

LC/MS/MS Screening Software

LabSolutions Insight Library Screening



Software Helps with Screening Target Components

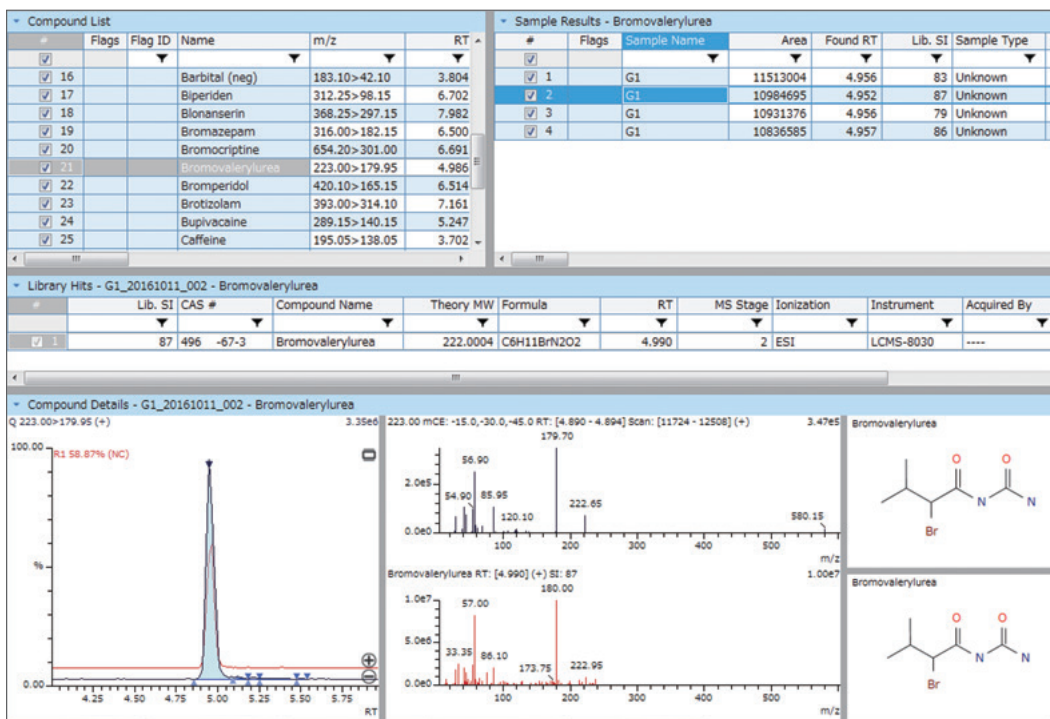
Screening Using the MRM-Automatic Product Ion Scan Method

By using a method with three product ion scan events specified at different collision energies (CE) for MRM events, three MS/MS spectra can be obtained while simultaneously detecting compounds with high sensitivity. Consequently, by searching the library using a merged spectrum of the three spectra, highly accurate identification results can be obtained.

Type	Event#	+/-	Compound Name	m/z	Time (1.623 min - 8.982 min)
MRM	21	+	Bromovalerylurea	223.00>17	
- Product Ion Scan	22	+	> CE--15.0, 20.00:1000.00		
(Product Ion Scan)	23	+	> CE--30.0, 20.00:1000.00		
(Product Ion Scan)	24	+	> CE--45.0, 20.00:1000.00		
MRM	25	+	Chlorpheniramine	275.00>23	
- Product Ion Scan	26	+	> CE--15.0, 20.00:1000.00		
(Product Ion Scan)	27	+	> CE--30.0, 20.00:1000.00		
(Product Ion Scan)	28	+	> CE--45.0, 20.00:1000.00		
MRM	29	+	7-aminonimetazepam	266.10	
- Product Ion Scan	30	+	> CE--15.0, 20.00:1000.00		

Ch	Precursor m/z	Product m/z	Pause Time	Dwell Time	Q1 Pre Bias	CE	Q3 Pre Bias	Use for Survey
Ch1	223.00	179.95	1.0	1.0	-11.0	-12.0	-20.0	<input checked="" type="checkbox"/>
Ch2	223.00	57.10	1.0	1.0	-11.0	-20.0	-23.0	<input checked="" type="checkbox"/>
Ch3								
Ch4								
Ch5								

The Insight Library Screening software can display library search results for multiple analytes at the same time. It can display the MRM chromatogram, MS/MS spectrum, library search results for compounds contained in the sample, and structural formulas of identified compounds.



Screening Results for Toxicological Substances Added to Whole Blood

The sedative hypnotic drug bromovalerylurea was identified from the MRM chromatogram and library search results (similarity score 87).

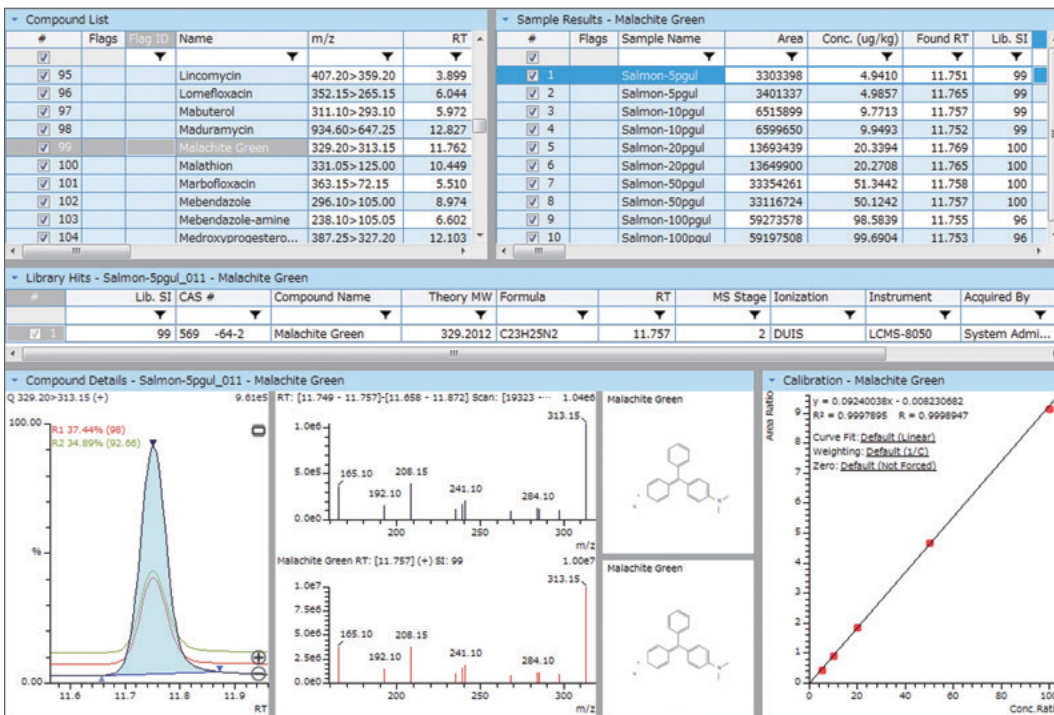
Screening Using Multi-MRM Method

MS/MS spectra can be obtained by specifying multiple channels for MRM events and plotting the intensity of each channel as MS/MS spectrum peaks. By searching the library using the MS/MS spectrum obtained, samples can be screened with high accuracy.

Type	Event#	+/-	Compound Name	m/z	Time (0.800 min - 13.247 min)
MRM	194	+	Decoquinat	418.25>372.20	
MRM	195	+	Virginiamycin S1	824.35>205	
MRM	196	+	Malachite Green	329.20>313.15	
MRM	197	+	Norgestimate	370.25>124.10	
MRM	198	+	Coumaphos	363.00>227.00, 3	

Ch	Precursor m/z	Product m/z	Pause Time	Dwell Time	Q1 Pre Bias(V)	CE	Q3 Pre Bias(V)
Ch1	329.20	313.15	1.0	3.0	-13.0	-38.0	-22.0
Ch2	329.20	208.15	1.0	3.0	-12.0	-36.0	-21.0
Ch3	329.20	165.10	1.0	3.0	-16.0	-65.0	-29.0
Ch4	329.20	241.10	1.0	3.0	-10.0	-55.0	-25.0
Ch5	329.20	239.10	1.0	3.0	-16.0	-65.0	-23.0
Ch6	329.20	192.10	1.0	3.0	-16.0	-60.0	-19.0
Ch7	329.20	284.10	1.0	3.0	-10.0	-45.0	-13.0
Ch8	329.20	235.15	1.0	3.0	-16.0	-47.0	-24.0
Ch9	329.20	285.15	1.0	3.0	-12.0	-36.0	-13.0
Ch10	329.20	297.10	1.0	3.0	-12.0	-53.0	-30.0
Ch11	329.20	268.15	1.0	3.0	-10.0	-62.0	-27.0
Ch12							
Ch13							
Ch14							

The Insight Library Screening software can display library search results for multiple analytes at the same time. It can display the MRM chromatogram, multi-channel MRM-based MS/MS spectrum, library search results, structural formulas, and MRM-based quantitative calibration curves for compounds contained in the sample.

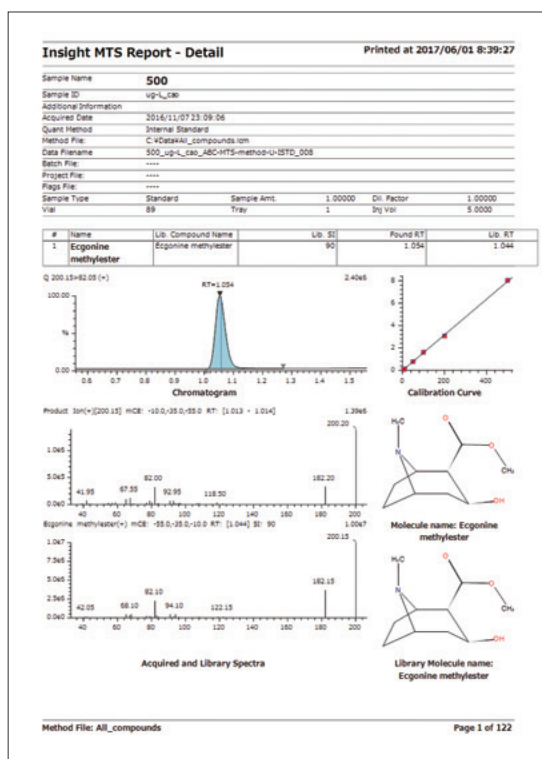


Results from Screening for Veterinary Drugs Added to Foods (Salmon Extract)

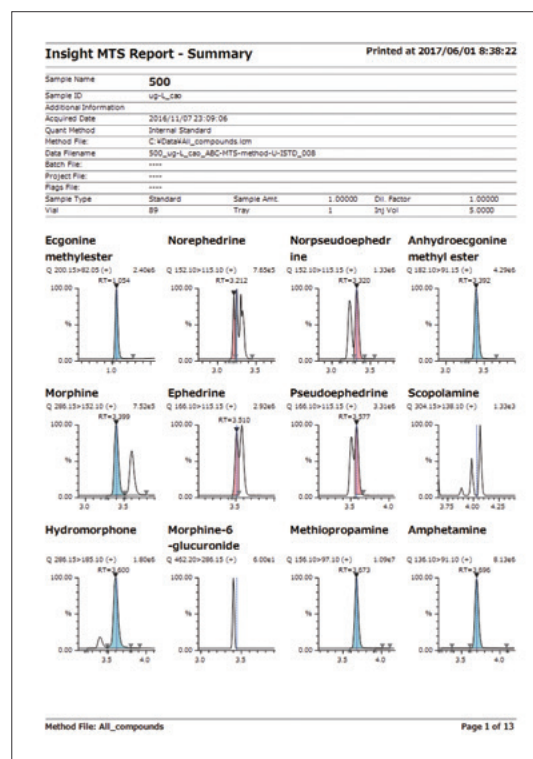
Malachite green disinfectant identified from the MRM chromatogram and library search results (similarity score 99).

▶ Printing Sophisticated Reports

Using the Library Screening software, separate reports can be printed for each data file. Summary reports or detailed results for each compound can also be printed.



Detailed results



Summary report



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