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Mass Spectral Libraries for Food Analysis

**Pesticides High Resolution MS/MS Spectral Library
Version 1.0 for Use in MasterView™ Software and
LibraryView™ Software**

Pesticides High Resolution MS/MS Library Version 1.0

An overview of the licensed mass spectral library for pesticides compatible with MasterView™ and LibraryView™ software

The MasterView™ and LibraryView™ software package is a fast way to analyze large batches of MS/MS data for accurate and efficient MS/MS library searching, data mining, and compound database management. We have assembled a high resolution, accurate mass MS/MS spectral library containing 557 pesticide and pesticide metabolite entries. This library was created using certified reference materials and can be used in MasterView™ and LibraryView™ software to perform MS/MS library searching or to create custom screening and/or quantitation methods using the integrated MS and MS/MS information.

Features of this high resolution MS/MS spectra library:

- Includes data on 557 pesticides and metabolites commonly tested for in fruits, vegetables and other food products.
- Includes 1310 high resolution MS/MS spectral library entries including individual spectra acquired using distinct collision energies, as well as a single spectra using collision energy spread representing the sum of three collision energies.
- Contains spectra for both positive and negative ionization for compounds that ionize in both polarities.

Advantages of using this MS/MS spectral library:

- Use the integrated MS and MS/MS information to build methods without the need to infuse standards and optimize conditions for a given compound.
- Easily create processing methods for a TOF-MS-IDA-MS/MS workflow for use on TripleTOF® LC/MS/MS systems.
- Quickly set-up XIC tables for quantitation and identification in MasterView™ software.
- Set-up smaller customer libraries by simply selecting only the compounds of interest from the list in LibraryView™ Software.

The following is a list of the compounds currently in the library. This library is verified for use on AB SCIEX TripleTOF® and QTRAP® LC/MS/MS systems.

Please note that this library is continuously being expanded to include additional compounds.

Compound	Formula	Formula Weight	CAS Number	# of Spectra
2,6-Dichlorbenzamide	C7H5Cl2NO	190.0285	2008-58-4	1
3-Hydroxycarbofuran	C12H15NO4	237.2554	16655-82-6	3
3-Keto-carbofuran	C12H13NO4	235.2395	16709-30-1	1
3,4,5-Trimethacarb	C11H15NO2	193.2457	2686-99-9	1
5-Hydroxy-clethodim-sulfone	C17H26ClNO6S	407.9135	N/A	2
5-Hydroxy-imidacloprid	C9H10ClN5O3	271.6631	N/A	1
5-Hydroxythiabendazole	C10H7N3OS	217.2499	948-71-0	1
6-Chlor-3-phenyl-pyridazin-4-ol	C10H7ClN2O	206.6314	40020-01-7	3
Acephate	C4H10NO3PS	183.1663	30560-19-1	4
Acetamiprid	C10H11ClN4	222.6773	135410-20-7	3
Acetochlor	C14H20ClNO2	269.7712	34256-82-1	1
Acibenzolar-S-methyl	C8H6N2OS2	210.2775	135158-54-2	2
Aclonifen	C12H9ClN2O3	264.668	74070-46-5	1
Alachlor	C14H20ClNO2	269.7712	15972-60-8	2
Alanycarb	C17H25N3O4S2	399.5321	83130-01-2	2
Aldicarb	C7H14N2O2S	190.2648	116-06-3	1
Aldicarb-sulfoxide	C7H14N2O3S	206.2641	1646-87-3	5
Aldoxycarb	C7H14N2O4S	222.2634	1646-88-4	3
Alloxydim	C17H25NO5	323.3892	55634-91-8	2
Ametryn	C9H17N5S	227.3323	834-12-8	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Amicarbazone	C10H19N5O2	241.2934	129909-90-6	1
Amidosulfuron	C9H15N5O7S2	369.3761	120923-37-7	2
Aminocarb	C11H16N2O2	208.2604	2032-59-9	3
Amitraz	C19H23N3	293.4123	33089-61-1	1
Amitrole	C2H4N4	84.0808	61-82-5	1
Anilofos	C13H19ClNO3PS2	367.8541	64249-01-0	2
Aramite	C15H23ClO4S	334.8623	140-57-8	1
Aspon	C12H28O5P2S2	378.4273	3244-90-4	1
Atrazine	C8H14ClN5	215.6858	1912-24-9	3
Atrazine-desethyl-desisopropyl-2-hydroxy	C3H5N5O	127.1059	645-92-1	1
Atrazine-desisopropyl-2-hydroxy	C5H9N5O	155.1597	7313-54-4	1
Atrazine-2-hydroxy	C8H15N5O	197.2403	2163-68-0	2
Atrazine-d5	C8H9(2H)5ClN5	220.7167		1
Atrazine-desethyl	C6H10ClN5	187.632	6190-65-4	2
Atrazine-desethyl-2-hydroxy	C6H11ON5	169.1865	19988-24-0	4
Atrazine-desisopropyl	C5H8N5Cl	173.6051	1007-28-9	2
Avermectin B1a	C48H72O14	873.091	65195-55-3	1
Azaconazole	C12H11Cl2N3O2	300.144	60207-31-0	1
Azamethiophos	C9H10ClN2O5PS	324.6796	35575-96-3	1
Azimsulfuron	C13H16N10O5S	424.3989	120162-55-2	1
Azinphos-ethyl	C12H16N3O3PS2	345.3801	2642-71-9	2
Azinphos-methyl	C10H12N3O3PS2	317.3263	86-50-0	2
Azoxystrobin	C22H17N3O5	403.3945	131860-33-8	4
Beflubutamid	C18H17F4NO2	355.3324	113614-08-7	1
Benalaxyl	C20H23NO3	325.4078	71626-11-4	5
Benazolin	C9H6ClNO3S	243.6688	3813-05-6	2
Bendiocarb	C11H13NO4	223.2285	22781-23-3	3
Benfuracarb	C20H30N2O5S	410.533	82560-54-1	3
Benoxacor	C11H11Cl2NO2	260.1195	98730-04-2	2
Bensulfuron-methyl	C16H18N4O7S	410.406	83055-99-6	3
Bensulide	C14H24NO4PS3	397.5157	741-58-2	1
Benthiavalicarb-isopropyl	C18H24FN3O3S	381.4699	177406-68-7	1
Benzoximate	C18H18ClNO5	363.7975	29104-30-1	3
Bifenazate	C17H20N2O3	300.3576	149877-41-8	3
Bifenox	C14H9Cl2NO5	342.1347	42576-02-3	1
Bifenthrin	C23H22ClF3O2	422.8748	82657-04-3	1
Bioallethrin	C19H26O3	302.4137	84030-86-4	1
Bioresmethrin	C22H26O3	338.4469	28434-01-7	1
Bitertanol	C20H23N3O2	337.422	55179-31-2	3
Boscalid	C18H12Cl2N2O	343.2121	188425-85-6	4
brodifacoum	C31H23BrO3	523.4259	56073-10-0	2
Bromacil	C9H13BrN2O2	261.1181	314-40-9	2
Bromophos	C8H8BrCl2O3PS	365.9968	2104-96-3	1
Bromophos-ethyl	C10H12BrCl2O3PS	394.0506	4824-78-6	1
Bromuconazole	C13H12BrCl2N3O	377.0672	116255-48-2	5
Bupirimate	C13H24N4O3S	316.4231	41483-43-6	4
Buprofezin	C16H23N3OS	305.4429	69327-76-0	3
Butafenacil	C20H18ClF3N2O6	474.8208	134605-64-4	3

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Butamifos	C13H21N2O4PS	332.3589	36335-67-8	4
Butocarboxim-sulfoxide	C7H14N2O3S	206.2641	34681-24-8	2
Butoxycarboxim	C7H14N2O4S	222.2634	34681-23-7	1
Butralin	C14H21N3O4	295.3385	33629-47-9	2
Buturon	C12H13CIN2O	236.7011	3766-60-7	1
Butylate	C11H23NOS	217.3742	2008-41-5	2
Cadusafos	C10H23O2PS2	270.3939	95465-99-9	2
Captafol	C10H9Cl4NO2S	349.0625	2425-06-1	1
Carbaryl	C12H11NO2	201.225	63-25-2	4
Carbendazim	C9H9N3O2	191.1896	10605-21-7	5
Carbetamide	C12H16N2O3	236.2708	16118-49-3	4
Carbofuran	C12H15NO3	221.2561	1563-66-2	4
Carbosulfan	C20H32N2O3S	380.5502	55285-14-8	2
Carboxin	C12H13NO2S	235.3053	5234-68-4	3
Carfentrazone-ethyl	C15H14Cl2F3N3O3	412.1955	128639-02-1	2
Carpropamid	C15H18Cl3NO	334.6725	104030-54-8	1
Chlorantraniliprole	C18H14BrCl2N5O2	483.1511	500008-45-7	2
Chlorbromuron	C9H10BrClN2O2	293.547	13360-45-7	1
Chlordimeform	C10H13CIN2	196.6797	6164-98-3	1
Chlorfenvinphos	C12H14Cl3O4P	359.5727	470-90-6	3
Chlorfluazuron	C20H9Cl3F5N3O3	540.6606	71422-67-8	4
Chloridazon	C10H8CIN3O	221.6461	1698-60-8	2
Chlorimuron-ethyl	C15H15CIN4O6S	414.8246	90982-32-4	1
Chlorophacinone	C23H15ClO3	374.8234	3691-35-8	3
Chlorotoluron	C10H13CIN2O	212.679	15545-48-9	4
Chloroxuron	C15H15CIN2O2	290.7494	1982-47-4	4
Chlorpyrifos-methyl	C7H7Cl3NO3PS	322.5338	5598-13-0	1
Chlorsulfuron	C12H12CIN5O4S	357.7758	64902-72-3	2
Chlorthiamid	C7H5Cl2NS	206.0935	1918-13-4	1
Chlorthiophos	C11H15Cl2O3PS2	361.2463	60238-56-4	1
Cinidon-ethyl	C19H17Cl2NO4	394.254	142891-20-1	2
Cinosulfuron	C15H19N5O7S	413.4096	94593-91-6	2
Clethodim	C17H26CINO3S	359.9156	99129-21-2	4
Clethodim-imin-sulfone	C14H23NO4S	301.4053	N/A	1
Clethodim-imin-sulfoxide	C14H23NO3S	285.4059	N/A	1
Clethodim-sulfone	C17H26CINO5S	391.9142	N/A	1
Clethodim-sulfoxide	C17H26CINO4S	375.9149	N/A	1
Clodinafop-propargyl	C17H13ClFNO4	349.7459	105512-06-9	3
Clofentezine	C14H8Cl2N4	303.1504	74115-24-5	4
clomazone	C12H14CINO2	239.7016	81777-89-1	2
Clomeprop	C16H15Cl2NO2	324.2064	84496-56-0	1
Clopyralid	C6H3Cl2NO2	192.0009	1702-17-6	3
Clothianidin	C6H8CIN5O2S	249.6792	210880-92-5	4
Coumaphos	C14H16ClO5PS	362.7688	56-72-4	2
Coumatetralyl	C19H16O3	292.3345	5836-29-3	2
Crotoxyphos	C14H19O6P	314.2748	7700-17-6	1
Cumyluron	C17H19CIN2O	302.8038	99485-76-4	2
Cyanazine	C9H13CIN6	240.6957	21725-46-2	3

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Cyanofenphos	C15H14NO2PS	303.3201	13067-93-1	1
Cyazofamid	C13H13ClN4O2S	324.7893	120116-88-3	4
Cycloate	C11H21NOS	215.3583	1134-23-2	1
Cycloxydim	C17H27NO3S	325.4707	101205-02-1	4
Cycluron	C11H22N2O	198.3086	2163-69-1	2
Cyflufenamid	C20H17F5N2O2	412.3597	180409-60-3	1
Cyfluthrin	C22H18Cl2FNO3	434.2941	68359-37-5	1
Cyhalofop-butyl	C20H20FNO4	357.3817	122008-85-9	1
Cymoxanil	C7H10N4O3	198.1815	57966-95-7	2
Cypermethrin	C22H19Cl2NO3	416.3036	52315-07-8	1
Cyphenothrin	C24H25NO3	375.4678	39515-40-7	1
Cyproconazole	C15H18ClN3O	291.7806	113096-99-4	3
Cyprodinil	C14H15N3	225.2937	121552-61-2	4
Cyromazine	C6H10N6	166.1861	66215-27-8	4
Daimuron	C17H20N2O	268.359	42609-52-9	3
Daminozide	C6H12N2O3	160.1728	1596-84-5	1
DEET	C12H17NO	191.2733	134-62-3	1
Deltamethrin	C22H19Br2NO3	505.2052	52918-63-5	1
Demeton-S-methyl-sulfone	C6H15O5PS2	262.2843	17040-19-6	2
Desethyl-desisopropyl-atrazine	C3H4ClN5	145.5514	3397-62-4	1
Desmedipham	C16H16N2O4	300.3142	13684-56-5	2
Desmethyl-formamido-pirimicarb	C11H16N4O3	252.2732	59333-83-4	2
Desmethyl-pirimicarb	C10H16N4O2	224.2629	30614-22-3	2
Desmetryn	C8H15N5S	213.3054	1014-69-3	5
Desphenyl-chloridazon	C4H4ClN3O	145.5482	6339-19-1	1
Di-allate	C10H17Cl2NOS	270.2211	2303-16-4	2
Dialifos	C14H17ClNO4PS2	393.8486	10311-84-9	1
Diamidafos	C8H13N2O2P	200.1773	1754-58-1	1
Diazinon	C12H21N2O3PS	304.3485	333-41-5	3
Dichlofenthion	C10H13Cl2O3PS	315.155	97-17-6	2
Dichlofluanid	C9H11Cl2FN2O2S2	333.2313	1085-98-9	1
Dichlorvos	C4H7Cl2O4P	220.9762	62-73-7	4
Diclobutrazol	C15H19Cl2N3O	328.2412	75736-33-3	2
Diclofop-methyl	C16H14Cl2O4	341.1903	51338-27-3	1
Diclosulam	C13H10Cl2FN5O3S	406.2228	145701-21-9	2
Dicrotophos	C8H16NO5P	237.1923	3735-78-3	4
Dicyclanil	C8H10N6	190.2081	112636-83-6	2
Diethofencarb	C14H21NO4	267.325	87130-20-9	4
Difenacoum	C31H24O3	444.5303	56073-07-5	4
Difenoconazole	C19H17Cl2N3O3	406.2682	119446-68-3	4
Difenoxyuron	C16H18N2O3	286.3308	14214-32-5	1
Difenzoquat	C17H17N2	249.3359	43222-48-6	1
Diflubenzuron	C14H9ClF2N2O2	310.6876	35367-38-5	6
Diflufenican	C19H11F5N2O2	394.3011	83164-33-4	1
Diflufenzopyr	C15H12F2N4O3	334.2825	109293-97-2	2
Dimefuron	C15H19ClN4O3	338.7939	34205-21-5	2
Dimepiperate	C15H21NOS	263.4025	61432-55-1	2
Dimethachlor	C13H18ClNO2	255.7443	50563-36-5	2

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Dimethametryn	C11H21N5S	255.386	22936-75-0	2
Dimethenamide	C12H18ClNO2S	275.7976	87674-68-8	4
Dimethoate	C5H12NO3PS2	229.2576	60-51-5	4
Dimethomorph	C21H22ClNO4	387.8629	110488-70-5	4
Dimetilan	C10H16N4O3	240.2622	644-64-4	1
Dimoxystrobin	C19H22N2O3	326.3956	149961-52-4	5
Diniconazole	C15H17Cl2N3O	326.2254	83657-24-3	5
Dinotefuran	C7H14N4O3	202.2132	165252-70-0	2
Dioxacarb	C11H13NO4	223.2285	6988-21-2	2
Dioxathion	C12H26O6P2S4	456.5395	78-34-2	1
Diphacinone	C23H16O3	340.3786	82-66-6	2
Diphenamid	C16H17NO	239.3174	957-51-7	2
Diphenylamine	C12H11N	169.2264	122-39-4	2
Dipropetryn	C11H21N5S	255.386	4147-51-7	4
Disulfoton-sulfon	C8H19O4PS3	306.4031	2497-06-5	1
Disulfoton-sulfoxide	C8H19O3PS3	290.4038	2497-07-6	5
Dithiopyr	C15H16F5NO2S2	401.4186	97886-45-8	3
Diuron	C9H10Cl2N2O	233.0969	330-54-1	3
Dodemorph	C18H35NO	281.4822	1593-77-7	2
Dodine	C15H33N3O2	287.446	2439-10-3	1
Doramectin	C50H74O14	899.1289	117704-25-3	1
Edifenphos	C14H15O2PS2	310.3746	17109-49-8	1
Emamectin B1a	C49H75NO13	886.1332	123997-28-4	1
Emamectin B1b	C48H73NO13	872.1063	137335-79-6	1
EPN	C14H14NO4PS	323.3077	2104-64-5	1
Epoxiconazole	C17H13ClFN3O	329.7614	106325-08-0	4
Eprinomectin B1a	C50H75NO14	914.1436	133305-88-1	1
EPTC	C9H19NOS	189.3204	759-94-4	2
Esfenvalerate	C25H22ClNO3	419.9078	66230-04-4	1
Esprocarb	C15H23NOS	265.4183	85785-20-2	2
Etaconazole	C14H15Cl2N3O2	328.1978	60207-93-4	1
Ethaboxam	C14H16N4OS2	320.4365	162650-77-3	1
Ethametsulfuron-methyl	C15H18N6O6S	410.4091	97780-06-8	1
Ethidimuron	C7H12N4O3S2	264.3262	30043-49-3	3
Ethiofencarb	C11H15NO2S	225.3101	29973-13-5	3
Ethiofencarb-sulfone	C11H15NO4S	257.3087	53380-23-7	1
Ethiofencarb-sulfoxide	C11H15NO3S	241.3094	53380-22-6	1
Ethiolate	C7H15NOS	161.2666	2941-55-1	4
Ethion	C9H22O4P2S4	384.4761	563-12-2	3
Ethion monooxon	C9H22O5P2S3	368.411	17356-42-2	1
Ethiprole	C13H9Cl2F3N4OS	397.2063	181587-01-9	2
Ethirimol	C11H19N3O	209.2916	23947-60-6	5
Ethofumesate	C13H18O5S	286.3472	26225-79-6	5
Ethoprophos	C8H19O2PS2	242.3401	13194-48-4	3
Ethoxysulfuron	C15H18N4O7S	398.3949	126801-58-9	2
Ethylenthiourea	C3H6N2S	102.1586	96-45-7	2
Etofenprox	C25H28O3	376.4958	80844-07-1	3
Etoazole	C21H23F2NO2	359.4163	153233-91-1	3

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Etrimfos	C10H17N2O4PS	292.2941	38260-54-7	1
Famoxadone	C22H18N2O4	374.3963	131807-57-3	3
Famphur	C10H16NO5PS2	325.3431	52-85-7	1
Fenamidone	C17H17N3OS	311.4064	161326-34-7	3
Fenamiphos	C13H22NO3PS	303.3607	22224-92-6	1
Fenamiphos-sulfone	C13H22NO5PS	335.3594	31972-44-8	4
Fenamiphos-sulfoxide	C13H22NO4PS	319.3601	31972-43-7	4
Fenarimol	C17H12Cl2N2O	331.2011	60168-88-9	3
Fenazaquin	C20H22N2O	306.408	120928-09-8	4
Fenbuconazole	C19H17ClN4	336.8242	114369-43-6	4
Fenfuram	C12H11NO2	201.225	24691-80-3	1
Fenhexamid	C14H17Cl2NO2	302.2001	126833-17-8	3
Fenitrothion	C9H12NO5PS	277.236	122-14-5	2
Fenobucarb	C12H17NO2	207.2726	3766-81-2	3
Fenofibric acid	C17H15ClO4	318.7565	42017-89-0	1
Fenothiocarb	C13H19NO2S	253.3639	62850-32-2	1
Fenoxanil	C15H18Cl2N2O2	329.2259	115852-48-7	1
Fenoxaprop-P-ethyl	C18H16ClNO5	361.7816	71283-80-2	1
fenoxycarb	C17H19NO4	301.3423	79127-80-3	3
Fenpiclonil	C11H6Cl2N2	237.088	74738-17-3	2
Fenpropathrin	C22H23NO3	349.4298	39515-41-8	2
Fenpropidin	C19H31N	273.4622	67306-00-7	1
Fenpropimorph	C20H33NO	303.4884	67306-03-0	4
Fenpyroximate	C24H27N3O4	421.4965	111812-58-9	4
Fenthion	C10H15O3PS2	278.3298	55-38-9	2
Fenthion-sulfone	C10H15O5PS2	310.3284	3761-42-0	4
Fenthion-sulfoxide	C10H15O4PS2	294.3291	3761-41-9	5
Fentin	C18H15Sn	350.003	668-34-8	1
Fenuron	C9H12N2O	164.2073	101-42-8	4
Fenvalerate	C25H22ClNO3	419.9078	51630-58-1	1
Fipronil	C12H4Cl2F6N4OS	437.1508	120068-37-3	5
Flamprop-M-isopropyl	C19H19ClFNO3	363.8162	63782-90-1	1
Flamprop-M-methyl	C17H15ClFNO3	335.7624	63729-98-6	1
Flazasulfuron	C13H12F3N5O5S	407.3286	104040-78-0	2
Flonicamid	C9H6F3N3O	229.1617	158062-67-0	3
Fluazifop-butyl	C19H20F3NO4	383.3675	69806-50-4	1
Fluazifop (free acid)	C15H12F3NO4	327.2599	83066-88-0	3
Flucycloxuron	C25H20ClF2N3O3	483.9022	113036-88-7	2
Flucythrinate	C26H23F2NO4	451.4701	70124-77-5	1
Fludioxonil	C12H6F2N2O2	248.189	131341-86-1	1
Flufenacet	C14H13F4N3O2S	363.3345	142459-58-3	4
Flufenoxuron	C21H11ClF6N2O3	488.7736	101463-69-8	3
Flumetsulam	C12H9F2N5O2S	325.2974	98967-40-9	3
Fluometuron	C10H11F3N2O	232.2056	2164-17-2	3
Fluoroglycofene-ethyl	C18H13ClF3NO7	447.7517	77501-90-7	1
Fluoxastrobin	C21H16ClF4NO5	458.8334	361377-29-9	4
Flupyr-sulfuron-methyl	C15H14F3N5O7S	465.3652	144740-54-5	3
Fluquinconazole	C16H8Cl2FN5O	376.177	136426-54-5	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Fluridone	C19H14F3NO	329.322	59756-60-4	1
Flurochloridone	C12H10Cl2F3NO	312.1185	61213-25-0	1
Fluroxypyr	C7H5Cl2FN2O3	255.0323	69377-81-7	4
Fluroxypyr-meptyl	C15H21Cl2FN2O3	367.2474	81406-37-3	1
Flurprimidole	C15H15F3N2O2	312.2918	56425-91-3	2
Flurtamone	C18H14F3NO2	333.3102	96525-23-4	2
Flusilazole	C16H15F2N3Si	315.3981	85509-19-9	3
Fluthiacet-methyl	C15H15ClFN3O3S2	403.8826	117337-19-6	3
Flutolanil	C17H16F3NO2	323.3151	66332-96-5	2
Flutriafol	C16H13F2N3O	301.296	76674-21-0	3
Fomesafen	C15H10ClF3N2O6S	438.7666	72178-02-0	1
Fonofos	C10H15OPS2	246.3311	944-22-9	1
Foramsulfuron	C17H20N6O7S	452.4464	173159-57-4	2
Forchlorfenuron	C12H10ClN3O	247.6841	68157-60-8	1
Formetanate	C11H15N3O2	221.2592	22259-30-9	2
Fosthiazate	C9H18NO3PS2	283.3493	98886-44-3	3
Fuberidazole	C11H8N2O	184.1977	3878-19-1	3
Furalaxyl	C17H19NO4	301.3423	57646-30-7	3
Furathiocarb	C18H26N2O5S	382.4793	65907-30-4	3
Glufosinate	C5H12NO4P	181.1281	77182-82-2	3
Halofenozide	C18H19ClN2O2	330.8142	112226-61-6	2
Halosulfuron-methyl	C13H15ClN6O7S	434.8153	100784-20-1	2
Haloxypop-etotyl	C19H19ClF3NO5	433.8116	87237-48-7	1
Haloxypop-P	C15H11ClF3NO4	361.7047	95977-29-0	1
Haloxypop-P-methyl	C16H13ClF3NO4	375.7316	72619-32-0	1
Heptenophos	C9H12ClO4P	250.6182	23560-59-0	2
Hexaconazole	C14H17Cl2N3O	314.2143	79983-71-4	4
Hexaflumuron	C16H8Cl2F6N2O3	461.1474	86479-06-3	2
Hexazinone	C12H20N4O2	252.3167	51235-04-2	2
Hexythiazox	C17H21ClN2O2S	352.8834	78587-05-0	4
Hydramethylnon	C25H24F6N4	494.4836	67485-29-4	4
Imazalil	C14H14Cl2N2O	297.1838	35554-44-0	4
Imazamethabenz-methyl	C16H20N2O3	288.3466	81405-85-8	2
Imazapic	C14H17N3O3	275.3075	104098-48-8	2
Imazapyr	C13H15N3O3	261.2806	81334-34-1	2
Imazaquin	C17H17N3O3	311.3406	81335-37-7	2
Imazethapyr	C15H19N3O3	289.3344	81335-77-5	1
Imibenconazole	C17H13Cl3N4S	411.7403	86598-92-7	3
Imidacloprid	C9H10ClN5O2	255.6638	138261-41-3	4
Imidacloprid-Olefin	C9H8ClN5O2	253.6479	N/A	1
Inabenfide	C19H15ClN2O2	338.7935	82211-24-3	1
Indoxacarb	C22H17ClF3N3O7	527.8411	173584-44-6	4
Iodosulfuron-methyl	C14H13IN5O6S	506.2562	185119-76-0	1
Ipconazole	C18H24ClN3O	333.8612	125225-28-7	2
Iprobenfos	C13H21O3PS	288.346	26087-47-8	1
Iprodione	C13H13Cl2N3O3	330.1703	36734-19-7	2
Iprovalicarb	C18H28N2O3	320.4321	140923-17-7	4
Isazofos	C9H17ClN3O3PS	313.7432	42509-80-8	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Isocarbamid	C8H15N3O2	185.2261	30979-48-7	1
Isofenphos	C15H24NO4PS	345.398	25311-71-1	3
Isofenphos-methyl	C14H22NO4PS	331.3711	99675-03-3	1
Isofenphos-oxon	C15H24NO5P	329.3329	31120-85-1	1
isoprocarb	C11H15NO2	193.2457	2631-40-5	3
Isoprothiolane	C12H18O4S2	290.4012	50512-35-1	1
Isoproturon	C12H18N2O	206.288	34123-59-6	4
Isoxaben	C18H24N2O4	332.3997	82558-50-7	3
Isoxadifen-ethyl	C18H17NO3	295.3381	163520-33-0	1
Isoxaflutole	C15H12F3NO4S	359.3243	141112-29-0	3
Isoxathion	C13H16NO4PS	313.3125	18854-01-8	1
Ivermectin B1a	C48H74O14	875.1068	70288-86-7	1
Kresoxim-methyl	C18H19NO4	313.3533	143390-89-0	4
lambda-Cyhalothrin	C23H19ClF3NO3	449.8571	91465-08-6	1
Lenacil	C13H18N2O2	234.2983	2164-08-1	2
Linuron	C9H10Cl2N2O2	249.0962	330-55-2	4
Lufenuron	C17H8Cl2F8N2O3	511.1552	103055-07-8	4
Malaoxon	C10H19O7PS	314.2944	1634-78-2	2
Malathion	C10H19O6PS2	330.3594	121-75-5	2
Maleic hydrazide	C4H4N2O2	112.088	123-33-1	2
Mandipropamid	C23H22ClNO4	411.885	374726-62-2	3
MCPA-butotyl	C15H21ClO4	300.782	19480-43-4	1
Mecarbam	C10H20NO5PS2	329.3748	2595-54-2	1
Mefenacet	C16H14N2O2S	298.3641	73250-68-7	4
Mefenpyr-diethyl	C16H18Cl2N2O4	373.2356	135590-91-9	2
Mepanipyrim	C14H13N3	223.2778	110235-47-7	4
Mepiquat	C7H16N	114.2108	15302-91-7	1
Mepronil	C17H19NO2	269.3436	55814-41-0	4
Mesosulfuron-methyl	C17H21N5O9S2	503.5106	208465-21-8	3
Mesotrione	C14H13NO7S	339.324	104206-82-8	3
Metaflumizone	C24H16F6N4O2	506.4078	139968-49-3	1
Metalaxyl	C15H21NO4	279.3361	57837-19-1	5
Metamitron	C10H10N4O	202.216	41394-05-2	2
Metazachlor	C14H16ClN3O	277.7537	67129-08-2	3
Metazachlor-Metabolite BH 479-11	C15H19N3O2S	305.3995		1
Metconazole	C17H22ClN3O	319.8343	125116-23-6	3
Methabenzthiazuron	C10H11N3OS	221.2816	18691-97-9	4
Methacrifos	C7H13O5PS	240.2151	30864-28-9	2
Methamidophos	C2H8NO2PS	141.129	10265-92-6	4
Methfuroxam	C14H15NO2	229.2788	28730-17-8	1
Methidathion	C6H11N2O4PS3	302.3312	950-37-8	2
Methiocarb	C11H15NO2S	225.3101	2032-65-7	3
Methomyl	C5H10N2O2S	162.211	16752-77-5	3
Methomyl-oxime	C3H7NOS	105.1591	13749-94-5	2
Methoprotryne	C11H21N5OS	271.3854	841-06-5	2
Methoxyfenozide	C22H28N2O3	368.4762	161050-58-4	5
Metobromuron	C9H11BrN2O2	259.1022	3060-89-7	4
Metolachlor	C15H22ClNO2	283.7981	51218-45-2	2

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Metolcarb	C9H11NO2	165.1919	1129-41-5	1
Metosulam	C14H13Cl2N5O4S	418.2585	139528-85-1	1
Metoxuron	C10H13ClN2O2	228.6783	19937-59-8	2
Metrafenone	C19H21BrO5	409.2763	220899-03-6	3
Metribuzin	C8H14N4OS	214.29	21087-64-9	4
Metsulfuron-methyl	C14H15N5O6S	381.3676	74223-64-6	2
Mevinphos	C7H13O6P	224.15	7786-34-7	3
Mexacarbate	C12H18N2O2	222.2873	315-18-4	2
Molinate	C9H17NOS	187.3045	2212-67-1	2
Monocrotophos	C7H14NO5P	223.1654	6923-22-4	4
Monolinuron	C9H11ClN2O2	214.6514	1746-81-2	4
Monuron	C9H11ClN2O	198.6521	150-68-5	2
Moxidectin	C37H53NO8	639.8298	113507-06-5	2
Myclobutanil	C15H17ClN4	288.7801	88671-89-0	5
N,N-Dimethylamino-N-tolyl-sulfonamide	C9H14N2O2S	214.2869	66840-71-9	1
Napropamide	C17H21NO2	271.3595	15299-99-7	2
Neburon	C12H16Cl2N2O	275.1776	555-37-3	3
Nicosulfuron	C15H18N6O6S	410.4091	111991-09-4	1
Nicotine	C10H14N2	162.2349	54-11-5	1
Nitenpyram	C11H15ClN4O2	270.7187	120738-89-8	3
Norflurazon	C12H9ClF3N3O	303.6713	27314-13-2	2
Norflurazon-desmethyl	C11H7ClF3N3O	289.6444	23576-24-1	1
Novaluron	C17H9ClF8N2O4	492.7097	116714-46-6	4
Nuarimol	C17H12ClFN2O	314.7467	63284-71-9	4
Ofurace	C14H16ClNO3	281.7388	58810-48-3	1
Omethoate	C5H12NO4PS	213.1925	1113-02-6	5
Orbencarb	C12H16ClNOS	257.7825	34622-58-7	2
Oxadargyl	C15H14Cl2N2O3	341.1935	39807-15-3	1
Oxadiazon	C15H18Cl2N2O3	345.2252	19666-30-9	1
Oxadixyl	C14H18N2O4	278.308	77732-09-3	4
Oxamyl	C7H13N3O3S	219.2629	23135-22-0	2
Oxamyl-oxime	C5H10N2O2S	162.211	30558-43-1	1
Oxasulfuron	C17H18N4O6S	406.4177	144651-06-9	2
Oxydemeton-methyl	C6H15O4PS2	246.2849	301-12-2	2
Oxyfluorfen	C15H11ClF3NO4	361.7047	42874-03-3	1
Paclobutrazol	C15H20ClN3O	293.7964	76738-62-0	3
Paraoxon	C10H14NO6P	275.1978	311-45-5	2
Paraoxon-methyl	C8H10NO6P	247.144	950-35-6	6
Parathion	C10H14NO5PS	291.2629	56-38-2	2
Parathion-methyl	C8H10NO5PS	263.2091	298-00-0	2
Pebulate	C10H21NOS	203.3473	1114-71-2	1
Penconazole	C13H15Cl2N3	284.1881	66246-88-6	4
Pencycuron	C19H21ClN2O	328.8417	66063-05-6	4
Pendimethalin	C13H19N3O4	281.3117	40487-42-1	3
Penoxsulam	C16H14F5N5O5S	483.3744	219714-96-2	1
Permethrin	C21H20Cl2O3	391.2937	52645-53-1	1
Pethoxamid	C16H22ClNO2	295.8091	106700-29-2	3
Phenmedipham	C16H16N2O4	300.3142	13684-63-4	5

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Phenthoate	C12H17O4PS2	320.367	2597-03-7	2
Phorate	C7H17O2PS3	260.3776	298-02-2	1
Phorate-sulfone	C7H17O4PS3	292.3762	2588-04-7	2
Phorate-sulfoxide	C7H17O3PS3	276.3769	2588-03-6	1
Phosalone	C12H15CINO4PS2	367.8107	2310-17-0	4
Phosfolan	C7H14NO3PS2	255.2955	947-02-4	4
Phosphamidon	C10H19CINO5P	299.6908	13171-21-6	2
Phoxim	C12H15N2O3PS	298.301	14816-18-3	2
Picolinafen	C19H12F4N2O2	376.3106	137641-05-5	1
Picoxystrobin	C18H16F3NO4	367.3247	117428-22-5	3
Piperonyl-butoxide	C19H30O5	338.4441	51-03-6	4
Piperophos	C14H28NO3PS2	353.4837	24151-93-7	3
Pirimicarb	C11H18N4O2	238.2898	23103-98-2	4
Pirimiphos-ethyl	C13H24N3O3PS	333.3901	23505-41-1	2
Pirimiphos-methyl	C11H20N3O3PS	305.3363	29232-93-7	2
Primisulfuron-methyl	C15H12F4N4O7S	468.341	86209-51-0	1
Prochloraz	C15H16Cl3N3O2	376.6695	67747-09-5	4
Procymidone	C13H11Cl2NO2	284.1416	32809-16-8	3
Profenofos	C11H15BrClO3PS	373.6327	41198-08-7	2
Prohexadione	C10H12O5	212.2021	88805-35-0	1
Promecarb	C12H17NO2	207.2726	2631-37-0	2
Prometon	C10H19N5O	225.2941	1610-18-0	2
Prometryn	C10H19N5S	241.3592	7287-19-6	3
Propachlor	C11H14ClNO	211.6912	1918-16-7	3
Propamocarb	C9H20N2O2	188.27	24579-73-5	4
Propanil	C9H9Cl2NO	218.0822	709-98-8	3
Propaquizafop	C22H22ClN3O5	443.8868	111479-05-1	1
propargite	C19H26O4S	350.4775	2312-35-8	3
Propazine	C9H16ClN5	229.7127	139-40-2	3
Propazine-2-hydroxy	C9H17N5O	211.2672	7374-53-0	2
Propazine-d14	C9H2(2H)14ClN5	243.7992		1
Propetamphos	C10H20NO4PS	281.3111	31218-83-4	1
Propham	C10H13NO2	179.2188	122-42-9	2
Propiconazole	C15H17Cl2N3O2	342.2247	60207-90-1	4
Propisochlor	C15H22NO2Cl	283.7981	86763-47-5	4
propoxur	C11H15NO3	209.245	114-26-1	4
Propoxycarbazone	C15H18N4O7S	398.3949	181274-15-7	3
Propyzamide	C12H11Cl2NO	256.1312	23950-58-5	2
Prosulfocarb	C14H21NOS	251.3914	52888-80-9	2
Prosulfuron	C15H16F3N5O4S	419.3831	94125-34-5	2
Prothioconazole	C14H15Cl2N3OS	344.2629	178928-70-6	2
Prothioconazole Desthiometabolite	C14H15Cl2N3O	312.1985	N/A	2
Prothiofos	C11H15Cl2O2PS2	345.247	34643-46-4	2
Pymetrozine	C10H11N5O	217.2307	123312-89-0	4
Pyracarbolid	C13H15NO2	217.2678	24691-76-7	3
Pyraclufos	C14H18ClN2O3PS	360.7996	89784-60-1	1
Pyraclostrobin	C19H18ClN3O4	387.8227	175013-18-0	4
Pyraflufen-ethyl	C15H13Cl2F3N2O4	413.1801	129630-17-7	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Pyrazophos	C14H20N3O5PS	373.3681	13457-18-6	2
Pyridaben	C19H25CIN2OS	364.9378	96489-71-3	4
Pyridalyl	C18H14Cl4F3NO3	491.1205	179101-81-6	1
Pyridaphenthion	C14H17N2O4PS	340.3382	119-12-0	2
Pyridate	C19H23CIN2O2S	378.9213	55512-33-9	1
Pyrifenox	C14H12Cl2N2O	295.168	88283-41-4	2
Pyrimethanil	C12H13N3	199.2558	53112-28-0	5
Pyriproxyfen	C20H19NO3	321.3761	95737-68-1	4
Pyroquilon	C11H11NO	173.2147	57369-32-1	3
Pyroxsulam	C14H13F3N6O5S	434.3544	422556-08-9	1
Quinalphos	C12H15N2O3PS	298.301	13593-03-8	2
Quinmerac	C11H8CINO2	221.643	90717-03-6	2
Quinoclamine	C10H6CINO2	207.6161	2797-51-5	1
Quinoxyfen	C15H8Cl2FNO	308.1389	124495-18-7	4
Quizalofop-ethyl	C19H17CIN2O4	372.808	76578-14-8	3
Resmethrin	C22H26O3	338.4469	10453-86-8	1
Rimsulfuron	C14H17N5O7S2	431.4471	122931-48-0	2
Rotenone	C23H22O6	394.4242	83-79-4	4
Sebuthylazine	C9H16CIN5	229.7127	7286-69-3	3
Sebuthylazine-desethyl	C7H12CIN5	201.6589	N/A	3
Sethoxydim	C17H29NO3S	327.4866	74051-80-2	2
Siduron	C14H20N2O	232.3259	1982-49-6	3
Simazine	C7H12CIN5	201.6589	122-34-9	3
Simazine-2-hydroxy	C7H13N5O	183.2134	2599-11-3	2
Simetryn	C8H15N5S	213.3054	1014-70-6	4
Spinetoram A	C42H69NO10	748.0104	187166-40-1	2
Spinetoram B	C43H69NO10	760.0215	187166-15-0	1
Spinosyn A	C41H65NO10	731.9677	131929-60-7	4
Spinosyn D	C42H67NO10	745.9946	131929-63-0	2
Spirodiclofen	C21H24Cl2O4	411.3248	148477-71-8	4
Spiromesifen	C23H30O4	370.4889	283594-90-1	2
Spirotetramat	C21H27NO5	373.4492	203313-25-1	2
Spiroxamine	C18H35NO2	297.4815	118134-30-8	5
Sulcotrione	C14H13ClO5S	328.7713	99105-77-8	2
Sulfentrazone	C11H10Cl2F2N4O3S	387.1924	122836-35-5	2
Sulfometuron-methyl	C15H16N4O5S	364.3804	74222-97-2	2
Sulfosulfuron	C16H18N6O7S2	470.4839	141776-32-1	2
Sulfotep	C8H20O5P2S2	322.3197	3689-24-5	1
Sulprofos	C12H19O2PS3	322.4486	35400-43-2	1
tau-Fluvalinate	C26H22ClF3N2O3	502.9208	102851-06-9	2
Tebuconazole	C16H22CIN3O	307.8233	107534-96-3	4
Tebufenozide	C22H28N2O2	352.4769	112410-23-8	4
Tebufenpyrad	C18H24CIN3O	333.8612	119168-77-3	4
Tebupirimfos	C13H23N2O3PS	318.3754	96182-53-5	2
Tebutam	C15H23NO	233.3539	35256-85-0	1
Tebuthiuron	C9H16N4OS	228.3169	34014-18-1	3
Teflubenzuron	C14H6Cl2F4N2O2	381.1133	83121-18-0	4
Temephos	C16H20O6P2S3	466.4717	3383-96-8	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
TEPP	C8H20O7P2	290.1896	107-49-3	1
Terbufos	C9H21O2PS3	288.4314	13071-79-9	2
Terbufos-sulfone	C9H21O4PS3	320.43	56070-16-7	4
Terbumeton	C10H19N5O	225.2941	33693-04-8	2
Terbuthylazine	C9H16CIN5	229.7127	5915-41-3	3
Terbuthylazine-2-hydroxy	C9H17N5O	211.2672	N/A	2
Terbuthylazine-desethyl	C7H12CIN5	201.6589	30125-63-4	3
Terbutryn	C10H19N5S	241.3592	886-50-0	3
Tetrachlorvinphos	C10H9Cl4O4P	365.9637	22248-79-9	1
Tetraconazole	C13H11Cl2F4N3O	372.1494	112281-77-3	4
Tetramethrin	C19H25NO4	331.4119	7696-12-0	3
Thiabendazole	C10H7N3S	201.2505	148-79-8	4
Thiacloprid	C10H9CIN4S	252.7259	111988-49-9	4
Thiamethoxam	C8H10CIN5O3S	291.7165	153719-23-4	4
Thidiazuron	C9H8N4OS	220.2535	51707-55-2	3
Thiencarbazone-methyl	C12H14N4O7S2	390.3945	317815-83-1	1
Thifensulfuron-methyl	C12H13N5O6S2	387.394	79277-27-3	2
Thiobencarb	C12H16CINOS	257.7825	28249-77-6	5
Thiodicarb	C10H18N4O4S3	354.4706	59669-26-0	1
Thiofanox-sulfone	C9H18N2O4S	250.3172	39184-59-3	3
Thiofanox-sulfoxide	C9H18N2O3S	234.3179	39184-27-5	1
Thionazin	C8H13N2O3PS	248.241	297-97-2	4
Thiophanate	C14H18N4O4S2	370.4503	23564-06-9	1
Thiophanate-methyl	C12H14N4O4S2	342.3965	23564-05-8	4
Tolclofos-methyl	C9H11Cl2O3PS	301.1281	57018-04-9	2
Tolyfluanid	C10H13Cl2FN2O2S2	347.2582	731-27-1	2
Topramezone	C16H17N3O5S	363.3926	210631-68-8	1
Tralkoxydim	C20H27NO3	329.4395	87820-88-0	3
Tri-allate	C10H16Cl3NOS	304.6659	2303-17-5	2
Triadimefon	C14H16CIN3O2	293.753	43121-43-3	4
Triadimenol	C14H18CIN3O2	295.7689	55219-65-3	2
Triasulfuron	C14H16CIN5O5S	401.8289	82097-50-5	2
Triazamate	C13H22N4O3S	314.4073	112143-82-5	1
Triazophos	C12H16N3O3PS	313.3157	24017-47-8	3
Triazoxide	C10H6CIN5O	247.6438	72459-58-6	2
Tribenuron-methyl	C15H17N5O6S	395.3944	101200-48-0	1
Trichlorfon	C4H8Cl3O4P	257.4368	52-68-6	3
Tricyclazole	C9H7N3S	189.2395	41814-78-2	2
Tridemorph	C19H39NO	297.5249	24602-86-6	1
Trietazine	C9H16CIN5	229.7127	1912-26-1	1
Trifloxystrobin	C20H19F3N2O4	408.3774	141517-21-7	4
Trifloxystrobin CGA 321113	C19H17F3N2O4	394.3505	252913-85-2	1
Trifloxystrobin NOA 413161	C19H15F3N2O6	424.3333		1
Trifloxystrobin NOA 413163	C19H15F3N2O6	424.3333		1
Triflumizole	C15H15ClF3N3O	345.752	68694-11-1	4
Triflumuron	C15H10ClF3N2O3	358.7043	64628-44-0	2
Trifluralin	C13H16F3N3O4	335.2831	1582-09-8	1
Triflusulfuron-methyl	C17H19F3N6O6S	492.4343	126535-15-7	2

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Trinexapac-ethyl	C ₁₃ H ₁₆ O ₅	252.2669	95266-40-3	2
Triphenylphosphate	C ₁₈ H ₁₅ O ₄ P	326.2886	115-86-6	2
Triticonazole	C ₁₇ H ₂₀ CIN ₃ O	317.8185	131983-72-7	2
Tritosulfuron	C ₁₃ H ₉ F ₆ N ₅ O ₄ S	445.3007	142469-14-5	2
Tritosulfuron BH 635-5	C ₅ H ₅ F ₃ N ₄ O	194.1164		1
Uniconazole	C ₁₅ H ₁₈ CIN ₃ O	291.7806	83657-22-1	1
Vamidothion	C ₈ H ₁₈ NO ₄ PS ₂	287.3376	2275-23-2	4
Warfarin	C ₁₉ H ₁₆ O ₄	308.3338	81-81-2	4
Zoxamide	C ₁₄ H ₁₆ Cl ₃ NO ₂	336.645	156052-68-5	5

Product Name	License	Part Number
Pesticides High Resolution MS/MS Spectral Library Version 1.0	permanent	5038645
	one-year	5038646

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