

# Mycotoxin Spectral LC/MS/MS Library Version 1.0

## *iMethods™ Test for Mycotoxin Spectral Library Version 1.0 for Cliquant® Software*

The following description outlines the approximately 235 mycotoxins available in the MRM catalogue and LC/MS/MS library. This library and MRM catalogue, created using certified reference materials, can be used stand-alone to create custom screening and/or quantitation methods or in conjunction with the iMethod™ Test for Mycotoxin Screening. The iMethod test provides a pre-configured test for the screening of 171 mycotoxins in positive ion mode and 72 mycotoxins in negative ion mode. This library is verified for use on AB SCIEX 4000 QTRAP® and AB SCIEX QTRAP 5500® LC/MS/MS systems.

The MRM catalogue and spectral library both contain information on the most common mycotoxins and their metabolites that are required to be monitored in grains, cereals or other food products. The MRM catalogue contains up to three transitions per compound. Each compound in the library has 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. If compounds ionize in both polarities, spectra for both are also included, bringing the potential total number of spectra per compound to eight.

The MRM catalogue can be used to build methods without the need to re-infuse standards and optimize MRM transitions for a given compound. Screening and/or quantitation methods can be created for use with either an MRM triggered EPI workflow, for use on QTRAP instruments, or for traditional quantitation where the ratio of the response of two or more transitions is used for compound confirmation. The latter MRM approach can be performed on either an API triple quadrupole or a QTRAP series instrument. Users simply need to select the compounds of interest as well as the number of transitions to be monitored from the MRM catalogue. Once selected, the Cliquant® Software automatically creates the acquisition and processing methods.

The following is a list of the mycotoxins currently in the library. Please note that this library is continuously being expanded to include additional compounds.

Compound	Formula	MW	CAS Number	# of Spectra
15-Acetyl-deoxynivalenol	C17H22O7	338.1	88337-96-6	4
15-Monoacetoxyscirpenol	C17H24O6	324.1	2623-22-5	4
16-Ketoaspergillimide	C20H27N3O4	373.2	199784-50-4	4
2-Amino-14,16-dimethyloctadecan-3-ol	C20H43ON	313.3	540770-33-0	4
3-Acetyl-deoxynivalenol	C17H22O7	338.1	50722-38-8	8
3-O-Methylviridicatin	C16H13NO2	251	6152-51-4	4
A23187	C29H37N3O6	523.2	52665-69-7	8
AAL-TA1 Toxin	C25H47NO10	521.3	79367-52-5	4
Actinomycin D	C62H86N12O16	1254.6	50-76-0	4
Aflatoxin B1	C17H12O6	312	1162-65-8	4
Aflatoxin B2	C17H14O6	314	7220-81-7	4
Aflatoxin G1	C17H12O7	328	1165-39-5	4
Aflatoxin G2	C17H14O7	330	7241-98-7	4
Aflatoxin M1	C17H12O7	328	6795-23-9	4
Aflatoxin M2	C17H14O7	330	6885-57-0	4
Agroclavine	C16H18N2	238.1	548-42-5	4
Alamethicin F30	C92H150N22O25	1963.1	27061-78-5	4
alpha-Zearalenol	C18H24O5	320.1	36455-72-8	8
alpha-Zearalenol-4-O-glucoside	C24H34O10	482.2	135626-94-7	8
Altenuene	C15H16O6	292	29752-43-0	8
Altenuisin	C15H14O6	290	31186-12-6	8

Compound	Formula	MW	CAS Number	# of Spectra
Alternariol	C14H10O5	258	641-38-3	8
Alternariolmethylether	C15H12O5	272	26894-49-5	8
Altersolanol	C16H16O7	320	22268-16-2	8
Altartoxin-I	C20H16O6	352	56258-32-3	4
Anisomycin	C14H19NO4	265.1	22862-76-6	4
Apicidin	C34H49N5O6	623.3	183506-66-3	8
Ascomycin	C43H69NO12	791.4	104987-12-4	4
Aspercilorin	C25H28N4O5	464.2	29123-52-2	8
Aspergillimide	C20H29N3O3	359.2	195966-93-9	4
Asperlactone	C9H12O4	184	76375-62-7	4
Asperloxine A	C21H19N3O5	393.1	223130-52-7	4
Aspinonene	C9H16O4	188.1	157676-96-5	4
Aspyrone	C9H12O4	184	17398-00-4	4
Asteric acid	C17H16O8	348	577-64-0	8
Atpenin A5	C15H21Cl2NO5	365	119509-24-9	8
Aureobasidin A	C60H92N8O11	1100.6	127757-30-6	4
Aurofusarin	C30H18O12	570	13191-64-5	8
Austdiol	C12H12O5	236	53043-28-0	8
Austocystin A	C19H13ClO6	372	55256-58-1	4
Avenacein Y	C15H10O8	318	102426-44-8	4
Bacitracin	C66H103N17O16S	1421.7	22601-59-8	4
Bafilomycin A1	C35H58O9	622.4	88899-55-2	4
Beauvericin	C45H57N3O9	783.4	26048-05-5	4
beta-Ergocryptine	C32H41N5O5	575.3	511-09-1	4
beta-Ergocryptinine	C32H41N5O5	575.3	511-10-4	4
beta-Zearalenol	C18H24O5	320.1	71030-11-0	8
beta-Zearalenol-4-O-glucoside	C24H34O10	482.2	135626-93-6	8
Brefeldin A	C16H24O4	280.1	20350-15-6	4
Brevicompanine B	C22H29N3O2	367.2	215121-47-4	4
Calphostin C	C44H38O14	790.2	121263-19-2	8
Cephalosporin C	C16H21N3O8S	415.1	61-24-5	4
Cerulenin	C12H17NO3	223.1	17397-89-6	4
Chaetocin	C30H28N6O6S4	696	28097-03-2	8
Chaetoglobosin A	C32H36N2O5	528.2	50335-03-0	4
Chanoclavine	C16H20N2O	256.1	2390-99-0	4
Chetomin	C31H30O6N6S4	710.1	1403-36-7	4
Chlamydosporol	C11H14O5	226	135063-30-8	4
Chloramphenicol	C11H12Cl2N2O5	322	56-75-7	4
Citreoviridin	C23H30O6	402.2	25425-12-1	4
Citrinin	C13H14O5	250	518-75-2	8
Citromycetin	C14H10O7	290	478-60-4	4
Cochliodinol	C32H30N2O4	506.2	11051-88-0	8
Curvularin	C16H20O5	292.1	10140-70-2	8
Cycloaspeptide A	C36H43N5O6	641.3	109171-13-3	8
Cycloechinulin	C20H21N3O3	351.1	143086-29-7	8
Cycloheximide	C15H23NO4	281.1	66-81-9	8
Cyclopenin	C17H14N2O3	294.1	19553-26-5	8
Cyclopeptide	C17H16N2O2	280.1	50886-63-0	4

Compound	Formula	MW	CAS Number	# of Spectra
Cyclopiazonic acid	C20H20N2O3	336.1	18172-33-3	8
Cyclosporin A	C62H111N11O12	1201.8	59865-13-3	8
Cyclosporin C	C62H111N11O13	1217.8	59787-61-0	4
Cyclosporin D	C63H113N11O12	1215.8	63775-96-2	4
Cyclosporin H	C62H111N11O12	1201.8	83602-39-5	4
Cytochalasin A	C29H35O5N	477.2	14110-64-6	4
Cytochalasin B	C29H37O5N	479.2	14930-96-2	4
Cytochalasin C	C30H37O6N	507.2	22144-76-9	4
Cytochalasin D	C30H37O6N	507.2	22144-77-0	4
Cytochalasin E	C28H33O7N	495.2	36011-19-5	4
Cytochalasin H	C30H39NO5	493.2	53760-19-3	4
Cytochalasin J	C28H37NO4	451.2	56144-22-0	4
Decarestrictine	C10H16O5	216	127393-89-9	4
Dechlorogriseofulvin	C17H18O6	318.1	3680-32-8	4
Deepoxy-deoxynivalenol	C15H20O5	280.1	88054-24-4	8
Deoxybrevianamide E	C21H25N3O2	351.1	34610-68-9	8
Deoxynivalenol	C15H20O6	296.1	51481-10-8	8
Deoxynivalenol-3-glucoside	C21H30O11	458.1	131180-21-7	8
Diacetoxyscirpenol	C19H26O7	366.1	2270-40-8	4
Dihydroergosine	C30H39N5O5	549.2	7288-61-1	4
Dihydroergotamine	C33H37N5O5	583.2	511-12-6	4
Dihydrolysergol	C16H20N2O	256.1	18051-16-6	4
Elymoclavine	C16H18N2O	254.1	548-43-6	4
Elymoclavine fructoside	C22H28N2O6	416.1	12379-50-9	4
Emodin	C15H10O5	270	518-82-1	8
Enniatin A	C36H63N3O9	681.4	144446-20-8	4
Enniatin A1	C35H61N3O9	667.4	4530-21-6	4
Enniatin B	C33H57N3O9	639.4	917-13-5	4
Enniatin B1	C34H59N3O9	653.4	19914-20-6	4
Enniatin B2	C32H55N3O9	625.3	632-91-7	4
Enniatin B3	C31H53N3O9	611.3	864-99-3	4
Equisetin	C22H31NO4	373.2	57749-43-6	8
Ergine	C16H17N3O	267.1	478-94-4	4
Erginine	C16H17N3O	267.1		4
Ergocornine	C31H39N5O5	561.2	564-36-3	4
Ergocorninine	C31H39N5O5	561.2	564-37-4	4
Ergocristine	C35H39N5O5	609.2	511-08-0	4
Ergocristinine	C35H39N5O5	609.2	511-07-9	4
Ergocryptine	C32H41N5O5	575.3	511-09-1	4
Ergocryptinine	C32H41N5O5	575.3	511-10-4	4
Ergometrine	C19H23N3O2	325.1	60-79-7	4
Ergometrinine	C19H23N3O2	325.1	479-00-5	4
Ergosine	C30H37N5O5	547.2	561-94-4	4
Ergosinine	C30H37N5O5	547.2	596-88-3	4
Ergotamine	C33H35N5O5	581.2	113-15-5	4
Ergotaminine	C33H35N5O5	581.2	639-81-6	4
Ergovaline	C29H35N5O5	533.2	2873-38-3	4
Erythromycin	C37H67NO13	733.4	114-07-8	8

Compound	Formula	MW	CAS Number	# of Spectra
Festuclovine	C16H20N2	240.1	569-26-6	4
FK 506	C44H69NO12	803.4	104987-11-3	8
Fulvic acid	C14H12O8	308	479-66-3	8
Fumagillin	C26H34O7	458.2	23110-15-8	8
Fumigaclavine A	C18H22N2O2	298.1	6879-59-0	4
Fumitremorgin C	C22H25N3O3	379.1	118974-02-0	4
Fumonisin B1	C34H59NO15	721.3	116355-83-0	8
Fumonisin B2	C34H59NO14	705.3	116355-84-1	8
Fumonisin B3	C34H59NO14	705.3	136379-59-4	8
Fusaproliferin	C27H40O5	444.2	152469-17-5	4
Fusarenon-X	C17H22O8	354.1	23255-69-8	8
Fusarielin A	C25H38O4	402.2	132341-17-5	4
Fusidic acid	C31H48O6	516.2	6990-06-3	4
Geldanamycin	C29H40N2O9	560.2	30562-34-6	4
Geodin	C17H12Cl2O7	397.9	427-63-4	8
Gibberellic acid	C19H22O6	346.1	77-06-5	8
Gliotoxin	C13H14O4N2S2	326	67-99-2	4
Griseofulvin	C17H17O6Cl	352	126-07-8	4
HC-Toxin	C21H32N4O6	436.2	83209-65-8	8
HT-2-Toxin	C22H32O8	424.2	26934-87-2	4
hydrolyzed Fumonisin B1	C22H47NO5	405.3	145040-09-1	4
Ionomycin	C41H72O9	708.5	56092-82-1	4
K252a	C27H21N3O5	467.1	97161-97-2	4
K252b	C26H19N3O5	453.1	99570-78-2	8
Kojic acid	C6H6O4	142	501-30-4	4
Lincomycin	C18H34N2O6S	406.2	154-21-2	4
Lolitrein B	C42H55NO7	685.3	81771-19-9	8
Lysergol	C16H18N2O	254.1	602-85-7	4
Macrosporin	C16H12O5	284	22225-67-8	8
Malformin C	C23H39N5O5S2	529.2	59926-78-2	4
Marcfortine A	C28H35N3O4	477.2	75731-43-0	4
Meleagrins	C23H23N5O4	433.1	71751-77-4	8
Methysergide	C21H27N3O2	353.2	361-37-5	4
Mevastatin	C23H34O5	390.2	73573-88-3	4
Mevinolin	C24H36O5	404.2	75330-75-5	4
Mithramycin	C52H76O24	1084.4	18378-89-7	4
Mitomycin C	C15H18N4O5	334.1	50-07-7	4
Monactin	C41H66O12	750.4	7182-54-9	4
Mycophenolic acid	C17H20O6	320.1	24280-93-1	8
Myriocin	C21H39NO6	401.2	35891-70-4	4
Neosolaniol	C19H26O8	382.1	36519-25-2	4
Neoxaline	C23H25N5O4	435.1	71812-10-7	8
NG012	C32H38O15	662.2	141731-76-2	8
Nidulin	C20H17Cl3O5	442	10089-10-8	4
Nigericin	C40H68O11	724.4	28643-80-3	4
Nivalenol	C15H20O7	312.1	23282-20-4	8
Nonactin	C40H64O12	736.4	6833-84-7	4
Normidulin	C19H15Cl3O5	427.9	33403-37-1	4

Compound	Formula	MW	CAS Number	# of Spectra
Ochratoxin A	C20H18NO6Cl	403	303-47-9	8
Ochratoxin alpha	C11H9ClO5	256	19165-63-0	8
Ochratoxin B	C20H19NO6	369.1	4825-86-9	8
Oligomycin A	C45H74O11	790.5	579-13-5	8
Oligomycin B	C45H72O12	804.5	11050-94-5	4
O-Methylsterigmatocystin	C19H14O6	338	17878-69-2	4
Ophiobolin A	C25H36O4	400.2	4611-05-6	4
Ophiobolin B	C25H38O4	402.2	5601-74-1	8
Oxaspirodion	C13H14O5	250	774538-95-3	4
oxidized Elymoclavine		258.1		4
oxidized Luol		290.5		4
Paraherquamide A	C28H35N3O5	493.2	77392-58-6	6
Paspaline	C28H39NO2	421.2	11024-56-9	4
Paspalinine	C27H31NO4	433.2	63722-91-8	8
Paspalitre A	C32H39NO4	501.2	63722-90-7	4
Paspalitre B	C32H39NO5	517.2	63764-58-9	4
Paxilline	C27H33NO4	435.2	57186-25-1	8
Penicillic acid	C8H10O4	170	90-65-3	4
Penicillin G	C16H18O4N2S	334	61-33-6	4
Penicillin V	C16H18N2O5S	350	87-08-1	4
Penigequinolone A	C27H33NO6	467.2	180045-91-4	8
Penitre A	C37H44O6NCl	633.2	12627-35-9	8
Pentoxifylline	C13H18N4O3	278.1	6493-05-6	4
Pestalotin	C11H18O4	214.1	34565-32-7	4
Phomopsin A	C36H45ClN6O12	788.2	64925-80-0	6
Physcion	C16H12O5	284	521-61-9	8
Pseurotin A	C22H25NO8	431.1	58523-30-1	7
Puromycin	C22H29N7O5	471.2	53-79-2	4
Pyrenophorol	C16H24O6	312.1	22248-41-5	4
Pyripyropene A	C31H37NO10	583.2	147444-03-9	4
Radicicol	C18H17ClO6	364	12772-57-5	8
Rapamycin	C51H79NO13	913.5	53123-88-9	8
Roquefortine C	C22H23N5O2	389.1	58735-64-1	8
Roridin A	C29H40O9	532.2	14729-29-4	4
Rubellin D	C30H22O10	542.1	121325-49-3	8
Rugulosin	C30H22O10	542.1	23537-16-8	8
Secalonic acid	C32H30O14	638.1	56283-72-8	8
Setosusin	C29H38O8	514.2	182926-45-0	4
Stachybotrylactam	C23H31NO4	385.2	163391-76-2	4
Staurosporine	C28H26N4O3	466.2	62996-74-1	4
Sterigmatocystin	C18H12O6	324	10048-13-2	4
Sulochrin	C17H16O7	332	519-57-3	8
T2-Tetraol	C15H22O6	298.1	34114-99-3	4
T2-Toxin	C24H34O9	466.2	21259-20-1	4
T2-Triol	C20H30O7	382.1	34114-98-2	4
Taxol	C47H51NO14	853.3	33069-62-4	8
Tentoxin	C22H30N4O4	414.2	28540-82-1	8
Tenuazonic acid	C10H15O3N	197.1	610-88-8	8

Compound	Formula	MW	CAS Number	# of Spectra
Terphenyllin	C20H18O5	338.1	52452-60-5	8
Territrem B	C29H34O9	526.2	70407-20-4	4
Tetracycline	C22H24N2O8	444.1	64-75-5	8
Thiolutin	C8H8N2O2S2	228	87-11-6	4
Trichodermin	C17H24O4	292.1	4682-50-2	4
Trichostatin A	C17H22N2O3	302.1	58880-19-6	4
Tryprostatin A	C22H27N3O3	381.2	171864-80-5	4
Ustiloxin A	C28H43N5O12S	673.2	143557-93-1	4
Ustiloxin B	C26H39N5O12S	645.2	151841-41-7	4
Ustiloxin D	C23H34N4O8	494.2	158243-18-6	8
Valinomycin	C54H90N6O18	1110.6	2001-95-8	8
Vancomycin	C66H75Cl2N9O24	1447.4	1404-93-9	4
Verrucaric acid	C27H34O9	502.2	3148-09-2	4
Verrucarol	C15H22O4	266.1	2198-92-7	4
Verrucofortine	C24H31N3O3	409.2	113706-21-1	4
Verruculogen	C27H33O7N3	511.2	12771-72-1	8
Viomellein	C30H24O11	560.1	55625-78-0	8
Viridicatin	C15H11NO2	237	129-24-8	4
Wortmannin	C23H24O8	428.1	19545-26-7	4
Zearalenone	C18H22O5	318.1	17924-92-4	8
Zearalenone-4-glucoside	C24H32O10	480.1	105088-14-0	8
Zearalenone-4-sulfate	C18H22O8S	398.1	132505-04-5	4

## Ordering Information

Product Name	Part Number
iMethods™ Tests for Mycotoxin Spectral Library Version 1.0 for Cliquant® Software	5011866

## Legal Acknowledgements/Disclaimers

The iMethod™ Test described above has been developed by AB SCIEX to provide all the sample prep and instrument parameters required to accelerate the adoption of this method for routine testing. The performance of this method will need to be verified in a given lab due to potential variations in instrument performance, maintenance, chemicals and procedures used, technical experience, sample matrices and environmental conditions. It is the responsibility of the end user to make adjustments to this method to account for slight differences in equipment and/or materials from lab to lab as well as to determine and validate the performance of this method for a given instrument and sample type. Please note that a working knowledge of Analyst® Software may be required to do so.

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