Mycotoxin Spectral Library Version 1.1 for LibraryView™ Software

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An overview of the licensed mass spectral library for mycotoxins compatible with LibraryView™ Software

LibraryView™ Software 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've assembled an MS/MS spectral library compatible with LibraryView™ Software containing 248 mycotoxin residue entries. This library was created using certified reference materials and can be used in LibraryView™ Software to perform MS/MS library searching or to create custom screening and/or quantitation methods using the integrated MRM information.

Features of this MS/MS spectra library:

- Includes data on 245 mycotoxins and other fungal/bacterial metabolites commonly tested for in grains, cereals, or other food products.
- Contains 245 integrated MRM entries with up to 3 transitions per compound.
- Includes 236 full MS/MS spectral library entries including individual spectra acquired using three distinct collision energies (20 eV, 35 eV, 50 eV), as well as a single spectra representing the sum of all 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 MRM information to build methods without the need to re-infuse standards and optimize MRM transitions for a given compound.
- Easily create screening methods for an MRM triggered EPI workflow for use on QTRAP® LC/MS/MS systems.
- Quickly set-up MRM quantitation methods for traditional MRM ratio quantitation and confirmation on a QTRAP® or Triple Quad™ LC/MS/MS system.
- Set-up smaller customer libraries by simply selecting only the compounds of interest from the list in LibraryView™ Software.
- Use LibraryView™ Software to automatically create your custom acquisition and quantitation methods.

The following is a list of the antibiotics currently in the library. This library is verified for use on AB SCIEX 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
15-Acetyl-deoxynivalenol	C17H22O7	338.3573	88337-96-6	4
15-Monoacetoxyscirpenol	C17H24O6	324.3738	2623-22-5	4
16-Ketoaspergillimide	C20H27N3O4	373.4523	199784-50-4	4
2-Amino-14,16-dimethyloctadecan-3-ol	C20H43ON	313.5676	540770-33-0	4
3-Acetyl-deoxynivalenol	C17H22O7	338.3573	50722-38-8	8
3-Nitropropionic acid	C3H5NO4	119.0768	504-88-1	0
3-O-Methylviridicatin	C16H13NO2	251.285	6152-51-4	4
A23187	C29H37N3O6	523.6296	52665-69-7	8
AAL-TA1 Toxin	C25H47NO10	521.6484	79367-52-5	4
Actinomycin D	C62H86N12O16	1255.436	50-76-0	4
Aflatoxin B1	C17H12O6	312.2787	1162-65-8	4
Aflatoxin B2	C17H14O6	314.2945	7220-81-7	4
Aflatoxin G1	C17H12O7	328.278	1165-39-5	4
Aflatoxin G2	C17H14O7	330.2939	7241-98-7	4
Aflatoxin M1	C17H12O7	328.278	6795-23-9	4
Aflatoxin M2	C17H14O7	330.2939	6885-57-0	4
Agroclavine	C16H18N2	238.3328	548-42-5	4
Alamethicin F30	C92H150N22O25	1964.336	27061-78-5	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
alpha-Zearalenol	C18H24O5	320.3855	36455-72-8	8
alpha-Zearalenol-4-O-glucoside	C24H34O10	482.5276	135626-94-7	8
Altenuene	C15H16O6	292.2883	29752-43-0	8
Altenusin	C15H14O6	290.2725	31186-12-6	8
Alternariol	C14H10O5	258.2304	641-38-3	8
Alternariolmethylether	C15H12O5	272.2573	26894-49-5	8
Altersolanol	C16H16O7	320.2987	22268-16-2	8
Altertoxin-I	C20H16O6	352.3435	56258-32-3	4
Altertoxin-II	C20H14O6	350.3276	56257-59-1	0
Amphotericin B	C47H73NO17	924.0926	1397-89-3	0
Anisomycin	C14H19NO4	265.3092	22862-76-6	4
Apicidin	C34H49N5O6	623.7934	183506-66-3	8
Ascomycin	C43H69NO12	792.0201	104987-12-4	4
Aspercolorin	C25H28N4O5	464.5215	29123-52-2	8
Aspergillimide	C20H29N3O3	359.4688	195966-93-9	4
Asperlactone	C9H12O4	184.1917	76375-62-7	4
Asperloxine A	C21H19N3O5	393.3993	223130-52-7	4
Aspinonene	C9H16O4	188.2234	157676-96-5	4
Aspyrone	C9H12O4	184.1917	17398-00-4	4
Asterric acid	C17H16O8	348.309	577-64-0	8
Atpenin A5	C15H21Cl2NO5	366.2409	119509-24-9	8
Aureobasidin A	C60H92N8O11	1101.438	127757-30-6	4
Aurofusarin	C30H18O12	570.4657	13191-64-5	8
Austdiol	C12H12O5	236.2242	53043-28-0	8
Austocystin A	C19H13ClO6	372.7614	55256-58-1	4
Avenacein Y	C15H10O8	318.2394	102426-44-8	4
Bacitracin	C66H103N17O16S	1422.713	22601-59-8	4
Bafilomycin A1	C35H58O9	622.8399	88899-55-2	4
Beauvericin	C45H57N3O9	783.9626	26048-05-5	4
beta-Ergocryptine	C32H41N5O5	575.7086	511-09-1	4
beta-Ergocryptinine	C32H41N5O5	575.7086	511-10-4	4
beta-Zearalenol	C18H24O5	320.3855	71030-11-0	8
beta-Zearalenol-4-O-glucoside	C24H34O10	482.5276	135626-93-6	8
Brefeldin A	C16H24O4	280.3641	20350-15-6	4
Brevicompanine B	C22H29N3O2	367.4916	215121-47-4	4
Calphostin C	C44H38O14	790.7773	121263-19-2	8
Cephalosporin C	C16H21N3O8S	415.4223	61-24-5	4
Cerulenin	C12H17NO3	223.2719	17397-89-6	4
Chaetocin	C30H28N6O6S4	696.8471	28097-03-2	8
Chaetoglobosin A	C32H36N2O5	528.6487	50335-03-0	4
Chanoclavine	C16H20N2O	256.348	2390-99-0	4
Chetomin	C31H30O6N6S4	710.874	1403-36-7	4
Chlamydosporol	C11H14O5	226.229	135063-30-8	4
Chloramphenicol	C11H12Cl2N2O5	323.1321	56-75-7	5
Chromomycin A3	C57H82O26	1183.261	7059-24-7	0
Citreoviridin	C23H30O6	402.4876	25425-12-1	4
Citrinin	C13H14O5	250.2511	518-75-2	8
Citromycetin	C14H10O7	290.229	478-60-4	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Cochliodinol	C32H30N2O4	506.6018	11051-88-0	8
Curvularin	C16H20O5	292.3317	10140-70-2	8
Cycloaspeptide A	C36H43N5O6	641.7679	109171-13-3	8
Cycloechinulin	C20H21N3O3	351.4054	143086-29-7	8
Cycloheximide	C15H23NO4	281.3519	66-81-9	8
Cyclopenin	C17H14N2O3	294.3101	19553-26-5	8
Cyclopeptine	C17H16N2O2	280.3266	50886-63-0	4
Cyclopiazonic acid	C20H20N2O3	336.3908	18172-33-3	8
Cyclosporin A	C62H111N11O12	1202.63	59865-13-3	8
Cyclosporin C	C62H111N11O13	1218.63	59787-61-0	4
Cyclosporin D	C63H113N11O12	1216.657	63775-96-2	4
Cyclosporin H	C62H111N11O12	1202.63	83602-39-5	4
Cytochalasin A	C29H35O5N	477.6009	14110-64-6	4
Cytochalasin B	C29H37O5N	479.6167	14930-96-2	4
Cytochalasin C	C30H37O6N	507.6271	22144-76-9	4
Cytochalasin D	C30H37O6N	507.6271	22144-77-0	4
Cytochalasin E	C28H33O7N	495.5726	36011-19-5	4
Cytochalasin H	C30H39NO5	493.6436	53760-19-3	4
Cytochalasin J	C28H37NO4	451.6063	56144-22-0	4
Decarestrictine	C10H16O5	216.2338	127393-89-9	4
Dechlorogriseofulvin	C17H18O6	318.3262	3680-32-8	4
Deepoxy-deoxynivalenol	C15H20O5	280.3207	88054-24-4	7
Deoxybrevianamide E	C21H25N3O2	351.4489	34610-68-9	8
Deoxynivalenol	C15H20O6	296.32	51481-10-8	6
Deoxynivalenol-3-glucoside	C21H30O11	458.4621	131180-21-7	8
Diacetoxyscirpenol	C19H26O7	366.411	2270-40-8	4
Dihydroergosine	C30H39N5O5	549.6706	7288-61-1	4
Dihydroergotamine	C33H37N5O5	583.6879	511-12-6	4
Dihydrolysergol	C16H20N2O	256.348	18051-16-6	4
Dinactin	C42H68O12	764.9944	20261-85-2	0
Elymoclavine	C16H18N2O	254.3321	548-43-6	4
Elymoclavine fructoside	C22H28N2O6	416.4742	12379-50-9	4
Emodin	C15H10O5	270.2414	518-82-1	8
Enniatin A	C36H63N3O9	681.9109	144446-20-8	4
Enniatin A1	C35H61N3O9	667.884	4530-21-6	4
Enniatin B	C33H57N3O9	639.8302	917-13-5	4
Enniatin B1	C34H59N3O9	653.8571	19914-20-6	4
Enniatin B2	C32H55N3O9	625.8033	632-91-7	4
Enniatin B3	C31H53N3O9	611.7764	864-99-3	4
Equisetin	C22H31NO4	373.4926	57749-43-6	8
Ergine	C16H17N3O	267.3309	478-94-4	4
Erginine	C16H17N3O	267.3309	N/A	4
Ergocornine	C31H39N5O5	561.6817	564-36-3	4
Ergocorninine	C31H39N5O5	561.6817	564-37-4	4
Ergocristine	C35H39N5O5	609.7258	511-08-0	4
Ergocristinine	C35H39N5O5	609.7258	511-07-9	4
Ergocryptine	C32H41N5O5	575.7086	511-09-1	4
Ergocryptinine	C32H41N5O5	575.7086	511-10-4	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Ergometrine	C19H23N3O2	325.4109	60-79-7	5
Ergometrinine	C19H23N3O2	325.4109	479-00-5	5
Ergosine	C30H37N5O5	547.6548	561-94-4	4
Ergosinine	C30H37N5O5	547.6548	596-88-3	4
Ergotamine	C33H35N5O5	581.6721	113-15-5	4
Ergotaminine	C33H35N5O5	581.6721	639-81-6	4
Ergovaline	C29H35N5O5	533.6279	2873-38-3	4
Ergovalinine	C29H35N5O5	533.6279	3263-56-7	0
Erythromycin	C37H67NO13	733.9374	114-07-8	8
Festuclavine	C16H20N2	240.3486	569-26-6	4
FK 506	C44H69NO12	804.0312	104987-11-3	8
Fulvic acid	C14H12O8	308.2442	479-66-3	8
Fumagillin	C26H34O7	458.5517	23110-15-8	8
Fumigaclavine A	C18H22N2O2	298.3852	6879-59-0	4
Fumitremorgin C	C22H25N3O3	379.4592	118974-02-0	4
Fumonisin B1	C34H59NO15	721.8395	116355-83-0	8
Fumonisin B2	C34H59NO14	705.8402	116355-84-1	8
Fumonisin B3	C34H59NO14	705.8402	136379-59-4	8
Fumonisin B4	C34H59NO13	689.8409	136379-60-7	0
Fusaproliferin	C27H40O5	444.6116	152469-17-5	4
Fusarenon-X	C17H22O8	354.3566	23255-69-8	8
Fusaric acid	C10H13NO2	179.2188	536-69-6	0
Fusarielin A	C25H38O4	402.5744	132341-17-5	4
Fusidic acid	C31H48O6	516.7185	6990/06/03	4
Geldanamycin	C29H40N2O9	560.6445	30562-34-6	4
Geodin	C17H12Cl2O7	399.1835	427-63-4	8
Gibberellic acid	C19H22O6	346.38	1977/06/05	8
Gliotoxin	C13H14O4N2S2	326.394	67-99-2	4
Griseofulvin	C17H17O6Cl	352.7711	126-07-8	4
HC-Toxin	C21H32N4O6	436.5084	83209-65-8	8
HT-2-Toxin	C22H32O8	424.491	26934-87-2	4
hydrolyzed Fumonisin B1	C22H47NO5	405.6187	145040-09-1	4
Ionomycin	C41H72O9	709.0171	56092-82-1	4
K252a	C27H21N3O5	467.4813	97161-97-2	4
K252b	C26H19N3O5	453.4545	99570-78-2	8
Kojic acid	C6H6O4	142.1111	501-30-4	4
Lincomycin	C18H34N2O6S	406.542	154-21-2	4
Lolitrem B	C42H55NO7	685.9015	81771-19-9	8
Lysergol	C16H18N2O	254.3321	602-85-7	4
Macrosporin	C16H12O5	284.2683	22225-67-8	8
Malformin C	C23H39N5O5S2	529.7222	59926-78-2	4
Marcfortine A	C28H35N3O4	477.604	75731-43-0	4
Meleagrin	C23H23N5O4	433.4673	71751-77-4	8
Methysergide	C21H27N3O2	353.4647	361-37-5	4
Mevastatin	C23H34O5	390.5199	73573-88-3	4
Mevinolin	C24H36O5	404.5468	75330-75-5	4
Mithramycin	C52H76O24	1085.16	18378-89-7	4
Mitomycin C	C15H18N4O5	334.3319	1950/07/07	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Monactin	C41H66O12	750.9675	7182-54-9	4
Moniliformin	C4H2O3	98.05797	71376-34-6	0
Mycophenolic acid	C17H20O6	320.3421	24280-93-1	7
Myriocin	C21H39NO6	401.5436	35891-70-4	4
Neosolaniol	C19H26O8	382.4104	36519-25-2	4
Neoxaline	C23H25N5O4	435.4831	71812-10-7	8
NG012	C32H38O15	662.6442	141731-76-2	8
Nidulin	C20H17Cl3O5	443.7103	10089-10-8	4
Nigericin	C40H68O11	724.973	28643-80-3	4
Nivalenol	C15H20O7	312.3193	23282-20-4	8
Nonactin	C40H64O12	736.9406	6833-84-7	4
Nornidulin	C19H15Cl3O5	429.6834	33403-37-1	4
Ochratoxin A	C20H18NO6Cl	403.8188	303-47-9	8
Ochratoxin alpha	C11H9ClO5	256.6421	19165-63-0	7
Ochratoxin B	C20H19NO6	369.374	4825-86-9	8
Oligomycin A	C45H74O11	791.0757	579-13-5	8
Oligomycin B	C45H72O12	805.0592	11050-94-5	4
O-Methylsterigmatocystin	C19H14O6	338.3166	17878-69-2	4
Ophiobolin A	C25H36O4	400.5585	4611/05/06	4
Ophiobolin B	C25H38O4	402.5744	5601-74-1	8
Oxaspirodion	C13H14O5	250.2511	774538-95-3	4
oxidized Elymoclavine	N/A	N/A	N/A	4
oxidized Luol	N/A	N/A	N/A	4
Paraherquamide A	C28H35N3O5	493.6033	77392-58-6	6
Paspaline	C28H39NO2	421.6235	11024-56-9	4
Paspalinine	C27H31NO4	433.5478	63722-91-8	8
Paspalitrem A	C32H39NO4	501.6663	63722-90-7	4
Paspalitrem B	C32H39NO5	517.6657	63764-58-9	4
Patulin	C7H6O4	154.1221	149-29-1	0
Paxilline	C27H33NO4	435.5636	57186-25-1	8
Penicillic acid	C8H10O4	170.1649	90-65-3	4
Penicillin G	C16H18O4N2S	334.3945	61-33-6	4
Penicillin V	C16H18N2O5S	350.3938	1987/08/01	4
Penigequinolone A	C27H33NO6	467.5623	180045-91-4	8
Penitrem A	C37H44O6NCl	634.2125	12627-35-9	8
Pentoxyfylline	C13H18N4O3	278.3112	6493/05/06	4
Pestalotin	C11H18O4	214.2614	34565-32-7	4
Phomopsin A	C36H45ClN6O12	789.2392	64925-80-0	6
Phomopsin B	C36H46N6O12	754.7944	64925-81-1	0
Physcion	C16H12O5	284.2683	521-61-9	8
Pseurotin A	C22H25NO8	431.4423	58523-30-1	7
Puromycin	C22H29N7O5	471.5166	53-79-2	4
Pyrenophorol	C16H24O6	312.3628	22248-41-5	4
Pyripyropene A	C31H37NO10	583.6354	147444-03-9	4
Radicicol	C18H17ClO6	364.7821	12772-57-5	8
Rapamycin	C51H79NO13	914.187	53123-88-9	8
Roquefortine C	C22H23N5O2	389.4576	58735-64-1	8
Roridin A	C29H40O9	532.631	14729-29-4	4

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Rubellin D	C30H22O10	542.4987	121325-49-3	8
Rugulosin	C30H22O10	542.4987	23537-16-8	8
Satratoxin G	C29H36O10	544.5986	53126-63-9	0
Satratoxin H	C29H36O9	528.5993	53126-64-0	0
Secalonic acid	C32H30O14	638.5815	56283-72-8	8
Setosusin	C29H38O8	514.6158	182926-45-0	4
Stachybotrylactam	C23H31NO4	385.5036	163391-76-2	4
Staurosporine	C28H26N4O3	466.5401	62996-74-1	4
Sterigmatocystin	C18H12O6	324.2897	10048-13-2	4
Sulochrin	C17H16O7	332.3097	519-57-3	8
T2-Tetraol	C15H22O6	298.3359	34114-99-3	4
T2-Toxin	C24H34O9	466.5283	21259-20-1	4
T2-Triol	C20H30O7	382.4538	34114-98-2	4
Taxol	C47H51NO14	853.9203	33069-62-4	8
Tentoxin	C22H30N4O4	414.5049	28540-82-1	8
Tenuazonic acid	C10H15O3N	197.234	610-88-8	8
Terphenyllin	C20H18O5	338.36	52452-60-5	8
Territrem B	C29H34O9	526.5835	70407-20-4	4
Tetracycline	C22H24N2O8	444.4412	64-75-5	9
Thiolutin	C8H8N2O2S2	228.2927	1987/11/06	4
Trichodermin	C17H24O4	292.3751	4682-50-2	4
Trichostatin A	C17H22N2O3	302.3735	58880-19-6	4
Tryprostatin A	C22H27N3O3	381.4751	171864-80-5	4
Ustiloxin A	C28H43N5O12S	673.7399	143557-93-1	4
Ustiloxin B	C26H39N5O12S	645.6862	151841-41-7	4
Ustiloxin D	C23H34N4O8	494.545	158243-18-6	8
Valinomycin	C54H90N6O18	1111.338	2001-95-8	8
Vancomycin	C66H75Cl2N9O24	1449.273	1404-93-9	4
Verrucarin A	C27H34O9	502.5614	3148/09/02	4
Verrucarol	C15H22O4	266.3372	2198-92-7	4
Verrucofortine	C24H31N3O3	409.5288	113706-21-1	4
Verruculogen	C27H33O7N3	511.5751	12771-72-1	8
Viomellein	C30H24O11	560.5139	55625-78-0	8
Viridicatin	C15H11NO2	237.2581	129-24-8	4
Wortmannin	C23H24O8	428.4387	19545-26-7	4
Zearalenone	C18H22O5	318.3697	17924-92-4	8
Zearalenone-4-glucoside	C24H32O10	480.5118	105088-14-0	8
Zearalenone-4-sulfate	C18H22O8S	398.432	132505-04-5	4

Product Name	Part Number
Mycotoxin Spectral Library Version 1.1	5023887

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