Time (min)	A (%)	B (%)
0	80	20
2	80	20
15	0	100
17	0	100
17.1	80	20
20	80	20

Electrospray ion source parameters:

- **Gas 1:** 40 psi
- **Gas2:** 50 psi
- **Curtain Gas:** 25 psi
- **Temperature:** 350 °C
- **Spray Voltage:** 5500 V
- **Polarity:** Positive

Settings for mass spectrometry

- **Workflow:** SWATH (Full Scan + MS^2)
- **Cycle time:** 0.78 s
- **ToF MS accumulation time:** 0.2 s
- **ToF MS mas range:** 100-950 m/z
- **Number of mass windows**: 10
- **ToF MS/MS: accumulation time:** 0.05 s
- **ToF MS/MS mas range:** 50-950 m/z

NOTE:
IF YOU NEED THIS DATABASE IN .csv, .xls, … PLEASE, CONTACT WITH
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3. LC-HRMS Database

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Acephate	C4H10NO3PS	183.0119	[M+H]+	184.0192
Acephate_F1	C2H8NO3PS			142.9928
Acephate_F2	C4H4NOP			113.0025
Acetamiprid	C10H11ClN4	222.0672	[M+H]+	223.0745
Acetamiprid_F1	C6H5ClN			126.0105
Acetamiprid_F2	C6H4N			90.0338
Aldicarb	C7H14N2O2S	190.0776	[M+Na]+	213.0668
Aldicarb_F1	C5H10NS			116.0529
Aldicarb_F2	C4H9S			89.0420
Aldicarb sulfone	C7H14N2O4S	222.0674	[M+H]+	223.0747
Aldicarb sulfone_F1	C3H4NS			86.0601
Aldicarb sulfone_F2	C5H10NO2S			148.0427
Aldicarb sulfoxide	C7H14N2O3S	206.0725	[M+H]+	207.0798
Aldicarb sulfoxide_F1	C4H9S			89.0420
Aldicarb sulfoxide_F2	C5H10NOS			132.0478
Ametoctradin	C15H25N5	275.2110	[M+H]+	276.2183
Ametoctradin_F1	C8H11N5			177.1009
Ametoctradin_F2	C6H7N5			149.0696
Avermectin B1a	C48H72O14	872.4922	[M+Na]+	895.4814
Avermectin B1a_F1	C34H47O7			576.3316
Avermectin B1a_F2	C7H13O3			145.0859
Avermectin B1b	C47H70O14	858.4766	[M+Na]+	881.4658
Avermectin B1b_F1	C33H45O7			553.3160
Avermectin B1b_F2	C16H19O5			291.1227
Azinphos-methyl	C10H12N3O3PS2	317.0058	[M+H]+	318.0131
Azinphos-methyl_F1	C7H6N3			132.0443
Azoxystrobin	C22H17N3O5	403.1168	[M+H]+	404.1241
Azoxystrobin_F1	C21H14N3O4			372.0979
Azoxystrobin_F2	C20H14N3O3			344.1030
Bifenazate	C17H20N2O3	300.1474	[M+H]+	301.1547
Bifenazate_F1	C12H12N			170.0961
Bitertanol	C20H23N3O2	337.1790	[M+H]+	338.1863
Bitertanol_F1	C18H21O2			269.1536

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Bitertanol_F2	C6H11O			99.1000
Boscalid	C18H12Cl2N2O	342.0327	[M+H]+	343.0399
Boscalid_F1	C18H12ClN2O			307.0636
Boscalid_F2	C6H3NOCl			139.9898
Bromuconazole_I	C13H12BrCl2N3O	374.9541	[M+H]+	375.9614
Bromuconazole_I_F1	C7H5Cl2			158.9763
Bromuconazole_I_F2	C2H4N3			70.0400
Bromuconazole_II	C13H12BrCl2N3O	374.9541	[M+H]+	375.9614
Bromuconazole_II_F1	C7H5Cl2			158.9763
Bromuconazole_II_F2	C2H4N3			70.0400
Bupirimate	C13H24N4O3S	316.1569	[M+H]+	317.1642
Bupirimate_F1	C8H12N3O			166.0969
Bupirimate_F2	C2H6NO2S			108.0114
Buprofezin	C16H23N3OS	305.1562	[M+H]+	306.1635
Buprofezin_F1	C7H8N			106.0651
Buprofezin_F2	C4H9			57.0699
Carbaryl	C12H11NO2	201.0790	[M+H]+	202.0863
Carbaryl_F1	C10H9O			145.0648
Carbaryl_F2	C9H9			117.0699
Carbendazim	C9H9N3O2	191.0695	[M+H]+	192.0768
Carbendazim_F1	C8H6N3O			160.0505
Carbendazim_F2	C7H6N3			132.0556
Carbofuran	C12H15NO3	221.1052	[M+H]+	222.1125
Carbofuran_F1	C10H13O2			165.0910
Carbofuran_F2	C7H7O2			123.0441
Carbosulfan	C20H32N2O3S	380.2133	[M+H]+	381.2206
Carbosulfan_F1	C5H12NS			118.0685
Carbosulfan_F2	C2H6NS			76.0216
Chlorantraniliprole	C18H14BrCl2N5O2	480.9708	[M+H]+	481.9781
Chlorantraniliprole_F1	C10H8BrClN3			283.9585
Chlorfenvinphos	C12H14Cl3O4P	357.9695	[M+H]+	358.9768
Chlorfenvinphos_F1	C8H4Cl3			204.9377
Chlorfenvinphos_F2	C8H4Cl2			169.9685
Chlorpyrifos	C9H11Cl3NO3PS	348.9263	[M+H]+	349.9336

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Chlorpyrifos_F1	C5H3Cl3NO			197.9275
Chlorpyrifos-methyl	C7H7Cl3NO3PS	320.8950	[M+H]+	321.9023
Chlorpyrifos-methyl_F1	C6H4Cl3NO2PS			289.8758
Clofentezine	C14H8Cl2N4	302.0126	[M+H]+	303.0199
Clofentezine_F1	C7H5NCl			138.0103
Clomazone	C12H14ClNO2	239.0713	[M+H]+	240.0786
Clomazone_F1	C7H6Cl			125.0140
Clothianidin	C6H8ClN5O2S	249.0087	[M+H]+	250.0160
Clothianidin_F1	C4H3NSCl			131.9669
Clothianidin_F2	C4H5N2S			113.0168
Coumaphos	C14H16ClO5PS	362.0145	[M+H]+	363.0217
Coumaphos_F1	C9H8O3PS			226.9934
Cyazofamid	C13H13ClN4O2S	324.0448	[M+H]+	325.0521
Cyazofamid_F1	C2H6NO2S			108.0114
Cymoxanil	C7H10N4O3	198.0753	[M+H]+	199.0826
Cymoxanil_F1	C4H6N3O2			128.0455
Cymoxanil_F2	C3H3N2O			83.0239
Cyproconazole	C15H18ClN3O	291.1138	[M+H]+	292.1211
Cyproconazole_F1	C7H6Cl			125.0153
Cyproconazole_F2	C2H4N3			70.0400
Cyprodinil	C14H15N3	225.1266	[M+H]+	226.1339
Cyprodinil_F1	C7H10N			108.0808
Cyromazine	C6H10N6	166.0967	[M+H]+	167.1040
Cyromazine_F1	C2H5N4			85.0508
Dazomet	C5H10N2S2	162.0285	[M+H]+	163.0358
Dazomet_F1	C3H6NS2			119.9936
Dazomet_F2	C3H8NS			90.0372
DEET	C12H17NO	191.1310	[M+H]+	192.1383
DEET_F1	C8H7O			119.0491
DEET_F2	C7H7			91.0542
Demeton-S-Methyl-Sulfone	C6H15O5PS2	262.0099	[M+H]+	263.0171
Demeton-S-Methyl-Sulfone_F1	C4H10O3PS			169.0084
Demeton-S-methylsulfoxide	C6H15O4PS2	246.0149	[M+H]+	247.0222
Demeton-S-methylsulfoxide_F1	C2H8O4P			127.0155

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Diazinon	C12H21N2O3PS	304.1010	[M+H]+	305.1083
Diazinon_F1	C4H10O3PS			169.0790
Dichlorvos	C4H7Cl2O4P	219.9459	[M+H]+	220.9532
Dichlorvos_F1	C2H8O4P			127.0155
Dicrotophos	C8H16NO5P	237.0766	[M+H]+	238.0839
Dicrotophos_F1	C6H10NO			112.0756
Diethofencarb	C14H21NO4	267.1471	[M+H]+	268.1543
Diethofencarb_F1	C6H6NO2			124.0392
Difenoconazole	C19H17Cl2N3O3	405.0647	[M+H]+	406.0720
Difenoconazole_F1	C13H9OCl2			251.0028
Diflubenzuron	C14H9ClF2N2O2	310.0321	[M+H]+	311.0393
Diflubenzuron_F1	C7H3OF2			141.0147
Dimethoate	C5H12NO3PS2	228.9996	[M+H]+	230.0069
Dimethoate_F1	C2H6O2PS			124.9813
Dimethomorph	C21H22ClNO4	387.1237	[M+H]+	388.1310
Dimethomorph_F1	C17H14O3Cl			301.0626
Diniconazole	C15H17Cl2N3O	325.0749	[M+H]+	326.0821
Diniconazole_F1	C2H4N3			70.0400
Diniconazole_F2	C7H5Cl2			158.9763
Diuron	C9H10Cl2N2O	232.0170	[M+H]+	233.0243
Diuron_F1	C3H6NO			72.0442
Dodine	C13H29N3	227.2361	[M+H]+	228.2434
Dodine_F1	CH6N3			60.0556
Dodine_F2	C4H9			57.0699
Emamectin B1a	C49H75NO13	885.5239	[M+H]+	886.5311
Emamectin B1a_F1	C8H16NO2			158.1178
Epoxiconazole	C17H13ClFN3O	329.0731	[M+H]+	330.0804
Epoxiconazole_F1	C8H6F			121.0444
Ethion	C9H22O4P2S4	383.9876	[M+H]+	384.9949
Ethion_F1	CH4O2PS2			142.9381
Ethirimol	C11H19N3O	209.1528	[M+H]+	210.1601
Ethirimol_F1	C8H14NO			140.1070
Ethoprophos	C8H19O2PS2	242.0564	[M+H]+	243.0637
Ethoprophos_F1	H4O2PS2			130.9377

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Etofenprox	C25H28O3	376.2039	[M+NH4]+	394.2377
Etofenprox_F1	C12H17O			177.1274
Etoxazole	C21H23F2NO2	359.1697	[M+H]+	360.1770
Etoxazole_F1	C7H3OF2			141.0146
Etoxazole_F2	C17H16NO2F2			304.1144
Famoxadone	C22H18N2O4	374.1266	[M+NH4]+	392.1605
Famoxadone_F1	C14H11O			195.0804
Famoxadone_F2	C6H7N2			107.0604
Fenamidone	C17H17N3OS	311.1092	[M+H]+	312.1165
Fenamidone_F1	C6H6N			92.0490
Fenamiphos	C13H22NO3PS	303.1058	[M+H]+	304.1131
Fenamiphos_F1	C8H10O3PS			217.0083
Fenamiphos_F2	C7H7O3PS			201.9848
Fenamiphos-sulfone	C13H22NO5PS	335.0956	[M+H]+	336.1029
Fenamiphos-sulfone_F1	C8H13NO5PS			266.0242
Fenamiphos-sulfoxide	C13H22NO4PS	319.1007	[M+H]+	320.1080
Fenamiphos-sulfoxide_F1	C8H10O4PS			233.0034
Fenarimol	C17H12Cl2N2O	330.0327	[M+H]+	331.0399
Fenarimol_F1	C16H11NOCl			268.0523
Fenazaquin	C20H22N2O	306.1732	[M+H]+	307.1805
Fenazaquin_F1	C12H17			161.1323
Fenbuconazole	C19H17ClN4	336.1142	[M+H]+	337.1215
Fenbuconazole_F1	C7H6Cl			125.0151
Fenhexamid	C14H17Cl2NO2	301.0636	[M+H]+	302.0709
Fenhexamid_F1	C7H13			97.1005
Fenitrothion	C9H12NO5PS	277.0174	[M+H]+	278.0247
Fenitrothion_F1	C2H8O3PS			142.9926
Fenitrothion_F2	C7H5			89.0386
Fenoxycarb	C17H19NO4	301.1314	[M+H]+	302.1387
Fenoxycarb_F1	C3H6NO2			88.0385
Fenpropathrin	C22H23NO3	349.1678	[M+H]+	350.1751
Fenpropathrin_F1	C8H13O			125.0950
Fenpropimorph	C20H33NO	303.2562	[M+H]+	304.2635
Fenpropimorph_F1	C11H15			147.1161

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Fenpyrazamine	C17H21N3O2S	331.1354	[M+H]+	332.1427
Fenpyrazamine_F1	C13H16N3O			230.1279
Fenpyroximate	C24H27N3O4	421.2002	[M+H]+	422.2074
Fenpyroximate_F1	C20H20N3O4			366.1427
Fenthion	C10H15O3PS2	278.0200	[M+H]+	279.0273
Fenthion_F1	C8H9O3PS			216.0005
Fenthion-oxon-sulfone	C10H15O6PS	294.0327	[M+H]+	311.0171
Fenthion-oxon-sulfone_F1	C9H14O4P			217.0624
Fenthion-oxon-sulfone_F2	C7H4O			104.0296
Fipronil	C12H4Cl2F6N4OS	435.9387	[M-H]-	434.9308
Fipronil_F1	C11H2N4OSClF			329.9593
Fipronil_F2	C8H2N2SClF			249.9582
Flonicamid	C9H6F3N3O	229.0463	[M+H]+	230.0536
Flonicamid_F1	C8H6N2OF3			203.0426
Fluazifop	C15H12F3NO4	327.0718	[M+H]+	328.0791
Fluazifop_F1	C14H11NO2F3			282.0736
Fluazifop_F2	C12H7NOF3			238.0499
Flubendiamide	C23H22F7IN2O4S	682.0233	[M-H]-	681.0154
Flubendiamide_F1	C10H10OSF4			254.0407
Flubendiamide_F2	C3H3NOF4I			271.9213
Fludioxynil	C12H6F2N2O2	248.0397	[M+NH4]+	266.0736
Fludioxynil_F1	C12H6FN2O2			229.0408
Fludioxynil_F2	C10H8NO			158.0600
Flufenacet	C14H13F4N3O2S	363.0665	[M+H]+	364.0737
Flufenacet_F1	C8H7NOF			152.0492
Flufenoxuron	C21H11ClF6N2O3	488.0362	[M+H]+	489.0435
Flufenoxuron_F1	C7H6F2NO			158.0409
Fluopyram	C16H11ClF6N2O	396.0464	[M+H]+	397.0537
Fluopyram_F1	C8H4F3O			173.0204
Fluquinconazole	C16H8Cl2FN5O	375.0090	[M+H]+	376.0163
Fluquinconazole_F1	C14H6Cl2FN2O			306.9847
Flusilazole	C16H15F2N3Si	315.1003	[M+H]+	316.1076
Flusilazole_F1	C8H8N3F			165.0699
Flutriafol	C16H13F2N3O	301.1027	[M+H]+	302.1099

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Flutriafol_F1	C2H4N3			70.0396
Formetanate	C11H15N3O2	221.1164	[M+H]+	222.1237
Formetanate_F1	C9H13N2O			165.1021
Fosthiazate	C9H18NO3PS2	283.0466	[M+H]+	284.0539
Fosthiazate_F1	C3H6NOS			104.0155
Haloxyfop	C15H11ClF3NO4	361.0329	[M+H]+	362.0402
Haloxyfop_F1	C14H10NO2ClF			316.0347
Hexaconazole	C14H17Cl2N3O	313.0749	[M+H]+	314.0821
Hexaconazole_F1	C7H5Cl2			158.9763
Hexythiazox	C17H21ClN2O2S	352.1012	[M+H]+	353.1085
Hexythiazox_F1	C9H11NCl			168.0574
Imazalil	C14H14Cl2N2O	296.0483	[M+H]+	297.0556
Imazalil_F1	C7H5Cl2			158.9763
Imazalil_F2	C3H5N2			69.0447
Imidacloprid	C9H10ClN5O2	255.0523	[M+H]+	256.0596
Imidacloprid_F1	C9H10N4Cl			209.0589
Indoxacarb	C22H17ClF3N3O7	527.0707	[M+H]+	528.0780
Indoxacarb_F1	C9H7F3NO2			218.0426
Ioxynil	C7H3I2NO	370.8304	[M-H]-	369.8224
Ioxynil_F1	I			126.9050
Iprovalicarb	C18H28N2O3	320.2100	[M+H]+	321.2173
Iprovalicarb_F1	C9H11			119.0850
Isocarbophos	C11H16NO4PS	289.0538	[M+H]+	290.0610
Isocarbophos_F1	C8H9NO3PS			230.0035
Isofenfos methyl	C14H22NO4PS	331.1007	[M+H]+	332.1080
Isofenfos methyl_F1	C9H13NO2PS			230.0399
Isofenfos methyl_F2	C7H5O2			121.0285
Isoprocarb	C11H15NO2	193.1103	[M+H]+	194.1176
Isoprocarb_F1	C6H7O			95.0491
Isoxaflutole	C15H12F3NO4S	359.0439	[M+H]+	360.0512
Isoxaflutole_F1	C9H6O3SF3			250.9987
Kresoxim-methyl	C18H19NO4	313.1314	[M+H]+	314.1387
Kresoxim-methyl_F1	C9H9N			131.0729
Kresoxim-methyl_F2	C8H6N			116.0495

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Linuron	C9H10Cl2N2O2	248.0119	[M+H]+	249.0192
Linuron_F1	C5H3Cl2			132.9606
Linuron_F2	C6H4NCl2			159.9715
Malaoxon	C10H19O7PS	314.0589	[M+H]+	315.0662
Malaoxon_F1	C4H3O3			99.0077
Malaoxon_F2	C3H3O2			71.0128
Malathion	C10H19O6PS2	330.0361	[M+H]+	331.0433
Malathion_F1	C2H8O3PS			124.9821
Mandipropamid	C23H22ClNO4	411.1237	[M+H]+	412.1310
Mandipropamid_F1	C19H19NO2Cl			328.1094
Mandipropamid_F2	C7H6Cl			125.0153
Mepanipyrim	C14H13N3	223.1109	[M+H]+	224.1182
Mepanipyrim_F1	C7H8N			106.0652
Mepanipyrim_F2	C6H7O			95.0491
Metaflumizone	C24H16F6N4O2	506.1177	[M+H]+	507.1250
Metaflumizone_F1	C16H11N3F3			302.0909
Metaflumizone_F2	C7H5N2			117.0459
Metalaxyl	C15H21NO4	279.1471	[M+H]+	280.1543
Metalaxyl_F1	C11H14N			160.1121
Metalaxyl_F2	C12H16NO			192.1383
Metconazole	C17H22ClN3O	319.1451	[M+H]+	320.1524
Metconazole_F1	C7H6Cl			125.0148
Metconazole_F2	C4H6O			70.0413
Methamidophos	C2H8NO2PS	141.0013	[M+H]+	142.0086
Methamidophos_F1	CH7BO3P			112.0158
Methamidophos_F2	H3NOP			63.9947
Methidathion	C6H11N2O4PS3	301.9619	[M+H]+	302.9691
Methidathion_F1	C3H5N2O			85.0394
Methidathion_F2	C3H7N2O2			103.0502
Methiocarb	C11H15NO2S	225.0824	[M+H]+	226.0896
Methiocarb_F1	C8H9O			121.0648
Methiocarb_F2	C7H7			91.0542
Methiocarb-sulfoxide	C11H15NO3S	241.0773	[M+H]+	242.0845
Methiocarb-sulfoxide_F1	C8H10O2S			170.0396

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Methiocarb-sulfoxide_F2	C8H10O			122.0726
Methomyl	C5H10N2O2S	162.0463	[M+H]+	163.0536
Methomyl_F1	C3H8NOS			106.0321
Methomyl_F2	C3H6NS			88.0216
Methoxyfenozide	C22H28N2O3	368.2100	[M+H]+	369.2173
Methoxyfenozide_F1	C9H9O2			149.0597
Methoxyfenozide_F2	C9H9O			133.0648
Metobromuron	C9H11BrN2O2	258.0004	[M+H]+	259.0077
Metobromuron_F1	C6H5NBr			169.9600
Metobromuron_F2	C6H5N			91.0417
Monocrotophos	C7H14NO5P	223.0610	[M+H]+	224.0682
Monocrotophos_F1	C2H8O4P			127.0155
Monocrotophos_F2	C2H4NO			58.0287
Myclobutanil	C15H17ClN4	288.1142	[M+H]+	289.1215
Myclobutanil_F1	C7H6Cl			125.0155
Myclobutanil_F2	C2H4N3			70.0400
Nitenpyram	C11H15ClN4O2	270.0883	[M+H]+	271.0956
Nitenpyram_F1	C6H5ClN			126.0106
Omethoate	C5H12NO4PS	213.0225	[M+H]+	214.0297
Omethoate_F1	C2H8O4P			127.0155
Omethoate_F2	C2H8O3PS			142.9926
Oxadixyl	C14H18N2O4	278.1266	[M+H]+	279.1339
Oxadixyl_F1	C9H10N			132.0808
Oxadixyl_F2	C8H7N			117.0573
Oxamyl	C7H13N3O3S	219.0678	[M+NH4]+	237.1016
Oxamyl_F1	C3H6NO			72.0444
Oxamyl_F2	C6H9N2O3S			189.0328
Oxyfluorfen	C15H11ClF3NO4	361.0329	[M+H]+	362.0402
Oxyfluorfen_F1	C12H6NOF3			237.0397
Oxyfluorfen_F2	C10H6N			140.0493
Paclobutrazol	C15H20ClN3O	293.1295	[M+H]+	294.1368
Paclobutrazol_F1	C2H4N3			70.0400
Paclobutrazol_F2	C7H6Cl			125.0153
Paraoxon methyl	C8H10NO6P	247.0246	[M+H]+	248.0319

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Paraoxon methyl_F1	C6H5NO5P			201.9900
Penconazole	C13H15Cl2N3	283.0643	[M+H]+	284.0716
Penconazole_F1	C7H5Cl2			158.9761
Penconazole_F2	C2H4N3			70.0400
Pencycuron	C19H21ClN2O	328.1342	[M+H]+	329.1415
Pencycuron_F1	C7H6Cl			125.0153
Pencycuron_F2	C6H8N			94.0651
Pendimethalin	C13H19N3O4	281.1375	[M+H]+	282.1448
Pendimethalin_F1	C8H10N3O4			212.0663
Pendimethalin_F2	C6H5N			91.0417
Phenthoate	C12H17O4PS2	320.0306	[M+H]+	321.0379
Phenthoate_F1	C8H7O2			135.0441
Phenthoate_F2	C6H7			79.0542
Phosalone	C12H15ClNO4PS2	366.9868	[M+H]+	367.9941
Phosalone_F1	C8H5NO2Cl			182.0003
Phosalone_F2	C3H7O4S			139.0057
Phosmet	C11H12NO4PS2	316.9945	[M+H]+	318.0018
Phosmet_F1	C9H6NO2			160.0393
Phosmet_F2	C8H5O2			133.0284
Phoxim	C12H15N2O3PS	298.0541	[M+H]+	299.0614
Phoxim_F1	C6H7O			95.0492
Phoxim_F2	C6H5			77.0378
Pirimicarb	C11H18N4O2	238.1430	[M+H]+	239.1503
Pirimicarb_F1	C3H6NO			72.0444
Pirimicarb_F2	C6H9N2			109.0760
Pirimicarb, desmethyl-	C10H16N4O2	224.1273	[M+H]+	225.1346
Pirimicarb, desmethyl-_F1	C3H6NO			72.0444
Pirimiphos-methyl	C11H20N3O3PS	305.0963	[M+H]+	306.1036
Pirimiphos-methyl_F1	C9H14N3			164.1178
Pirimiphos-methyl_F2	C5H6N3			108.0556
Prochloraz	C15H16Cl3N3O2	375.0308	[M+H]+	376.0381
Prochloraz_F1	C12H13NO2Cl3			308.0006
Prochloraz_F2	C4H8N			70.0651
Procymidone	C13H11Cl2NO2	283.0167	[M+H]+	284.0240

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Procymidone_F1	C12H12NOCl2			256.0291
Procymidone_F2	C5H7			67.0542
Profenofos	C11H15BrClO3PS	371.9351	[M+H]+	372.9424
Profenofos_F1	C6H6BrClO3PS			302.8638
Propamocarb	C9H20N2O2	189.1598	[M+H]+	189.1598
Propamocarb_F1	C4H8NO2			102.0548
Propamocarb_F2	C2H4NO2			74.0237
Propaquizafop	C22H22ClN3O5	443.1248	[M+H]+	444.1321
Propaquizafop_F1	C5H10NO			100.0757
Propaquizafop_F2	C16H12N2O2Cl			299.0582
Propargite	C19H26O4S	350.1552	[M+NH4]+	368.1890
Propargite_F1	C12H15O			175.1117
Propiconazole	C15H17Cl2N3O2	341.0698	[M+H]+	342.0771
Propiconazole_F1	C7H5Cl2			158.9763
Propiconazole_F2	C5H9			69.0699
Propoxur	C11H15NO3	209.1052	[M+H]+	210.1125
Propoxur_F1	C6H7O2			111.0441
Propoxur_F2	C5H5			65.0386
Propyzamide	C12H11Cl2NO	255.0218	[M+H]+	256.0291
Propyzamide_F1	C7H3OCl2			172.9558
Propyzamide_F2	C7H6NOCl2			189.9821
Proquinazid	C14H17IN2O2	372.0335	[M+H]+	373.0408
Proquinazid_F1	C8H6N2O2I			288.9467
Proquinazid_F2	C8H3NO2I			271.9203
Prothioconazole	C14H15Cl2N3OS	343.0313	[M+H]+	344.0386
Prothioconazole_F1	C7H6Cl			125.0153
Prothioconazole_F2	C14H15Cl2N3S			327.0778
Pymetrozine	C10H11N5O	217.0964	[M+H]+	218.1036
Pymetrozine_F1	C6H5N2			105.0447
Pymetrozine_F2	C5H5N			79.0417
Pyraclostrobin	C19H18ClN3O4	387.0986	[M+H]+	388.1059
Pyraclostrobin_F1	C9H9NO2			163.0628
Pyraclostrobin_F2	C8H7NO			133.0522
Pyrethrin I	C21H28O3	328.2039	[M+H]+	329.2111

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Pyrethrin I_F1	C10H13			133.1012
Pyrethrin I_F2	C8H9			105.0699
Pyrethrin II	C22H28O5	372.1937	[M+H]+	373.2010
Pyrethrin II_F1	C11H13O			161.0609
Pyrethrin II_F2	C10H13			133.1012
Pyridaben	C19H25ClN2OS	364.1376	[M+H]+	365.1449
Pyridaben_F1	C11H15			147.1160
Pyridaben_F2	C8H9			105.0699
Pyridate	C19H23ClN2O2S	379.1242	[M+H]+	379.1242
Pyridate_F1	C10H8N2OCl			207.0320
Pyridate_F2	C4H9			57.0699
Pyrimethanil	C12H13N3	199.1109	[M+H]+	200.1182
Pyrimethanil_F1	C6H7N2			107.0605
Pyrimethanil_F2	C5H8N			82.0651
Pyriproxyfen	C20H19NO3	321.1365	[M+H]+	322.1438
Pyriproxyfen_F1	C5H6NO			96.0444
Pyriproxyfen_F2	C8H7O			119.0491
Quinoclamine	C10H6ClNO2	207.0087	[M+H]+	208.0160
Quinoclamine_F1	C7H5O			105.0334
Quinoclamine_F2	C8H6N			116.0495
Quinoxyfen	C15H8Cl2FNO	306.9967	[M+H]+	308.0040
Quinoxyfen_F1	C9H5NCl2			196.9793
Quinoxyfen_F2	C15H8NOClF			272.0273
Rotenone	C23H22O6	394.1416	[M+H]+	395.1489
Rotenone_F1	C14H13O2			213.0910
Rotenone_F2	C11H12O3			192.0781
Spinosyn A	C41H65NO10	731.4609	[M+H]+	732.4681
Spinosyn A_F1	C8H16NO			142.1224
Spinosyn D	C42H67NO10	745.4765	[M+H]+	746.4838
Spinosyn D_F1	C8H16NO			142.1222
Spirodiclofen	C21H24Cl2O4	410.1052	[M+H]+	411.1124
Spirodiclofen_F1	C15H15O3Cl2			313.0391
Spirodiclofen_F2	C5H11			71.0855
Spiromesifen	C23H30O4	370.2144	[M+H]+	371.2217

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Spiromesifen_F1	C17H21O3			273.1490
Spirotetramat	C21H27NO5	373.1889	[M+H]+	374.1962
Spirotetramat_F1	C13H14NO2			216.1019
Spirotetramat_CisEnol	C18H23NO3	301.1678	[M+H]+	302.1751
Spirotetramat_CisEnol_F1	C17H20NO2			270.1489
Spirotetramat_CisEnol_F2	C13H14NO2			216.1019
Spirotetramat_EnolGlucoside	C24H33NO8	463.2206	[M+H]+	464.2279
Spirotetramat_EnolGlucoside_F1	C18H24NO3			302.1751
Spirotetramat_EnolGlucoside_F2	C17H20NO2			270.1489
Spirotetramat_KetoHydroxy	C18H23NO4	317.1627	[M+H]+	318.1700
Spirotetramat_KetoHydroxy_F1	C18H22NO3			300.1600
Spirotetramat_KetoHydroxy_F2	C17H18NO2			268.1338
Spirotetramat_MonoHydroxy	C18H25NO3	303.1834	[M+H]+	304.1907
Spirotetramat_MonoHydroxy_F1	C17H20NO			254.1539
Spirotetramat_MonoHydroxy_F2	C15H17N			211.1356
Spiroxamine	C18H35NO2	297.2668	[M+H]+	298.2741
Spiroxamine_F1	C8H18NO			144.1377
Spiroxamine_F2	C6H14N			100.1121
Tebuconazole	C16H22ClN3O	307.1451	[M+H]+	308.1524
Tebuconazole_F1	C7H6Cl			125.0153
Tebuconazole_F2	C2H4N3			70.0400
Tebufenozide	C22H28N2O2	352.2151	[M+H]+	353.2224
Tebufenozide_F1	C9H9O			133.0645
Tebufenozide_F2	C8H9			105.0699
Tebufenpyrad	C18H24ClN3O	333.1608	[M+H]+	334.1681
Tebufenpyrad_F1	C6H10ClN2			145.0527
Teflubenzuron	C14H6Cl2F4N2O2	379.9742	[M+H]+	380.9815
Teflubenzuron_F1	C7H6F2NO			158.0412
Teflubenzuron_F2	C7H3F2O			141.0147
Terbuthylazine	C9H16ClN5	229.1094	[M+H]+	230.1167
Terbuthylazine_F1	C5H9N5Cl			174.0541
Terbuthylazine_F2	C4H7N3Cl			132.0323
Tetraconazole	C13H11Cl2F4N3O	371.0215	[M+H]+	372.0288
Tetraconazole_F1	C7H5Cl2			158.9763

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Tetraconazole_F2	C2H4N3			70.0400
TFNA	C7H4F3NO2	191.0194	[M+H]+	192.0267
TFNA_F1	C6H5NF3			148.0369
TFNA_F2	C5H5NF			98.0396
TFNG	C9H7F3N2O3	248.0409	[M+H]+	249.0473
TFNG_F1	C8H6F3N2O			203.0427
TFNG_F2	C6H5NF3			148.0369
Thiabendazole	C10H7N3S	201.0361	[M+H]+	202.0433
Thiabendazole_F1	C9H7N2S			175.0327
Thiabendazole_F2	C9H7N2OS			191.0274
Thiacloprid	C10H9ClN4S	252.0237	[M+H]+	253.0309
Thiacloprid_F1	C6H5NCl			126.0105
Thiacloprid_F2	C6H4N			90.0338
Thiamethoxam	C8H10ClN5O3S	291.0193	[M+H]+	292.0266
Thiamethoxam_F1	C7H9N4S			181.0542
Thiamethoxam_F2	C4H3NSCl			131.9669
Thiobencarb	C12H16ClNOS	257.0641	[M+H]+	258.0714
Thiobencarb_F1	C7H6Cl			125.0153
Thiobencarb_F2	C7H5			89.0386
Thiodicarb	C10H18N4O4S3	354.0490	[M+H]+	355.0563
Thiodicarb_F1	C2H6NS2			107.9936
Thiodicarb_F2	C3H6NS			88.0216
Thiophanate-methyl	C12H14N4O4S2	342.0457	[M+H]+	343.0529
Thiophanate-methyl_F1	C7H7N2S			151.0325
Thiophanate-methyl_F2	C6H7N			93.0573
Tolclofos-methyl	C9H11Cl2O3PS	299.9543	[M+H]+	300.9616
Tolclofos-methyl_F1	C6H5O2Cl			174.9711
Tolclofos-methyl_F2	C2H8O3PS			142.9924
Triadimefon	C14H16ClN3O2	293.0931	[M+H]+	294.1004
Triadimefon_F1	C11H14OCl			197.0728
Triadimefon_F2	C5H4Cl			98.9996
Triadimenol	C14H18ClN3O2	295.1088	[M+H]+	296.1160
Triadimenol_F1	C4H6O			70.0413
Triadimenol_F2	C6H11O			99.0804

Compound	Molecular Formula	Neutral mass (Da)	Adduct	Exact mass (m/z)
Triazophos	C12H16N3O3PS	313.0650	[M+H]+	314.0723
Triazophos_F1	C8H8N3O			162.0662
Triazophos_F2	H4O3PS			114.9613
Trichlorfon	C4H8Cl3O4P	255.9226	[M+H]+	256.9299
Trichlorfon_F1	C2H8O4P			127.0155
Trichlorfon_F2	CH4O2P			78.9943
Trifloxystrobin	C20H19F3N2O4	408.1297	[M+H]+	409.1370
Trifloxystrobin_F1	C9H7NF3			186.0525
Trifloxystrobin_F2	C8H6N			116.0495
Triflumuron	C15H10ClF3N2O3	358.0332	[M+H]+	359.0405
Triflumuron_F1	C7H7NOCl			156.0211
Triflumuron_F2	C7H4OCl			138.9945
Triticonazole	C17H20ClN3O	317.1295	[M+H]+	318.1368
Triticonazole_F1	C4H6O			70.0407
Triticonazole_F2	C7H6Cl			125.0153
Zoxamide	C14H16Cl3NO2	335.0247	[M+H]+	336.0319
Zoxamide_F1	C8H5Cl2O			186.9709

F1: Fragment 1
F2: Fragment 2