

For LabSolutions™ LCMS

# High Resolution Accurate Mass Library for Forensic Toxicology



LCMS-9030

Perform forensic toxicology screening for drugs of abuse, psychotropic drugs, pharmaceuticals, pesticides, and natural toxins using this high-resolution accurate mass database.

## MS/MS Spectra for over 900 Toxicological Substances

The High Resolution Accurate Mass (HRAM) Library includes two MS/MS spectral libraries. Each library is built using two different separation conditions and is suitable for targeted or non-targeted screening of drugs of abuse, psychotropic drugs, pharmaceuticals, pesticides, and other compounds of toxicological interest.

### Library Contents

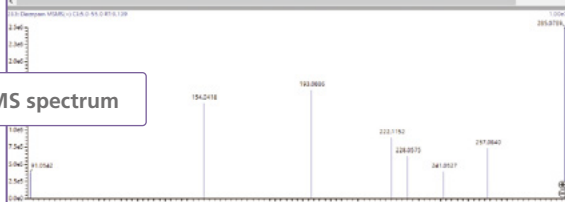
Library 1 includes 81 MS/MS spectra and ODS method retention times for various illegal drugs and pharmaceuticals commonly of interest to forensic laboratories. Library 2 includes MS/MS spectra for 901 potentially toxic substances of interest to forensic analysis and clinical research. Retention times and method conditions are based on a Biphenyl column.

#	Compound Name	Precursor m/z	Formula	RT	Synonym	Theory m/z	MS Stage	Ionization	Mass Range	Collision Energy	Collision Gas Vol.
266	Desamylamiodane	617.0997	C23H29NO3	9.949	(2-Butyl-1-benzofuran-3-yl)(14-(2-cyanoethyl)ethoxy)-3,5-dichlorophenylmethanone	616.0924	2	ESI	201.0910 - 617.0997	5.0 - 55.0	200.0000
267	Desipramine	267.1036	C19H23N	7.174	1-(10,11-Dihydro-5H-dibenz[b,f]azepin-5-yl)-N-methyl-1-propanamine	266.1763	2	ESI	72.0000 - 267.1036	5.0 - 55.0	200.0000
268	Desmethylamitriptyline	316.1448	C19H19N3O	7.256	3-(2-chlorophenyl)amino-N,N-dimethyl-1-propanamine	300.1110	2	ESI	103.0444 - 316.1448	5.0 - 55.0	200.0000
269	Desmethylclozapine	311.1554	C19H19N3O	6.111	1-(4-Fluorophenyl)-1-(3-methylphenyl)pyrrolidine	310.1481	2	ESI	83.0232 - 311.1554	5.0 - 55.0	200.0000
270	Desmethylclonidine	301.1466	C18H21ClN2	7.879	3-(3-Chloro-10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)-N-methyl-1-propanamine	300.1393	2	ESI	72.0000 - 301.1466	5.0 - 55.0	200.0000
271	Desmethylcitalopram	300.0779	C19H19FN3O	7.227	3-(2-Fluorophenyl)-7-methyl-1,4-dihydro-2H-1,4-benzodiazepin-2-one	299.0709	2	ESI	196.0714 - 300.0779	5.0 - 55.0	200.0000
272	Desmethylcitalopram	293.1543	C19H19N3O	6.914	1,2,3,4,9,10-hexahydrobenzodiazepino[2,1-b]pyridin-3-yl(2-thienyl)ethanone	292.1476	2	ESI	91.0242 - 293.1543	5.0 - 55.0	200.0000
273	Desmethylcitalopram	253.1495	C18H17N3O	5.727	1,2,3,4,9,10-hexahydrobenzodiazepino[2,1-b]pyridin-3-yl(2-thienyl)ethanone	251.1403	2	ESI	115.0242 - 253.1495	5.0 - 55.0	200.0000
274	Desmethylcitalopram	292.0634	C19H19N3O	7.058	(15,40)-(13,4-Dichlorophenyl)-1,2,3,4-tetrahydro-1-naphthalenamine	291.0562	2	ESI	91.0242 - 292.0634	5.0 - 55.0	200.0000
275	Desmethylcitalopram	266.1030	C19H19N3O	7.188	1-(2,4-Dichlorophenyl)pyrrolidine-N,N-dimethyl-1-propanamine	265.1197	2	ESI	89.0386 - 266.1030	5.0 - 55.0	200.0000
276	Desmethylcitalopram	264.1958	C18H17N3O	4.194	1-(2,4-Dichlorophenyl)pyrrolidine-N,N-dimethyl-1-propanamine	263.1885	2	ESI	105.0690 - 264.1958	5.0 - 55.0	200.0000
277	Desmethylcitalopram	214.1121	C8H11N3S	6.720	N-isopropyl-N-methyl-N-methylsulfonamide, 1,3,5-triazine-2,4-diamine	213.1048	2	ESI	68.0243 - 214.1121	5.0 - 55.0	200.0000
278	Desmethylcitalopram	275.1310	C19H19N3O	6.877	(20-(2,4-Dichlorophenyl)-N,N-dimethyl-1-(2-synthyl)-1-propanamine	274.1237	2	ESI	118.0937 - 275.1310	5.0 - 55.0	200.0000
279	Desmethylcitalopram	252.1538	C18H17N3O	4.844	(2S)-N-Ethyl-1-(3-chlorophenyl)pyrrolidine-2-propanamine	251.1235	2	ESI	109.0448 - 252.1538	5.0 - 55.0	200.0000
280	Desmethylcitalopram	272.2009	C18H19NO	6.913	(6a,13a)-3-Methoxy-17-methylmorpholin	271.1936	2	ESI	121.0548 - 272.2009	5.0 - 55.0	200.0000
281	Desmethylcitalopram	340.2271	C22H27NO2	7.056	(2S,3S)-2-(2-methylamino-3-methyl-1,2-diphenyl-2-oxoethyl)propanoate	339.2199	2	ESI	91.0242 - 340.2271	5.0 - 55.0	200.0000
282	Desmethylcitalopram	309.1809	C19H21NO4	3.624	N-(3-Isopropyl-4-(2-hydroxy-2-propoxyphenyl)phenyl)acetamide	308.1739	2	ESI	98.0964 - 309.1809	5.0 - 55.0	200.0000
283	Desmethylcitalopram	284.1958	C18H17N3O	9.199	7-Chloro-1-methyl-1-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one	283.0716	2	ESI	91.0242 - 284.1958	5.0 - 55.0	200.0000
284	Desmethylcitalopram	290.0990	C18H17NO2S	4.815	7-Chloro-3-methyl-2H-1,2,4-benzoxazine-1,1-dioxide	289.0917	2	ESI	43.0239 - 290.0990	5.0 - 55.0	200.0000
285	Desmethylcitalopram	220.9132	C8H11NO4P	5.099	1,2-Dichloro-N,N-dimethyl-1-propanamine	219.9049	2	ESI	79.9943 - 220.9132	5.0 - 55.0	200.0000
286	Desmethylcitalopram	318.0189	C19H19N3O	8.900	7-Chloro-5-(2-chlorophenyl)-1-methyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one	317.0127	2	ESI	154.0418 - 318.0189	5.0 - 55.0	200.0000
287	Desmethylcitalopram	296.0240	C18H17NO2S	8.284	(2S,4S)-2,4-Dichlorophenylamino-N,N-dimethyl-1-propanamine	295.0167	2	ESI	216.0418 - 296.0240	5.0 - 55.0	200.0000
288	Desmethylcitalopram	252.1530	C18H17N3O	7.287	3-(10,11-Dihydro-5H-dibenz[b,f]azepin-5-yl)-N,N-dimethyl-1-propanamine	249.1518	2	ESI	79.0242 - 252.1530	5.0 - 55.0	200.0000
289	Desmethylcitalopram	252.1514	C18H17N3O	7.192	1-(1-(4-Chlorophenyl)cyclobutyl)-1-methyl-1-propanamine	251.1441	2	ESI	89.0239 - 252.1514	5.0 - 55.0	200.0000
290	Desmethylcitalopram	268.1543	C18H17NO4	7.550	Isopropyl (3,4-dichlorophenyl)carbamate	267.1471	2	ESI	80.0495 - 268.1543	5.0 - 55.0	200.0000
291	Desmethylcitalopram	155.0488	C6H11O4P	1.150	Dimethyl hydrogen phosphate	154.0395	2	ESI	80.0736 - 155.0488	5.0 - 55.0	200.0000

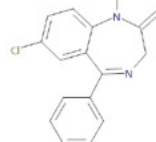
### Compound information

Each library contains key information critical to accurate identification of compounds, including precursor ion m/z, molecular formula, and monoisotopic mass, as well as spectral acquisition parameters, such as collision energy, ionization, and retention time.

### MS/MS spectrum



### Chemical structure



Example of Library Entry

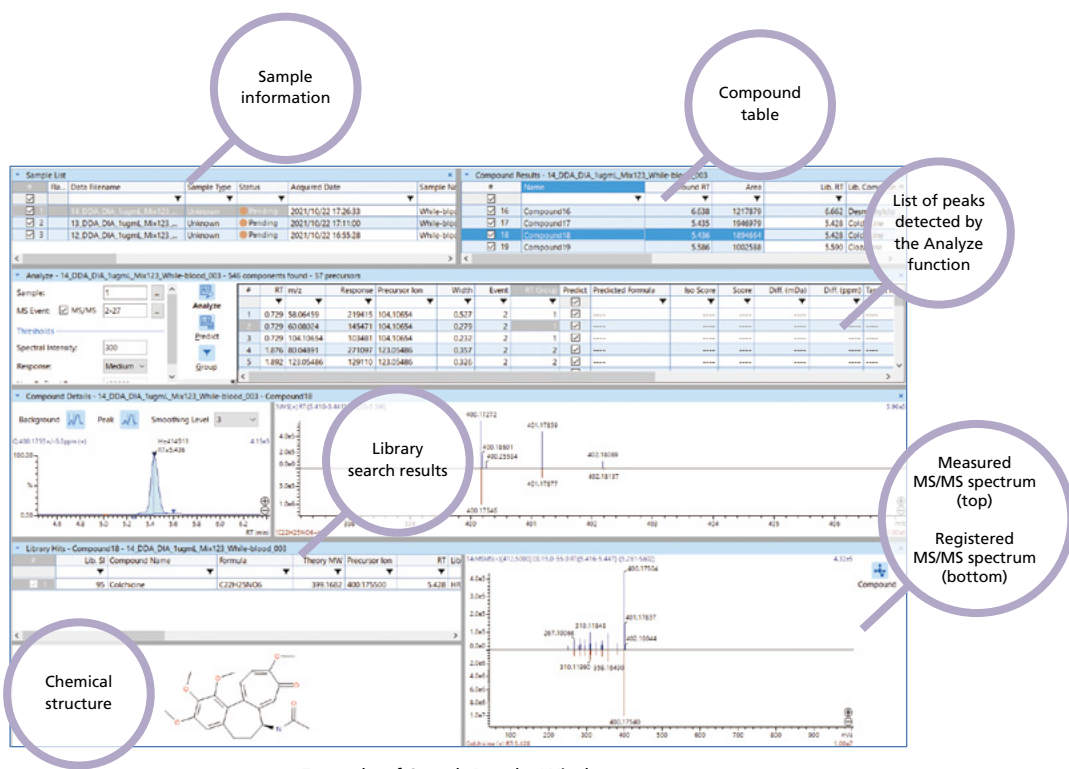
# High Resolution Accurate Mass Library for Forensic Toxicology

## Simple Data Analysis Using LabSolutions Insight Explore™

Data acquired with a Shimadzu Q-TOF system can be analyzed easily using LabSolutions Insight Explore software. Library searching and compound identification can be performed in just three steps. Search results are displayed in a format that is visually easy to understand.

### Procedure for Compound Identification by Searching the Library

- STEP 1** Use Insight's Analyze function to detect peaks in the mass spectrum and register results in the compound table.
- STEP 2** Search the MS/MS library for spectra with similarities to detected compounds.
- STEP 3** Check library search results along with library similarity score and chemical structure.



Example of Search Results Window

### Remarks and Precautions

1. LabSolutions LCMS Ver. 5.113 or later and LabSolutions Insight™ Ver. 3.85P4 or later are required.
2. This library is intended for research use only. It may not be used for clinical diagnostic applications.

LabSolutions, LabSolutions Insight Explore and LabSolutions Insight are trademarks of Shimadzu Corporation or its affiliated companies in Japan and/or other countries.



Shimadzu Corporation  
[www.shimadzu.com/an/](http://www.shimadzu.com/an/)

### For Research Use Only. Not for use in diagnostic procedures.

This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.

Company names, products/service names and logos used in this publication are trademarks and trade names of Shimadzu Corporation, its subsidiaries or its affiliates, whether or not they are used with trademark symbol "TM" or "®".

Third-party trademarks and trade names may be used in this publication to refer to either the entities or their products/services, whether or not they are used with trademark symbol "TM" or "®".

Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The contents of this publication are provided to you "as is" without warranty of any kind, and are subject to change without notice. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication.