

Application Data Sheet

No.44

LC-MS

Liquid Chromatograph Mass Spectrometer

Identification of Drugs in Urine Using Synchronized Survey Scan[®]

This report describes an analytical system using ultra-high-speed triple quadrupole mass spectrometry (LCMS-8030) for forensic analysis of drugs in urine. The LCMS-8030 has a Synchronized Survey Scan function that automatically performs MS/MS when a precursor threshold is exceeded, thereby producing a combined MRM and MRM-dependent product ion scan in a single analysis. Utilizing MRMs, it is possible to sensitively detect compounds while simultaneously performing a product ion scan, yielding MS/MS spectra. Furthermore, as the Collision Energy (CE) can be configured for each product scan, it is possible to optimize the CE for each compound, further increasing product ion scan spectra quality.

MRM mass chromatograms and library search results based on MS/MS spectra data from four compounds (allylisopropylacetylurea, diclofenac, amobarbital and thiamylal) spiked in urine are shown in this report.

Type	Event#	+/-	Compound Name	m/z	Time (0.000 min - 17.680 min)
MRM	85	+	093_Lidocaine	235.00>86.10	
- Product Ion Scan	86	+	> 50.00	245.00	
MRM	87	+	087_Aconitine	646.00>104.95	Positive
- Product Ion Scan	88	+	> 50.00	656.00	
MRM	193	-	072_Pentobarbital (neg)	225.	Negative
- Product Ion Scan	194	-	> 50.00	235.00	
MRM	195	-	051_Amobarbital (neg)	225.1	
- Product Ion Scan	196	-	> 50.00	235.00	
MRM	89	+	069_Nitrazepam	282.10>236.	
- Product Ion Scan	90	+	> 50.00	292.00	

MRM parameter

Product Ion Scan parameter

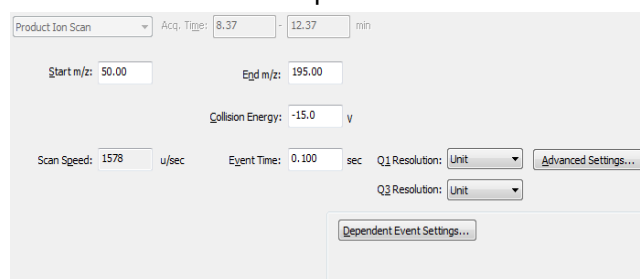
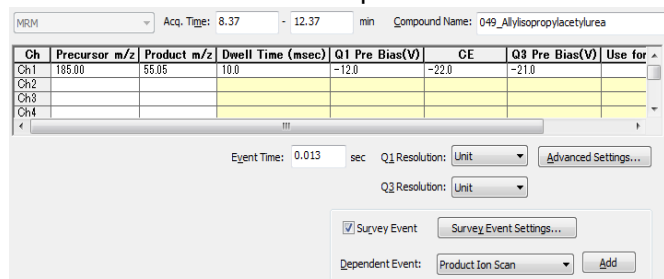


Figure 1: User Interface of MRM-Product Ion Scan Setting in LabSolutions Software

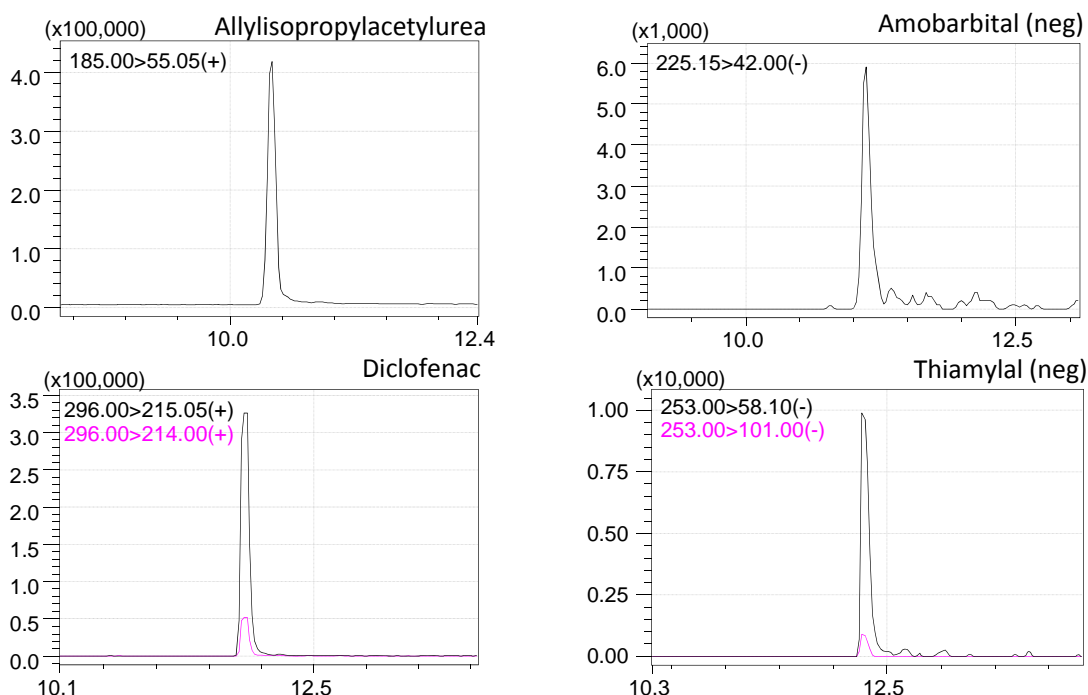


Figure 2: MRM Chromatograms of 4 Compounds Spiked into Urine

Figure 3 shows the LabSolutions Library Search Parameter Settings. Accurate results can be obtained using details, including precursor m/z and polarity, in addition to MS/MS spectral information (product m/z values and intensities).

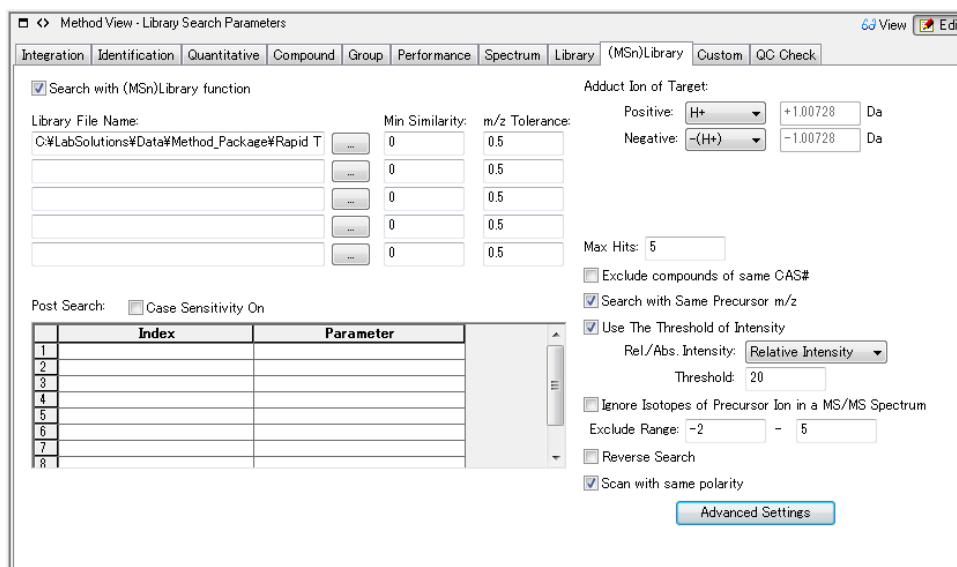


Figure 3: LabSolutions Library Search Parameter Settings interface

Alternatively, it is possible to retrieve inaccurate information from a library search when precursor m/z and polarity information is excluded (Fig.4 bottom), indicating precursor m/z and polarity are important values when searching the library.

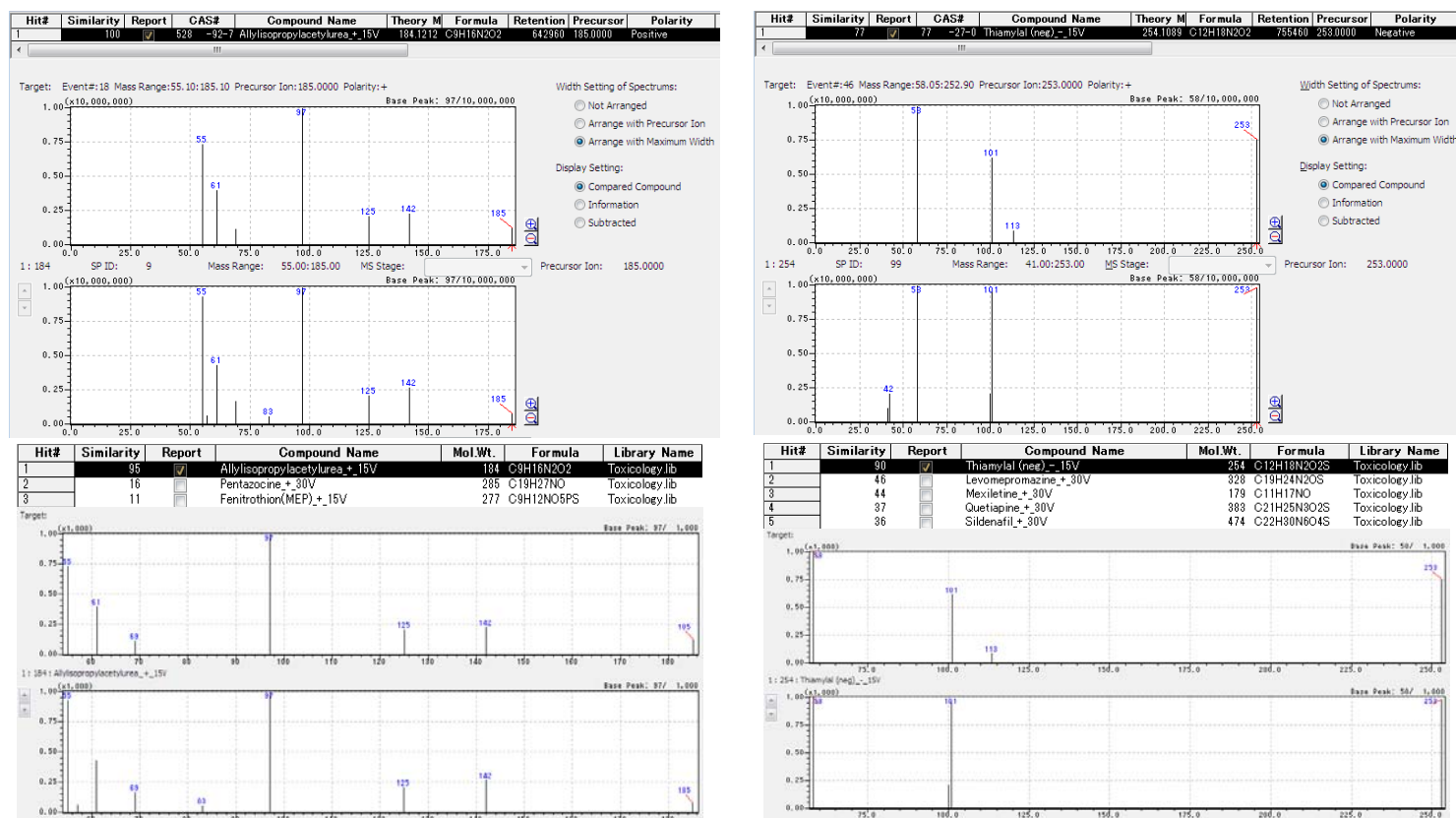


Figure 4: Library Search Results (top : parameter ON, bottom : parameter OFF)

First Edition: June, 2014



For Research Use Only. Not for use in diagnostic procedures.
The content of this publication shall not be reproduced, altered or sold for any commercial purpose without the written approval of Shimadzu. The information contained herein is provided to you "as is" without warranty of any kind including without limitation warranties as to its accuracy or completeness. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication. This publication is based upon the information available to Shimadzu on or before the date of publication, and subject to change without notice.