

For LabSolutions™ LCMS

High Resolution Accurate Mass Library for Forensic Toxicology Ver. 2



LCMS-9050

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

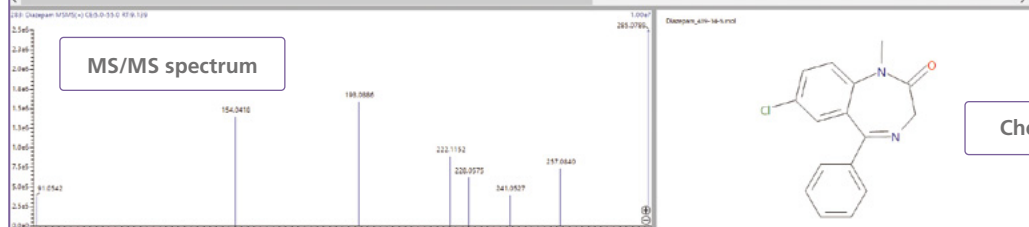
MS/MS Spectra for over 1,900 Toxicological Substances

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.

#	Compound Name	Precursor m/z	Formula	RT	Synonym	Theory MW	MS Stage	Ionization	Mass Range	Collision Energy	Collision Gas Vol.
256	Demethylamitriptyline	437.0997	C23H25N3O3	9.840	(2R)-N-(3-(dimethylamino)propyl)-1-(4-(2-methylamino)ethoxy)-3,5-dimethoxyphenylmethanone	416.9934	2	ESI	201.0910 - 617.9997	S.O. - 55.0	210.0000
257	Desipramine	267.1856	C18H21NO	7.174	3-(10,11-Dihydro-5H-dibenz[<i>b,h</i>]azepin-5-yl)-N-methyl-1-propanamine	266.1703	2	ESI	72.0800 - 267.1856	S.O. - 55.0	210.0000
258	Desmethylam	318.1448	C18H19N3O4	7.256	3-(1Ethoxycarbonylamino)phenyl phenylcarbamate	300.1110	2	ESI	108.0444 - 318.1448	S.O. - 55.0	210.0000
259	Desmethylclonidine	311.1554	C19H19N2O2	6.111	1-(4-Fluorophenyl)-1-(1-(methylamino)propyl)-1,3-dihydro-2-benzofuran-5-carbonitrile	310.1481	2	ESI	88.0292 - 311.1554	S.O. - 55.0	210.0000
270	Desmethylpropamine	301.1466	C18H21CN2	7.870	3-(3-Chloro-10,11-dihydro-5H-dibenz[<i>b,h</i>]azepin-5-yl)-N-methyl-1-propanamine	300.1399	2	ESI	72.0808 - 301.1466	S.O. - 55.0	210.0000
271	Desmethylbenzazepin	300.0779	C19H19N3O3	7.227	5-(4-Fluorophenyl)-7-oxo-1,3-dihydro-2H-1,4-benzodiazepin-2-one	296.0705	2	ESI	146.0714 - 300.0779	S.O. - 55.0	210.0000
272	Desmethylammonium	251.1543	C17H18N2	6.554	1,2,3,4,10,14-Hexahydroindeno[2,1-b]pyrido[2,3-d]benzoxazine	250.1470	2	ESI	91.0542 - 251.1543	S.O. - 55.0	210.0000
273	Desmethylazepine	252.1495	C16H17NO	5.727	1,2,3,4,10,14-Hexahydroindeno[2,1-b]pyrido[2,3-d]benzoxazine	251.1423	2	ESI	115.0542 - 252.1495	S.O. - 55.0	210.0000
274	Desmethylsertraline	250.0654	C18H19N2O2	7.850	115,451-4-(3,4-Dichlorophenyl)-1,2,3,4-tetrahydro-1-naphthalenamine	251.0562	2	ESI	91.0542 - 275.0289	S.O. - 55.0	210.0000
275	Desmethylbutoramine	266.1670	C18H24N2O	7.248	1-(1-(4-Chlorophenyl)cyclohexyl)-N,N-dimethyl-1-butylamine	265.1597	2	ESI	89.0386 - 266.1670	S.O. - 55.0	210.0000
276	Desmethylsertraline	254.1958	C18H19N2O2	4.194	4-(2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl)phenol	261.1885	2	ESI	105.0699 - 264.1958	S.O. - 55.0	210.0000
277	Desmethyl	234.1131	C18H19NO5	4.720	N-isopropyl-N-methyl-4-methyl-4-methyl-1,3,5-triazine-2,4-diamine	233.1048	2	ESI	68.0343 - 234.1131	S.O. - 55.0	210.0000
278	Deschlorpheniramine	275.1110	C18H19N3	5.877	(3S)-3-(4-Chlorophenyl)-N,N-dimethyl-3-(2-pyridinyl)-1-propanamine	274.1237	2	ESI	118.0051 - 270.0731	S.O. - 55.0	210.0000
279	Desfenbutamine	232.1308	C12H17FN3	4.844	(2S)-N-Ethyl-1-(2-(trifluoromethyl)phenyl)-2-propanamine	231.1235	2	ESI	109.0448 - 232.1308	S.O. - 55.0	210.0000
280	Dextromethorphan	272.2009	C18H25NO	6.913	(9S,13a,16a)-3-Methoxy-17-methylmorphinan	271.1936	2	ESI	121.0948 - 272.2009	S.O. - 55.0	210.0000
281	Diethylpropylamine	348.2271	C22H31NO2	7.036	(2S,3R)-4-(dimethylamino)-3-methyl-1,2-diphenyl-2-butanyl propionate	336.2198	2	ESI	91.0542 - 348.2271	S.O. - 55.0	210.0000
282	Diazepam	328.1809	C16H14N2O2	3.624	N-(3-allyl-4-(2-hydroxy-2-isopropylamino)propyl)phenylacetamide	326.1735	2	ESI	86.0964 - 328.1809	S.O. - 55.0	210.0000
283	Diazepam	303.0722	C16H13ClN2O2	9.130	7-Chloro-1-methyl-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one	284.0716	2	ESI	91.0542 - 285.0789	S.O. - 55.0	210.0000
294	Diazoxide	230.9990	C8H7ClN3O2S	4.815	7-Chloro-3-methyl-2H-1,2,4-benzoxadiazine 1,1-dioxide	229.9917	2	ESI	63.0229 - 230.9990	S.O. - 55.0	210.0000
295	Dichlorvos	220.0532	C4H7Cl2O4P	5.599	2,2-Dichlorovinyl dimethyl phosphite	219.0439	2	ESI	78.0943 - 220.0532	S.O. - 55.0	210.0000
296	Dichlorpropen	319.0399	C16H12Cl2N2O2	8.900	7-Chloro-5-(2-chlorophenyl)-1-methyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one	318.0327	2	ESI	154.0418 - 319.0399	S.O. - 55.0	210.0000
297	Diclofenac	296.0240	C14H11Cl2NO2	8.384	(2S,2R)-2-(2-(2-chlorophenyl)amino)phenylacetic acid	295.0167	2	ESI	214.0418 - 296.0240	S.O. - 55.0	210.0000
298	Diclofenac	250.1590	C18H19N	7.297	3-(10,11-Dihydro-5H-dibenz[<i>b,h</i>]azepin-5-ylidene)-1-propanamine	249.1518	2	ESI	79.0542 - 250.1590	S.O. - 55.0	210.0000
299	Diclofenac	252.1514	C15H22CN	7.192	1-(1-(4-Chlorophenyl)cyclohexyl)-3-methyl-1-butylamine	251.1441	2	ESI	89.0386 - 252.1514	S.O. - 55.0	210.0000
300	Difenhydramine	268.1543	C18H21NDO4	7.550	isopropyl (3,4-dihydroxyphenyl)carbamate	267.1471	2	ESI	80.0495 - 268.1543	S.O. - 55.0	210.0000
301	Diethylphosphate	155.0468	C4H11O4P	1.150	Diethyl hydrogen phosphate	154.0395	2	ESI	80.0336 - 155.0468	S.O. - 55.0	210.0000

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.



Chemical structure

Example of Library Entry

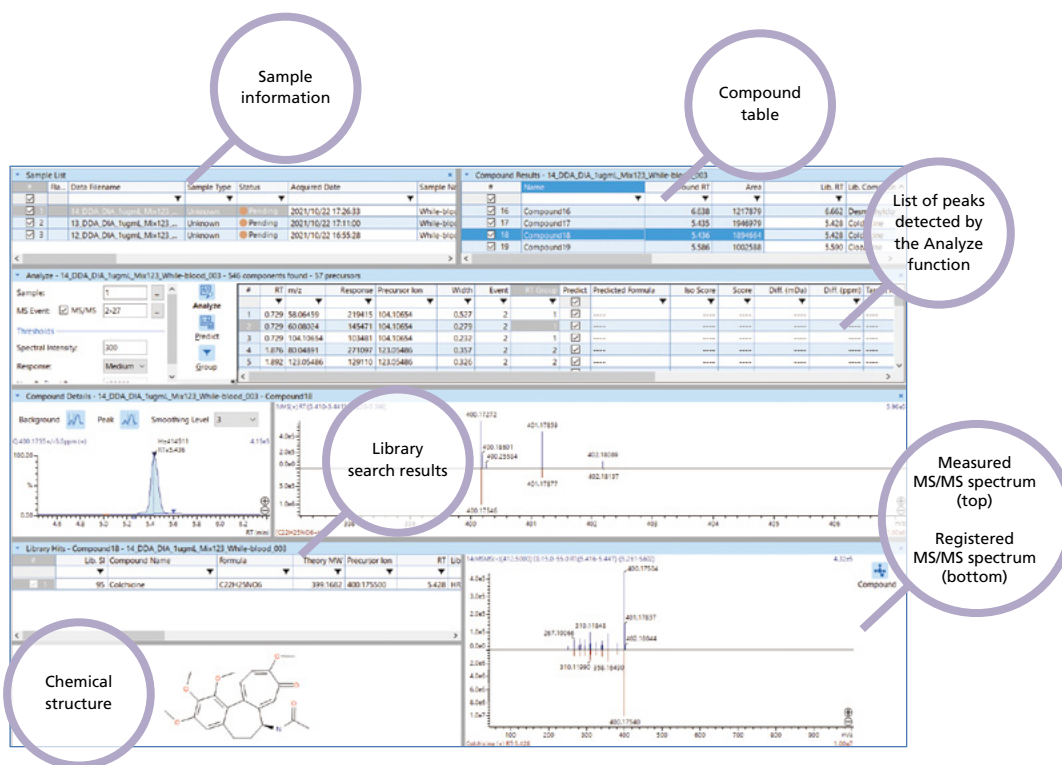
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Simple Data Analysis Using LabSolutions Insight Explore™

Data acquired with a Shimadzu QTOF 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. 5.128 or later and LabSolutions Insight™ Ver. 4.2 SP1 or later are required.
2. This library is intended for research use only. It may not be used for clinical diagnostic applications.

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