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Mass Spectral Libraries for Food Analysis

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

Antibiotics High Resolution MS/MS Library Version 1.0

An overview of the licensed mass spectral library for antibiotics and veterinary drugs 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 244 antibiotic and veterinary drug 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 244 antibiotics and veterinary drugs commonly tested for in food products of animal origin.
- Includes 259 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
17a-Methyltestosterone	C20H30O2	302.4572	58-18-4	1
4,6-Dimethyl-2-Hydroxypyrimidine	C6H8N2O	124.1425	108-79-2	1
5-Hydroxymebendazole	C16H15N3O3	297.3137	60254-95-7	1
5-Hydroxymebendazole-D3	C16H12(2H)3N3O3	300.3323		1
5-Hydroxythiabenzazole	C10H7N3OS	217.2499	948-71-0	1
a-Nortestosterone	C18H26O2	274.4034	68-22-4	1
Acepromazine	C19H22N2OS	326.4613	61-00-7	1
Acetoxyprogesterone-17a	C23H32O4	372.5048	302-23-8	1
Acetyltiylosin, 3-O-	C48H79NO18	958.1505	63409-10-9	1
Albendazole	C12H15N3O2S	265.3347	54965-21-8	1
Albendazole-2-amino-sulfone-D3	C10H10(2H)3N3O2S	242.3153		1
Albendazole-D3	C12H12 2H3N3O2S	268.3532		1
Albendazole sulfoxide	C12H15N3O3S	281.334	54029-12-8	1
Albendazole sulfoxide-d3	C12H12 2H3N3O3S	284.3525		1
Albendazolsulfon	C12H15N3O4S	297.3333	75184-71-3	1
Albendazolsulfon-D3	C12H12 2H3N3O4S	300.3518		1
Albendazolsulfonamin	C10H13N3O2S	239.2967	80983-34-2	1
Aminoflubendazol	C14H10FN3O	255.2518	82050-13-3	1
Aminomebendazol	C14H11N3O	237.2613	52329-60-9	1
Aminophenazon	C13H17N3O	231.2978	58-15-1	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Aminopropylon	C16H22N4O2	302.3767	3690-04-8	1
Amoxicillin	C16H19N3O5S	365.4085	26787-78-0	1
Ampicillin	C16H19N3O4S	349.4092	69-53-4	1
Arprinocid	C12H9CIFN5	277.6887	55779-18-5	1
Avermectin B1a	C48H72O14	873.091	71751-41-2	1
Azaperone	C19H22FN3O	327.4021	1649-18-9	1
b-Boldenone	C19H26O2	286.4144	846-48-0	1
Bamethan	C12H19NO2	209.2884	3703-79-5	1
Baquiloprim	C17H20N6	308.3867	102280-35-3	1
Benzylpenicillin, (Penicillin G)	C16H18N2O4S	334.3945	61-33-6	1
Brilliant green	C27H34N2O4S	482.6427	633-03-4	1
Brombuterol	C12H18Br2N2O	366.095	419337-02-4	1
Carazolol	C18H22N2O2	298.3852	57775-29-8	1
Carbuterol	C13H21N3O3	267.3282	34866-47-2	1
Carprofen	C15H12CINO2	273.7188	53716-49-7	1
Cefalonium	C20H18N4O5S2	458.5159	5575-21-3	1
Cefazolin	C14H14N8O4S3	454.51	25953-19-9	1
Cefoperazon	C25H27N9O8S2	645.6742	62893-20-3	1
Ceftiofur	C19H17N5O7S3	523.5667	80370-57-6	1
Cephalexin	C16H17N3O4S	347.3933	15686-71-2	1
Cephapirin	C17H17N3O6S2	423.4674	21593-23-7	1
Chloramphenicol	C11H12Cl2N2O5	323.1321	56-75-7	2
Chlorbrombuterol	C12H18BrClN2O	321.6442	37153-52-9	1
Chlormadinone acetate	C23H29ClO4	404.9337	302-22-7	1
Chlorprothixene	C18H18ClNS	315.8652	113-59-7	1
Chlortetracyclin	C22H23ClN2O8	478.886	57-62-5	1
Cimaterol	C12H17N3O	219.2868	54239-37-1	1
Cimbuterol	C13H19N3O	233.3137	54239-39-3	1
Ciprofloxacin	C17H18FN3O3	331.347	85721-33-1	1
Clenbuterol	C12H18Cl2N2O	277.1934	21898-19-1	1
Clencyclohexerol	C14H20Cl2N2O2	319.2307	157877-79-7	1
Clenhexerol	C14H22Cl2N2O	305.2472	78982-88-4	1
Clenisopenterol	C13H20Cl2N2O	291.2203	157664-68-1	1
Clenpenterol	C13H20Cl2N2O	291.2203	37158-47-7	1
Clenproperol	C11H16Cl2N2O	263.1665	38339-18-3	1
Clenproperol-D7	C11H9 2H7Cl2N2O	270.2098	1173021-09-4	1
Clobendazole	C16H12ClN3O3	329.7427		1
Clorprenaline	C11H16ClNO	213.707	3811-25-4	1
Clorsulon	C8H8Cl3N3O4S2	380.6563	60200-06-8	1
Closantel	C22H14Cl2I2N2O2	663.0804	57808-65-8	2
Closantel-13C(6)	(13C6)C16H14Cl2I2N2O2	669.0343		2
Cloxacillin	C19H18ClN3O5S	435.8864	61-72-3	1
Cyclopentylalbendazole	C14H17N3O2S	291.3726	77723-30-9	1
Danofloxacin	C19H20FN3O3	357.3849	112398-08-0	1
Dapson	C12H12N2O2S	248.3041	80-08-0	1
Decoquinat	C24H35NO5	417.5457	18507-89-6	1
Desacetylcephapirin	C15H15N3O5S2	381.4301	38115-21-8	1
Dexamethasone	C22H29FO5	392.4677	50-02-2	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Diclofenac	C14H11Cl2NO2	296.1526	15307-86-5	1
Dicloxacillin	C19H17Cl2N3O5S	470.3312	3116-76-5	1
Dienestrol	C18H18O2	266.34	84-17-3	1
Dienestrol-D2	C18H16O2(2H)2	268.3523		1
Diethylstilbestroldipropionat	C24H28O4	380.4841	130-80-3	1
Difloxacin	C21H19F2N3O3	399.3974	98106-17-3	1
Dimetridazol	C5H7N3O2	141.1296	551-92-8	1
Dimetridazol-D3	C5H4 2H3N3O2	144.1481	64678-69-9	1
Dinitrocarbanilid-D8	C13H2 2H8N4O5	310.2958		1
Doramectin	C50H74O14	899.1289	117704-25-3	2
Doxycycline (Tautomer)	C22H24N2O8	444.4412	564-25-0	1
Emamectin benzoate (B1a)	C49H75NO13	886.1332	155569-91-8	1
Enrofloxacin	C19H22FN3O3	359.4007	93106-60-6	1
Enrofloxacin-D5	C19(2H)5H17FN3O3	364.4316		1
epi-Chlortetracyclin	C22H23ClN2O8	478.886	14297-93-9	1
epi-Oxytetracyclin	C22H24N2O9	460.4405	35259-39-3	1
epi-Tetracyclin	C22H24N2O8	444.4412	23313-80-6	1
Eprinomectin B1a	C50H75NO14	914.1436	133305-88-1	1
Erythromycin A	C37H67NO13	733.9374	59319-72-1	1
Erythromycin A-(13C)2	(13C)2C35H67NO13	735.922	114-07-08	1
Erythromycin A Anhydrid	C37H65NO12	715.9222	23893-13-2	1
Ethidimuron	C7H12N4O3S2	264.3262	30043-49-3	1
Febantel	C20H22N4O6S	446.4825	58306-30-2	1
Fenbendazol-D3	C15H10 2H3N3O2S	302.3704	1228182-47-5	1
Fenbendazole	C15H13N3O2S	299.3519	43210-67-9	1
Fenbendazole sulfone-D3	C15H10 2H3N3O4S	334.3691	1228182-49-7	1
Fenoterol	C17H21NO4	303.3581	13392-18-2	1
Florfenicol	C12H14Cl2FNO4S	358.2157	73231-34-2	2
Flubendazole	C16H12FN3O3	313.2884	31430-15-6	1
Flubendazole-D3	C16H9 2H3FN3O3	316.3069	1173021-08-3	1
Flufenamic Acid	C14H10F3NO2	281.2344	530-78-9	1
Flumequine	C14H12FNO3	261.2528	42835-25-6	1
Flumethasone	C22H28F2O5	410.4582	2135-17-3	1
Flunixin	C14H11F3N2O2	296.2491	38677-85-9	1
Flunixin-D3	C14H8(2H)3F3N2O2	299.2676	1015856-60-6	2
Gamithromycin	C40H76N2O12	777.0493	145435-72-9	1
Halofuginon	C16H17BrClN3O3	414.6859	55837-20-2	1
Heliotrin	C16H27NO5	313.394	303-33-3	1
Hydroxy-Ipronidazole-D3	C7H8(2H)3N3O3	188.2012		1
Hydroxymethylclenbuterol	C12H18Cl2N2O2	293.1928	38339-18-3	1
Ipronidazole	C7H11N3O2	169.1834	14885-29-1	1
Ipronidazole-D3	C7H8(2H)3N3O2	172.2019		1
Ipronidazole-OH	C7H11N3O3	185.1827	35175-14-5	1
Isochlortetracyclin	C22H23ClN2O8	478.886	514-53-4	1
Isoxsuprine	C18H23NO3	301.3857	395-28-8	1
Ivermectin	C48H74O14	875.1068	70288-86-7	1
Josamycin	C42H69NO15	828.0071	56689-45-3	1
Ketoprofen	C16H14O3	254.2855	22071-15-4	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Ketotriclabendazole	C13H7Cl3N2O2	329.5693		2
Kristallviolett	C25H30ClN3	407.9867	548-62-9	1
Labetalol	C19H24N2O3	328.4114	36894-69-6	1
Lasalocid A	C34H53NaO8	612.7797	25999-20-6	1
Leuco Malachite Green	C23H26N2	330.4734	129-73-7	1
Leuco Malachite Green-D5	C23H21(2H)5N2	335.5043		1
Leucocrystal Violet	C25H31N3	373.5419	603-48-5	1
Leucomycin	C35H59NO13	701.8519	1392-21-8	1
Levamisole	C11H12N2S	204.2944	14769-73-4	1
Lincomycin	C18H34N2O6S	406.542	154-21-2	1
Mabuterol	C13H18ClF3N2O	310.7469	56341-08-3	1
Mapenterol	C14H20ClF3N2O	324.7738	95656-68-1	1
Marbofloxacin	C17H19FN4O4	362.361	115550-35-1	1
Mebendazol	C16H13N3O3	295.2979	31431-39-7	1
Mebendazol-D3	C16H10 2H3N3O3	298.3164		1
Meclofenamic acid	C14H11Cl2NO2	296.1526	644-62-2	1
Medroxyprogesterone acetate	C24H34O4	386.5317	71-58-9	1
Mefenamic acid	C15H15NO2	241.2899	61-68-7	1
Megestrol acetate	C24H32O4	384.5158	595-33-5	1
Melengestrol acetate	C25H32O4	396.5268	2919-66-6	1
Meloxicam	C14H13N3O4S2	351.4039	71125-38-7	1
Meloxicam-D3	C14H10 2H3N3O4S2	354.4224	942047-63-4	2
Methapyrilene	C14H19N3S	261.3898	135-23-9	1
Methicillin	C17H20N2O6S	380.42	61-32-5	1
Methotrimeprazine	C19H24N2OS	328.4772	851-68-3	1
Meticloprindol, (Clopidol)	C7H7Cl2NO	192.0443	2971-90-6	1
Metoprolol	C15H25NO3	267.3684	37350-58-6	1
Metronidazol	C6H9N3O3	171.1558	444-48-1	1
Metronidazol-D3	C6H6(2H)3N3O3	174.1743		1
Metronidazole-OH	C6H9N3O4	187.1551	4812-40-2	1
Monensin	C36H62O11	670.8813	17090-79-8	1
Monocrotalin	C16H23NO6	325.3616	315-22-0	1
Nafcillin	C21H22N2O5S	414.4807	147-52-4	1
Nalidixic acid	C12H12N2O3	232.239	389-08-2	1
Nandrolon	C18H26O2	274.4034	434-22-0	1
Naproxen	C14H14O3	230.2635	22204-53-1	1
Netobimin-Micronized	C14H20N4O7S2	420.4641	88255-01-0	1
Niflumic acid	C13H9F3N2O2	282.2222	4394-00-7	1
Nitroxinil	C7H3IN2O3	290.017	1689-89-0	1
Norfloxacin	C16H18FN3O3	319.3359	70458-96-7	1
Oleandomycin	C35H61NO12	687.8684	2751-09-9	1
Orciprenaline	C11H17NO3	211.2609	586-06-1	1
Oxacillin	C19H19N3O5S	401.4416	61-72-3	1
Oxfendazole	C15H13N3O3S	315.3512	53716-50-0	1
Oxfendazole-D3	C15H10 2H3N3O3S	318.3698	1228182-54-4	1
Oxfendazolsulfon	C15H13N3O4S	331.3506	54029-20-8	1
Oxibendazole	C12H15N3O3	249.2696	20559-55-1	1
Oxibendazole-D7	C12H8 2H7N3O3	256.3128	1173019-44-7	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Oxolinic acid	C13H11NO5	261.234	14698-29-4	1
Oxyphenbutazone	C19H20N2O3	324.3797	129-20-4	1
Oxytetracycline	C22H24N2O9	460.4405	79-57-2	1
Phenylbutazone	C19H20N2O2	308.3804	129-18-0	1
Phenylbutazone-D10	C19H10(2H)10N2O2	318.4422		1
Pirbuterol	C12H20N2O3	240.3025	38677-81-5	1
Pirlimycin	C17H31ClN2O5S	410.9606	79548-73-5	1
Praziquantel	C19H24N2O2	312.4121	55268-74-1	1
Prednisolone	C21H28O5	360.4503	50-24-8	1
Progesterone	C21H30O2	314.4682	57-83-0	1
Promethazine	C17H20N2S	284.4241	60-87-7	1
Propionylpromazine	C20H24N2OS	340.4882	3568-24-9	1
Ractopamine	C18H23NO3	301.3857	97825-25-7	1
Rafoxanide	C19H11Cl2I2NO3	626.0161	22662-39-1	2
Ramifenazon	C14H19N3O	245.3247	3615-24-5	1
Retrorsin	C18H25NO6	351.3995	480-54-6	1
Ritodrine	C17H21NO3	287.3588	26652-09-5	1
Robenidine	C15H13Cl2N5	334.2079	25875-51-8	1
Ronidazole	C6H8N4O4	200.154	7681-76-7	1
Ronidazole-D3	C6H5(2H)3N4O4	203.1725	1015855-87-4	1
Roxithromycin	C41H76N2O15	837.0583	80214-83-1	1
Salbutamol	C13H21NO3	239.3147	18559-94-9	1
Salmeterol	C25H37NO4	415.5732	89365-50-4	1
Salmeterol-D3	C25H34 2H3NO4	418.5918	497063-94-2	1
Sarafloxacin	C20H17F2N3O3	385.3705	98105-99-8	1
Secnidazol	C7H11N3O3	185.1827	3366-95-8	1
Selamectin	C43H63NO11	769.9732	220119-17-5	1
Semduramycin	C45H76O16	873.0882	113378-31-7	1
Senecionin	C18H25NO5	335.4002	130-01-8	1
Seneciophyllin	C18H23NO5	333.3843	480-81-9	1
Sotalol	C12H20N2O3S	272.3668	3930-20-9	1
Spectinomycin	C14H24N2O7	332.3535	1695-77-8	1
Spiramycin	C43H74N2O14	843.0652	8025-81-8	1
Stanozolol	C21H32N2O	328.4982	10418-03-8	1
Sulfabenzamide	C13H12N2O3S	276.3145	127-71-9	1
Sulfacetamide	C8H10N2O3S	214.2434	144-80-9	1
Sulfachloropyridazine	C10H9ClN4O2S	284.7245	80-32-0	1
Sulfadiazine	C10H10N4O2S	250.2797	68-35-9	1
Sulfadimethoxine	C12H14N4O4S	310.3321	122-11-2	1
Sulfadimethoxine-D6	C12H8 2H6N4O4S	316.3692		1
Sulfadimidin	C12H14N4O2S	278.3335	57-68-1	1
Sulfadoxine	C12H14N4O4S	310.3321	2447-57-6	1
Sulfaguanidin	C7H10N4O2S	214.2466	57-67-0	1
Sulfamerazine	C11H12N4O2S	264.3066	127-79-7	1
Sulfameter	C11H12N4O3S	280.3059	651-06-9	1
Sulfamethizol	C9H10N4O2S2	270.3331	144-82-1	1
Sulfamethoxazole	C10H11N3O3S	253.2802	723-46-6	1
Sulfamethoxy-pyridazine	C11H12N4O3S	280.3059	80-35-3	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Sulfamoxol	C11H13N3O3S	267.3071	729-99-7	1
Sulfanilamide	C6H8N2O2S	172.2062	63-74-1	1
Sulfaphenazole	C15H14N4O2S	314.3666	526-08-9	1
Sulfapyridin	C11H11N3O2S	249.2919	144-83-2	1
Sulfaquinoxaline	C14H12N4O2S	300.3397	59-40-5	1
Sulfathiazole	C9H9N3O2S2	255.3184	72-14-0	1
Terbutaline	C12H19NO3	225.2878	23031-25-6	1
Testosterone	C19H28O2	288.4303	58-22-0	1
Tetracycline	C22H24N2O8	444.4412	60-54-8	1
Tetramisole-D5	C11H7 2H5N2S	209.3253	1173021-85-6	1
Thiabendazole	C10H7N3S	201.2505	148-79-8	1
Thiamphenicol	C12H15Cl2NO5S	356.2246	15318-45-3	2
Tiamulin	C28H47NO4S	493.75	55297-95-5	1
Tilmicosin	C46H80N2O13	869.1465	108050-54-0	1
Tinidazol	C8H13N3O4S	247.2733	19387-91-8	1
Tolfenamic Acid	C14H12ClNO2	261.7078	13710-19-5	1
Tolfenamic Acid-(13C)6	C8(13C)6H12ClNO2	267.6617		2
Trenbolone	C18H22O2	270.3717	10161-33-8	1
Triamcinolone	C21H27FO6	394.4401	124-94-7	1
Triclabendazole	C14H9Cl3N2OS	359.6613	68786-66-3	2
Triclabendazole-D3	C14H6 2H3Cl3N2OS	362.6798		2
Triclabendazole sulfone	C14H9Cl3N2O3S	391.66	100648-14-4	2
Triclabendazole sulfoxide	C14H9Cl3N2O2S	375.6606	100648-13-3	2
Trimethoprim	C14H18N4O3	290.3222	738-70-5	1
Tulathromycin Marker		0		1
Tulobuterol	C12H18ClNO	227.7339	41570-61-0	1
Tylosin A	C46H77NO17	916.1133	8026-48-0	1
Tylosin B	C39H65NO14	771.9429	11032-98-7	1
Tylvylosin (Aivlosin)	C53H87NO19	1042.268	63409-12-1	1
Valnemulin	C31H52N2O5S	564.8288	101312-92-9	1
Xylazine	C12H16N2S	220.3372	23076-35-9	1
Zilpaterol	C14H19N3O2	261.324	117827-79-9	1

Product Name	License	Part Number
Antibiotics High Resolution MS/MS Spectral Library Version 1.0	permanent	5038640
	one-year	5038642

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Headquarters
500 Old Connecticut Path, Framingham, MA 01701 USA
Phone 508-383-7700
www.sciex.com

International Sales
For our office locations please call the division
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