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Mass Spectral Libraries for Forensic Analysis

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

Forensics High Resolution MS/MS Library Version 1.0

An overview of the licensed mass spectral library for forensics 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 370 compound 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 370 compounds commonly tested for in forensic samples.
- Includes 517 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
1-Hydroxytriazolam	C17H12Cl2N4O	359.2146	37115-45-0	1
10,11-Dihydro-10-hydroxycarbamazepine	C15H14N2O2	254.2887	29331-92-8	1
11-Hydroxy-THC	C21H30O3	330.4675	36557-05-8	1
17-Hydroxyprogesterone	C21H30O3	330.4675	604-09-1	1
2-Hydroxyethylflurazepam	C17H14ClFN2O2	332.7619		1
2C-H	C10H15NO2	181.2347	3600-86-0	1
2C-I	C10H14INO2	307.1312	69587-11-7	1
2C-T2	C12H19NO2S	241.3528	207740-24-7	1
2C-T4	C13H21NO2S	255.3797	207740-25-8	1
2C-T7	C13H21NO2S	255.3797	207740-26-9	1
4-Beta-hydroxystanozolol	C21H32N2O2	344.4976		1
4-Ethylamphetamine	C11H17N	163.2629	457-87-4	1
4-Fluoromethcathinone	C10H12FNO	181.21	7589-35-7	1
4-Hydroxytriazolam	C17H12Cl2N4O	359.2146	65686-11-5	1
4-MTA	C10H15NS	181.3004	14116-06-4	1
6-APB/5-APB	C11H13NO	175.2305	286834-85-3	1
6-Beta-Naltrexol	C20H25NO4	343.4229	49625-89-0	1
6-Monoacetylmorphine	C19H21NO4	327.3802	2784-73-8	2
6-Monocetylcodeine	C20H23NO4	341.4071	6703-27-1	1
7-Aminoclonazepam	C15H12ClN3O	285.733	4959-17-5	2

Compound	Formula	Formula Weight	CAS Number	# of Spectra
7-Aminoflunitrazepam	C16H14FN3O	283.3056	34084-50-9	1
7-Aminonitrazepam	C15H13N3O	251.2882	4928-02-3	1
9-Hydroxyrisperidone	C23H27FN4O3	426.4913	144598-75-4	1
Acetaminophen	C8H9NO2	151.165	103-90-2	3
Acetazolamide	C4H6N4O3S2	222.2455	59-66-5	1
Alfentanil	C21H32N6O3	416.5239	71195-58-9	1
Alpha-Hydroxyalprazolam	C17H13CIN4O	324.7698	37115-43-8	2
Alpha-hydroxymidazolam	C18H13CIFN3O	341.7725	59468-90-5	1
Alpha-Pyrrolidinopentiophenone	C15H21NO	231.3381	5485-65-4	1
Alprazolam	C17H13CIN4	308.7705	28981-97-7	5
Alprenolol	C15H23NO2	249.3533	13655-52-2	1
AM2201	C24H22FNO	359.4437	335161-24-5	1
AM2201 6-hydroxyindole metabolite	C24H22FNO2	375.4431		1
AM2201 N-(4-hydroxypentyl) metabolite	C24H22FNO2	375.4431		1
AM694	C20H19FINO	435.2803		1
Amiodarone	C25H29I2NO3	645.3195	1951-25-3	1
Amitriptyline	C20H23N	277.4098	50-48-6	3
Amobarbital	C11H18N2O3	226.2756	57-43-2	1
Amoxapine	C17H16CIN3O	313.7868	14028-44-5	1
Amphetamine	C9H13N	135.2091	300-62-9	1
Androstenedione	C19H26O2	286.4144	63-05-8	1
Aripiprazole	C23H27Cl2N3O2	448.3923	129722-12-9	2
Atenolol	C14H22N2O3	266.3404	29122-68-7	1
Atropine	C17H23NO3	289.3747	51-55-8	1
Azithromycin	C38H72N2O12	748.9955	83905-01-5	1
Baclofen	C10H12CINO2	213.6636	1134-47-0	2
BDB	C11H15NO2	193.2457	42542-07-4	1
Benzocaine	C9H11NO2	165.1919	94-09-7	1
Benzoyllecgonine	C16H19NO4	289.3312	519-09-5	2
Betaxolol	C18H29NO3	307.4332	63659-18-7	1
Bisoprolol	C18H31NO4	325.4484	66722-44-9	1
Brompheniramine	C16H19BrN2	319.2442	86-22-6	1
Bupivacaine	C18H28N2O	288.4334	2180-92-9	1
Buprenorphine	C29H41NO4	467.6491	52485-79-7	2
Buprenorphine-glucuronide	C35H49NO10	643.7747	101224-22-0	1
Bupropion	C13H18CINO	239.745	34841-39-9	2
Buspirone	C21H31N5O2	385.5099	36505-84-7	1
Butabarbital	C10H16N2O3	212.2487	125-40-6	1
Butalbital	C11H16N2O3	224.2597	77-26-9	1
Butorphanol	C21H29NO2	327.467	42408-82-2	2
Butylone	C12H15NO3	221.2561	17762-90-2	1
Cabazitaxel (sodiated)	C45H56NO14Na	857.9276	183133-96-2	1
Caffeine	C8H10N4O2	194.1933	58-08-2	2
Cannabinol	C21H26O2	310.4365	521-35-7	1
Carbamazepine	C15H12N2O	236.2735	298-46-4	2
Carisoprodol	C12H24N2O4	260.3335	78-44-4	3
Cathine	C9H13NO	151.2085	2153-98-2	1
Cathinone	C9H11NO	149.1926	5265-18-9	2

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Chloramphenicol	C ₁₁ H ₁₂ Cl ₂ N ₂ O ₅	323.1321	56-75-7	1
Chlordiazepoxide	C ₁₆ H ₁₄ CIN ₃ O	299.7599	58-25-3	2
Chlorpheniramine	C ₁₆ H ₁₉ CIN ₂	274.7934	132-22-9	3
Chlorpromazine	C ₁₇ H ₁₉ CIN ₂ S	318.8689	50-53-3	2
Chlorpropamide	C ₁₀ H ₁₃ CIN ₂ O ₃ S	276.742	94-20-2	1
Cimetidine	C ₁₀ H ₁₆ N ₆ S	252.3421	51481-61-9	3
Cindamycin	C ₁₈ H ₃₃ CIN ₂ O ₅ S	424.9875	18323-44-9	1
Citalopram	C ₂₀ H ₂₁ FN ₂ O	324.3984	59729-33-8	2
Clenbuterol	C ₁₂ H ₁₈ Cl ₂ N ₂ O	277.1934	37148-27-9	1
Clobazam	C ₁₆ H ₁₃ CIN ₂ O ₂	300.7445	22316-47-8	1
Clomipramine	C ₁₉ H ₂₃ CIN ₂	314.8583	303-49-1	1
Clonazepam	C ₁₅ H ₁₀ CIN ₃ O ₃	315.7158	1622-61-3	1
Clonidine	C ₉ H ₉ Cl ₂ N ₃	230.0964	4205-90-7	2
Clopamide	C ₁₄ H ₂₀ CIN ₃ O ₃ S	345.8484	636-54-4	1
Clozapine	C ₁₈ H ₁₉ CIN ₄	326.829	5786-21-0	2
Cocaethylene	C ₁₈ H ₂₃ NO ₄	317.385	529-38-4	1
Cocaine	C ₁₇ H ₂₁ NO ₄	303.3581	50-36-2	2
Codeine	C ₁₈ H ₂₁ NO ₃	299.3698	76-57-3	2
Cortisol	C ₂₁ H ₃₀ O ₅	362.4662	50-23-7	2
Cotinine	C ₁₀ H ₁₂ N ₂ O	176.2183	486-56-6	2
Cyclobenzaprine	C ₂₀ H ₂₁ N	275.3939	303-53-7	2
Demoxepam	C ₁₅ H ₁₁ CIN ₂ O ₂	286.7176	963-39-3	1
Desethylamiodarone	C ₂₃ H ₂₅ I ₂ NO ₃	617.2657	83409-32-9	1
Desipramine	C ₁₈ H ₂₂ N ₂	266.3866	50-47-5	3
Desmethyl-cis-tramadol	C ₁₅ H ₂₃ NO ₂	249.3533	1018989-94-0	1
Desmethylocitalopram	C ₁₉ H ₁₉ FN ₂ O	310.3715	144010-85-5	1
Desmethyldoxepin	C ₁₈ H ₁₉ NO	265.3553	1225-56-5	1
Dexamethasone	C ₂₂ H ₂₉ FO ₅	392.4677	50-02-2	1
Dextromethorphan	C ₁₈ H ₂₅ NO	271.4029	125-71-3	3
DHT	C ₁₉ H ₃₀ O ₂	290.4461	521-18-6	1
Diazepam	C ₁₆ H ₁₃ CIN ₂ O	284.7452	439-14-5	1
Dibutyl phthalate	C ₁₆ H ₂₂ O ₄	278.3483	84-74-2	1
Dibutyl phthalate (sodiated)	C ₁₆ H ₂₁ NaO ₄	300.3301		1
Diclofenac	C ₁₄ H ₁₁ Cl ₂ NO ₂	296.1526	15307-86-5	2
Diethylpropion	C ₁₃ H ₁₉ NO	205.3002	90-84-6	1
Dihydrocodeine	C ₁₈ H ₂₃ NO ₃	301.3857	125-28-0	1
Diltiazem	C ₂₂ H ₂₆ N ₂ O ₄ S	414.5241	42399-41-7	2
Diocetyl phthalate	C ₂₄ H ₃₈ O ₄	390.5634	117-84-0	1
Diphenhydramine	C ₁₇ H ₂₁ NO	255.3602	58-73-1	3
Diphenoxylate	C ₃₀ H ₃₂ N ₂ O ₂	452.5969	915-30-0	1
DMA	C ₁₁ H ₁₇ NO ₂	195.2616	2801-68-5	1
DMT	C ₁₂ H ₁₆ N ₂	188.2728	61-50-7	1
DOB	C ₁₁ H ₁₆ BrNO ₂	274.1572	43061-16-1	1
DOEt	C ₁₃ H ₂₁ NO ₂	223.3153	22004-32-6	1
DOM	C ₁₂ H ₁₉ NO ₂	209.2884	15588-95-1	1
Donepezil	C ₂₄ H ₂₉ NO ₃	379.4995	120014-06-4	1
Doxepin	C ₁₉ H ₂₁ NO	279.3822	1668-19-5	2
Doxylamine	C ₁₇ H ₂₂ N ₂ O	270.3748	469-21-6	3

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Duloxetine	C18H19NOS	297.4197	116539-59-4	1
Ecgonine methyl ester	C10H17NO3	199.2498	7143-09-1	1
EDDP	C20H23N	277.4098	66729-78-0	1
Ephedrine	C10H15NO	165.2353	299-42-3	3
Epimetendiol	C20H28	268.4427	132830-78-5	1
Epioxandrolone	C19H30O3	306.4454	26624-15-7	1
Erythromycin	C37H67NO13	733.9374	114-07-8	1
Esmolol	C16H25NO4	295.3788	81147-92-4	1
Estazolam	C16H11ClN4	294.7436	29975-16-4	1
Ethosuximide	C7H11NO2	141.1699	77-67-8	1
Ethylone	C12H15NO3	221.2561	1112937-64-0	1
Etomidate	C14H16N2O2	244.2935	33125-97-2	1
Fatty acid (C20:4)	C20H32O2	304.473		1
Felbamate	C11H14N2O4	238.2432	25451-15-4	1
Fenfluramine	C12H16F3N	231.2612	458-24-2	3
Fentanyl	C22H28N2O	336.4776	437-38-7	3
Flunitrazepam	C16H12FN3O3	313.2884	1622-62-4	2
Fluoroamphetamine	C9H12FN	153.1996	459-02-9	1
Fluoxetine	C17H18F3NO	309.3316	54910-89-3	2
Fluphenazine	C22H26F3N3OS	437.5281	69-23-8	1
Flurazepam	C21H23ClFN3O	387.8848	17617-23-1	3
Fluvoxamine	C15H21F3N2O2	318.3394	54739-18-3	1
Furosemide	C12H11ClN2O5S	330.7469	54-31-9	1
Gabapentin	C9H17NO2	171.2395	60142-96-3	2
Guaifenesin	C10H14O4	198.2186	93-14-1	1
Haloperidol	C21H23ClFN2O2	375.8706	52-86-8	2
Hydrochlorothiazide	C7H8ClN3O4S2	297.7398	58-93-5	1
Hydrocodone	C18H21NO3	299.3698	125-29-1	2
Hydromorphone	C17H19NO3	285.343	466-99-9	3
Hydromorphone glucuronide	C23H27NO9	461.4685	40505-76-8	1
Hydroxyzine	C21H27ClN2O2	374.9107	68-88-2	1
Ibuprofen	C13H18O2	206.2848	15687-27-1	1
Imipramine	C19H24N2	280.4134	50-49-7	2
Indomethacin	C19H16ClNO4	357.7933	53-86-1	1
JWH-018	C24H23NO	341.4533	209414-07-3	1
JWH-018 5-hydroxy or 6-hydroxy metabolite	C24H23NO2	357.4526		2
JWH-018 N-(5-hydroxypentyl) metabolite	C24H23NO2	357.4526		1
JWH-018 N-pentanoic acid	C24H21NO3	371.4361		1
JWH-019	C25H25NO	355.4802		1
JWH-019 5-hydroxyindole or N-(6-hydroxyhexyl) metabolite	C25H25NO2	371.4795		1
JWH-073	C23H21NO	327.4264	208987-48-8	2
JWH-073 Hydroxy Metabolite 1	C23H21NO2	343.4257		1
JWH-073 Hydroxy Metabolite 2	C23H21NO2	343.4257		1
JWH-073 Hydroxy Metabolite 3	C23H21NO2	343.4257		1
JWH-073N-Butanoic acid	C23H19NO3	357.4092		1
JWH-081	C25H25NO2	371.4795	210179-46-7	1
JWH-081-N-5-OH-pentyl	C25H25NO3	387.4788		1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
JWH-122	C25H25NO	355.4802	619294-47-2	1
JWH-122 N-(5-hydroxypentyl) metabolite	C25H25NO2	371.4795		1
JWH-200	C25H24N2O2	384.4783		1
JWH-200-OH-indole Metabolite 1	C25H24N2O3	400.4776		1
JWH-200-OH-indole Metabolite 2	C25H24N2O3	400.4776		1
JWH-203	C21H22CINO	339.865		1
JWH-210	C26H27NO	369.507	824960-64-7	2
JWH-210 6-hydroxyindole metabolite	C26H27NO2	385.5064		1
JWH-210 N-(4 or 5-hydroxypentyl) metabolite	C26H27NO2	385.5064		1
JWH-210 N-(5-carboxypentyl) metabolite	C26H25NO3	399.4898		1
JWH-250	C22H25NO2	335.4464	864445-43-2	1
JWH-250 5-hydroxyindole metabolite	C22H25NO3	351.4457		2
JWH-250 N-(4 or 5-hydroxypentyl) metabolite	C22H25NO3	351.4457		2
JWH-250 N-(carboxypentyl) metabolite	C22H23NO4	365.4292		1
JWH-398	C24H22CINO	375.8981		1
JWH-398 N-(5-hydroxypentyl) metabolite	C25H22CINO2	403.9084		1
JWH-398 N-pentanoic acid metabolite	C24H20CINO3	405.8809		1
JWH 210 N-(5-COOH-pentyl) Metabolite	C26H25NO3	399.4898		1
JWH122 N-(5-OH-pentyl) Metabolite	C25H25NO2	371.4795		1
Ketamine	C13H16CINO	237.7291	1867-66-9	2
Ketoprofen	C16H14O3	254.2855	22071-15-4	3
Ketorolac	C15H13NO3	255.2733	74103-06-3	1
Labetalol	C19H24N2O3	328.4114	36894-69-6	1
Lamotrigine	C9H7Cl2N5	256.0941	84057-84-1	2
Levamisole	C11H12N2S	204.2944	14769-73-4	1
Levetiracetam	C8H14N2O2	170.2114	102767-28-2	2
Levofloxacin	C18H20FN3O4	361.3732	100986-85-4	1
Levorphanol	C17H23NO	257.376	77-07-6	5
Lidocaine	C14H22N2O	234.3417	137-58-6	2
Loratadine	C22H23ClN2O2	382.89	79794-75-5	2
Lorazepam	C15H10Cl2N2O2	321.1625	846-49-1	2
Loxapine	C18H18ClN3O	327.8137	1977-10-2	1
MAM-2201	C25H24FNO	373.4706	1354631-24-5	1
MAM-2201 N-(4-hydroxypentyl) metabolite	C25H24FNO2	389.47		1
MAM-2201 N-pentanoic acid	C25H23NO3	385.463		1
Maprotiline	C20H23N	277.4098	10262-69-8	2
mCPP	C10H13ClN2	196.6797	6640-24-0	1
MDA	C10H13NO2	179.2188	4764-17-4	3
MDEA	C12H17NO2	207.2726	105-59-9	3
MDMA	C11H15NO2	193.2457	42542-10-9	4
MDPPP	C14H17NO3	247.294	24698-57-5	1
MDPV	C16H21NO3	275.3478	24622-62-6	1
Medazepam	C16H15ClN2	270.7617	2898-12-6	1
Mefenamic acid	C15H15NO2	241.2899	61-68-7	1
Melatonin	C13H16N2O2	232.2825	73-31-4	1
Meperidine	C15H21NO2	247.3374	57-42-1	5
Mephedrone	C11H15NO	177.2464	1189805-46-6	1
Mephobarbital	C13H14N2O3	246.2659	115-38-8	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Meprobamate	C9H18N2O4	218.2528	57-53-4	2
Mescaline	C11H17NO3	211.2609	54-04-6	1
Metaxalone	C12H15NO3	221.2561	1665-48-1	1
Methadone	C21H27NO	309.4519	76-99-3	3
Methamphetamine	C10H15N	149.236	537-46-2	2
Methaqualone	C16H14N2O	250.3004	72-44-6	1
Methcathinone	C10H13NO	163.2195	5650-44-2	1
Methedrone	C11H15NO2	193.2457	530-54-1	1
Methocarbamol	C11H15NO5	241.2437	532-03-6	1
Methsuximide	C12H13NO2	203.2409	77-41-8	1
Methylone	C11H13NO3	207.2292	191916-41-3	1
Methylphenidate	C14H19NO2	233.3105	113-45-1	2
Methyltestosterone	C20H30O2	302.4572	58-18-4	1
Metoclopramide	C14H22ClN3O2	299.8006	364-62-5	1
Metoprolol	C15H25NO3	267.3684	37350-58-6	1
Mianserin	C18H20N2	264.3707	24219-97-4	1
Midazolam	C18H13ClFN3	325.7731	59467-70-8	3
Mirtazapine	C17H19N3	265.3585	85650-52-8	1
Morphine	C17H19NO3	285.343	57-27-2	2
Morphine-3-glucuronide	C23H27NO9	461.4685	20290-09-9	1
N-Desmethyflunitrazepam	C15H10N3O3F	299.2615	2558-30-7	1
Nalbuphine	C21H27NO4	357.4498	20594-83-6	1
Naloxone	C19H21NO4	327.3802	465-65-6	4
Naltrexone	C20H23NO4	341.4071	16590-41-3	3
Naproxen	C14H14O3	230.2635	22204-53-1	2
Nefazadone	C25H32ClN5O2	470.0147	83366-66-9	1
Nicotine	C10H14N2	162.2349	54-11-5	2
Nitrazepam	C15H11N3O3	281.271	146-22-5	1
Norbuprenorphine	C25H35NO4	413.5574	78715-23-8	2
Norbuprenorphine glucuronide	C31H43NO10	589.683	469887-29-4	1
Norclomipramine	C18H21ClN2	300.8314	303-48-0	1
Norclozapine	C17H17ClN4	312.8022	6104-71-8	1
Norcocaine	C16H19NO4	289.3312	18717-72-1	1
Nordiazepam	C15H11ClN2O	270.7183	1088-11-5	2
Nordoxepin	C18H19NO	265.3553	1225-56-5	1
Norfentanyl	C14H20N2O	232.3259	1609-66-1	4
Norfludiazepam	C15H10ClFN2O	288.7088	2886-65-9	2
Norfluoxetine	C16H16F3NO	295.3047	57226-68-3	1
Norketamine	C12H14ClNO	223.7022	35211-10-0	2
Normeperidine	C14H19NO2	233.3105	77-17-8	2
Norpropoxyphene	C21H25NO	307.436	3376-94-1	2
Norsertaline	C16H15Cl2N	292.2077	91797-58-9	1
Nortramadol	C15H23NO2	249.3533	75377-45-6	1
Nortriptyline	C19H21N	263.3829	72-69-5	1
Noscapine	C22H23NO7	413.4271	128-62-1	1
O-Desmethylvenlafaxine	C16H25NO2	263.3801	93413-62-8	1
Olanzapine	C17H20N4S	312.4376	132539-06-1	1
Olanzapine-D3	C17H17(2H)3N4S	315.4561		1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Orphenadrine	C18H23NO	269.387	83-98-7	1
Oxaprozin	C18H15NO3	293.3223	21256-18-8	1
Oxazepam	C15H11ClN2O2	286.7176	604-75-1	2
Oxcarbazepine	C15H12N2O2	252.2728	28721-07-5	1
Oxycodone	C18H21NO4	315.3692	76-42-6	3
Oxymorphone	C17H19NO4	301.3423	76-41-5	3
Oxymorphone glucuronide	C23H27NO10	477.4679	770735-01-8	1
Papaverine	C20H22ClNO4	375.8519	58-74-2	1
Para-Methoxyamphetamine	C10H15NO	165.2353	64-13-1	1
Paroxetine	C19H20FNO3	329.3714	61869-08-7	1
PEG-10mer Ammonium adduct	C20H42O11NH3	475.5767		1
PEG-11mer Ammonium adduct	C22H46O12NH3	519.6298		1
PEG-12mer Ammonium adduct	C24H50O13NH3	563.6829		1
PEG-7mer Ammonium adduct	C14H30O8NH3	343.4174		1
PEG-8mer Ammonium adduct	C16H34O9NH3	387.4705		1
PEG-9mer Ammonium adduct	C18H38O10NH3	431.5236		1
Pentazocine	C19H27NO	285.4298	359-83-1	2
Pentobarbital Negative	C11H18N2O3	226.2756	76-74-4	1
Pentylone	C13H17NO3	235.283	698963-77-8	1
Perphenazine	C21H26ClN3OS	403.9746	58-39-9	1
Phenazepam	C15H10BrClN2O	349.6139	51753-57-2	1
Phenazepam (351 ion)	C15H10BrClN2O	349.6139	51753-57-2	1
Phencyclidine	C17H25N	243.3925	77-10-1	3
Phendimetrazine	C12H17NO	191.2733		1
Pheniramine	C16H20N2	240.3486	86-21-5	1
Phenmetrazine	C11H15NO	177.2464	134-49-6	1
Phenobarbital	C12H12N2O3	232.2391	50-06-6	1
Phenothiazine	C12H9NS	199.2749	92-84-2	1
Phentermine	C10H15N	149.236	122-09-8	2
Phenylephrine	C9H13NO2	167.2078	61-76-7	1
Phenylpropanolamine	C9H13NO	151.2085	14838-15-4	1
Phenytoin	C15H12N2O2	252.2728	57-41-0	1
Piperacillin	C23H27N5O7S	517.5613	61477-96-1	2
PMA	C10H15NO	165.2353	64-13-1	1
PMMA	C11H17NO	179.2622	3398-68-3	1
PPA	C9H13NO	151.2085	154-41-6	1
Pregabalin	C8H17NO2	159.2284	148553-50-8	1
Primidone	C12H14N2O2	218.2556	125-33-7	1
Primidone dimer	C24H28N4O4	436.5112	125-33-7	1
Proadifen	C23H32ClNO2	389.9656	62-68-0	1
Progesterone	C21H30O2	314.4682	57-83-0	1
Promazine	C17H20N2S	284.4241	58-40-2	1
Promethazine	C17H20N2S	284.4241	60-87-7	2
Propoxyphene	C22H29NO2	339.4781	469-62-5	3
Propranolol	C16H21NO2	259.3484	525-66-6	1
Protriptyline	C19H21N	263.3829	438-60-8	2
Pseudoephedrine	C10H15NO	165.2353	90-82-4	2
Psilocin	C12H16N2O	204.2721	520-53-6	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
Pyrilamine	C17H23N3O	285.3895	91-84-9	1
Quetiapine	C21H25N3O2S	383.5132	111974-69-7	1
Quinidine	C20H24N2O2	324.4231	56-54-2	1
Raloxifene	C28H27NO4S	473.5915	84449-90-1	1
Ramelteon	C16H21NO2	259.3484	196597-26-9	1
Ranitidine	C13H22N4O3S	314.4073	66357-35-5	1
RCS-4	C21H23NO2	321.4195	1345966-78-0	1
RCS-4-N-(5-CarboxyPentyl)	C21H21NO4	351.4023		1
RCS-4 M9/M10 Metabolite	C20H21NO3	323.3919		1
RCS-4 N-(5-hydroxypentyl) Metabolite	C21H23NO3	337.4188		1
RCS-8 or SR-18	C25H29NO2	375.5112		1
Reserpine	C33H40N2O9	608.6887	50-55-5	1
Risperidone	C23H27FN4O2	410.4919	106266-06-2	2
Ritalinic acid	C13H17NO2	219.2836	19395-41-6	2
Rocuronium	C32H53N2O4	529.7841	143558-00-3	1
Salicyclic Acid	C7H6O3	138.1228	69-72-7	1
Secobarbital	C12H18N2O3	238.2866	76-73-3	1
Selegiline	C13H17N	187.285	14611-51-9	1
Selegiline isomer	C13H17N	187.285	14611-51-9	1
Sertraline	C17H17Cl2N	306.2346	79617-96-2	2
Sildenafil	C22H30N6O4S	474.5828	139755-83-2	1
Sotalol	C12H20N2O3S	272.3668	3930-20-9	1
Strychnine	C21H22N2O2	334.4183	57-24-9	1
Sufentanil	C22H30N2O2S	386.5571	56030-54-7	1
Sulfadimethoxine	C12H14N4O4S	310.3321	122-11-2	1
Synephrine	C9H13NO2	167.2078	94-07-5	1
Tadalafil	C22H19N3O4	389.411	171596-29-5	1
Taxol	C47H51NO14	853.9203	33069-62-4	1
Taxotere (Sodiated)	C43H52NO14Na	829.8738	114977-28-5	1
Temazepam	C16H13ClN2O2	300.7445	846-50-4	3
Testosterone	C19H28O2	288.4303	58-22-0	1
TFMPP	C11H14ClF3N2	266.6938	16015-69-3	1
THC	C21H30O2	314.4682	1972-08-3	1
THC-COOH	C21H28O4	344.451	64280-14-4	1
Theobromine	C7H8N4O2	180.1664	83-67-0	1
Theophylline	C7H8N4O2	180.1664	58-55-9	1
Thiopental	C11H18N2O2S	242.3406	76-75-5	1
Thioridazine	C21H26N2S2	370.5801	50-52-2	2
Thiothixene	C23H29N3O2S2	443.6314	5591-45-7	1
Ticlopidine	C14H14ClNS	263.7894	55142-85-3	1
Timolol	C13H24N4O3S	316.4231	26839-75-8	1
Topiramate	C12H21NO8S	339.3646	97240-79-4	1
Tramadol	C16H25NO2	263.3801	27203-92-5	2
Trazadone	C19H22ClNSO	371.8699	19794-93-5	2
Triazolam	C17H12Cl2N4	343.2153	28911-01-5	1
Trifluoperazine	C21H24F3N3S	407.5019	117-89-5	1
Trimipramine	C20H26N2	294.4403	739-71-9	2
Tripolidine	C19H22N2	278.3976	486-12-4	1

Compound	Formula	Formula Weight	CAS Number	# of Spectra
UR-144	C ₂₁ H ₂₉ NO	311.4677		1
UR-144 N-(5-hydroxypentyl) metabolite	C ₂₁ H ₂₉ NO ₂	327.467		2
UR-144 N-pentanoic acid metabolite	C ₂₁ H ₂₇ NO ₃	341.4505		1
Valproic acid	C ₈ H ₁₆ O ₂	144.2138	99-66-1	1
Vardenafil	C ₂₃ H ₃₃ CIN ₆ O ₄ S	525.0704	224785-91-5	1
Venlafaxine	C ₁₇ H ₂₇ NO ₂	277.407	93413-69-5	1
Verapamil	C ₂₇ H ₃₈ N ₂ O ₄	454.61	52-53-9	2
Warfarin	C ₁₉ H ₁₆ O ₄	308.3338	81-81-2	1
XLR11	C ₂₁ H ₂₈ FNO	329.4582		1
Yohimbine	C ₂₁ H ₂₆ N ₂ O ₃	354.4493	146-48-5	1
Zaleplon	C ₁₇ H ₁₅ N ₅ O	305.3397	151319-34-5	2
Ziprasidone	C ₂₁ H ₂₁ CIN ₄ O ₅	412.9417	146939-27-7	2
Zolpidem	C ₁₉ H ₂₁ N ₃ O	307.3958	82626-48-0	4
Zonisamide	C ₈ H ₈ N ₂ O ₃ S	212.2276	68291-97-4	1
Zopiclone	C ₁₇ H ₁₇ CIN ₆ O ₃	388.8137	43200-80-2	1

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Publication number: 11120815-01 Document number: RUO-MKT-07-2101-A



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

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