SHIMADZU
Excellence in Science

For LabSolutions™ LCMS

LC/MS/MS Forensic Toxicology Database

Simplified Acquisition and Identification

The Forensic Toxicology Database includes optimized LC-MS/MS data acquisition parameters and a library database to help clinical and forensic researchers build screening and quantitation methods quickly, simplifying method development.

MRM & Spectral Library database contains information on more than 2,500 compounds

The spectral library database is built using two separation conditions (ODS and Biphenyl). Both methods have information on clinical and forensic compounds of interest in routine analysis. The ODS method contains information on 1,250 compounds and the Biphenyl method contains 1,281 compounds. Compound datasheet includes: monoisotopic mass, RT, CAS number, formula and compound class. This package provides Synchronized Survey Scan parameters (MRM parameters, MRM intensity threshold and triggered product ion scan parameters) optimized for screening analysis.

Enhanced identification by merged spectrum

Each certified reference material was acquired with three different collision energies to generate an information-rich merged-CE spectrum which can be used in library matching and compound verification. Matching with a merged-CE spectrum library can be a powerful tool to identify compounds with a library score.

Analytical Conditions for ODS column

Analytical column	:	Phenomenex Kinetex XB-C18 (2.1 mmI.D. x 100 mmL., 2.6um)
Guard column	:	Phenomenex SecurityGuard ULTRA C18 2.1mmID
Mobile phase A	:	10 mmol/L ammonium formate + 0.1% formic acid – water
Mobile phase B	:	10 mmol/L ammonium formate + 0.1% formic acid – methanol
Flow rate	:	0.3 mL / min
Column temp.	:	40 °C
Analytical time	:	15 min

Analytical Conditions for Biphenyl column

Analytical column	:	Restek Raptor Biphenyl (2.1 mmI.D. x 100 mmL., 2.7um)
Mobile phase A	:	2 mmol/L ammonium formate + 0.002% formic acid – water
Mobile phase B	:	2 mmol/L ammonium formate + 0.002% formic acid – methanol
Flow rate	:	0.3 mL/min (0.5 mL/min from 11 min to 14 min)
Column temp.	:	50 °C
Analytical time	:	17 min

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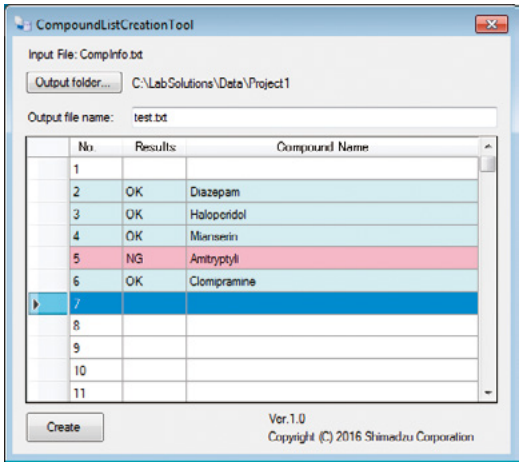
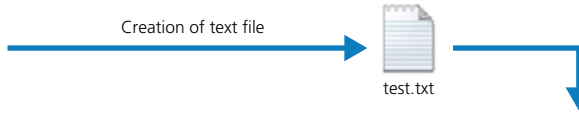
LC/MS/MS Forensic Toxicology Database

Method Creation by "Compound List Creation Tool"



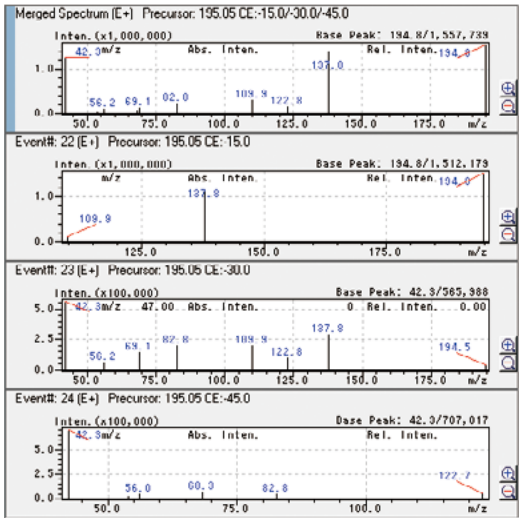
To accelerate customized method development, the 'Compound List Creation Tool' can be used to select specific panels of targets from the library for analysis by LC-MS/MS.



Type	Event#	+/−	Compound Name m/z	Time (0.000 min – 8.348 min)
MRM	5	+	Caffeine 195.10>138.05, 195.10>42.10	
├ Product Ion Scan	6	+	> CE=-15.0, 20.00>205.10	
├ (Product Ion Scan)	7	+	> CE=-30.0, 20.00>205.10	
└ (Product Ion Scan)	8	+	> CE=-45.0, 20.00>205.10	
MRM	9	+	Atropine 290.15>124.15, 290.15>93.20	
├ Product Ion Scan	10	+	> CE=-15.0, 20.00>300.15	
├ (Product Ion Scan)	11	+	> CE=-30.0, 20.00>300.15	
└ (Product Ion Scan)	12	+	> CE=-45.0, 20.00>300.15	
MRM	13	+	Fentanyl 337.20>105.10, 337.20>188.10	
├ Product Ion Scan	14	+	> CE=-15.0, 20.00>347.20	

Synchronized Survey Scan
(Including three Product Ion Scan events with three different CE)

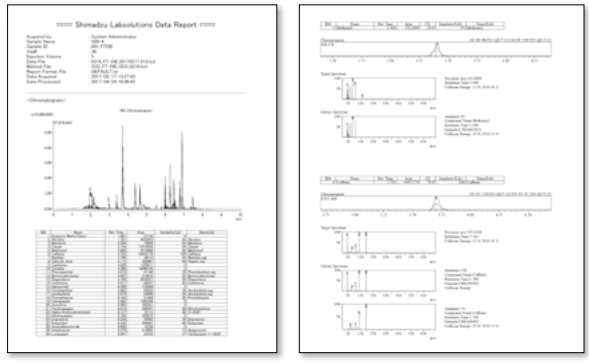
Compound Identification by Merged Spectra



Merged Spectrum

MS/MS Spectra with three different CE

Merged Spectra using three MS/MS spectra with three different CE help to increase the confidence in reporting results by using library searchable spectra.



Report by Library Search Results with Merged Spectra

Remarks and Precautions

1. LabSolutions LCMS Ver. 5.109 or later and LabSolutions Insight™ Ver. 3.8SP1 or later are required.
2. It is the user's responsibility to adopt appropriate quality control tests using standard samples to confirm qualitative and quantitative information obtained with the database.

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