

Application Data Sheet

No. 61

GC-MS

Gas Chromatograph Mass Spectrometer

Analysis of Metabolites in Rat Urine Using Scan/MRM via GC-MS/MS (2)

The GCMS-TQ8030 is a GC-MS/MS system equipped with Scan/MRM mode to allow simultaneous Scan and MRM data measurements. Using Scan/MRM mode, it is possible to perform high-sensitivity analysis through high selectivity via MRM, while simultaneously performing qualitative analysis utilizing the mass spectrum via Scan.

By making use of these features, the target components can be quantified reliably with MRM, and untargeted, unknown components can be qualified through a library search of the mass spectrum obtained with Scan. This Application Datasheet introduces the results of Scan/MRM measurements of metabolites extracted from rat urine. Five target components are measured with MRM, and unknown peaks are identified through a library search of the mass spectrum obtained with Scan.

Experimental

The urease-treated direct drying method [1] was used, and the rat urine was then subjected to trimethylsilylation prior to measurement.

Analysis Conditions

Scan/MRM was used as the measurement mode. Table 1 shows the analysis conditions.

Table 1: Analysis Conditions

GC-MS	:GCMS-TQ8030		
Column	:DB-5 (Length 30 m, 0.25 mm I.D., df=1.0 μm)		
[GC]		[MS]	
Injection Temp.	:280 °C	Interface Temp.	:280 °C
Column Oven Temp.	:100 °C (4 min) → (4 °C /min) → 320 °C (0 min)	Ion Source Temp.	:200 °C
Injection Mode	:Splitless	Tuning Mode	:Standard
Sampling Time	:1 min	Acquisition Mode	:Scan / MRM
Flow Control Mode	:Linear velocity (39.0 cm/sec)	Scan Mass Range	:m/z 45 - 600
Injection volume	:1 μL	Scan Event Time	:0.2 sec
		Scan Speed	:3,333 u/sec

MRM monitoring m/z

Compound name	RT (min)	Quantitative Transition		Qualitative Transition	
		Precursor>Product	CE (V)	Precursor>Product	CE (V)
Lactic acid-2TMS	7.51	219 > 149	8	219 > 191	5
Glycerol-3TMS	14.711	218 > 159	6	218 > 113	14
Glutaric acid-2TMS	18.827	158 > 116	8	158 > 101	15
Adipic acid-2TMS	22.078	275 > 141	8	275 > 111	10
Suberic acid-2TMS	27.76	303 > 109	12	303 > 191	4

[1] I. Matsumoto, T. Kuhara, Mass Spectrom. Rev. 15 (1996) 43.

Analysis Results

Metabolites in rat urine were measured in Scan/MRM mode. The Scan total ion chromatogram and the MRM mass chromatogram are shown in Fig. 1. Figs. 2 & 3 show the mass spectra measured with Scan and the library mass spectra identified through the library search.

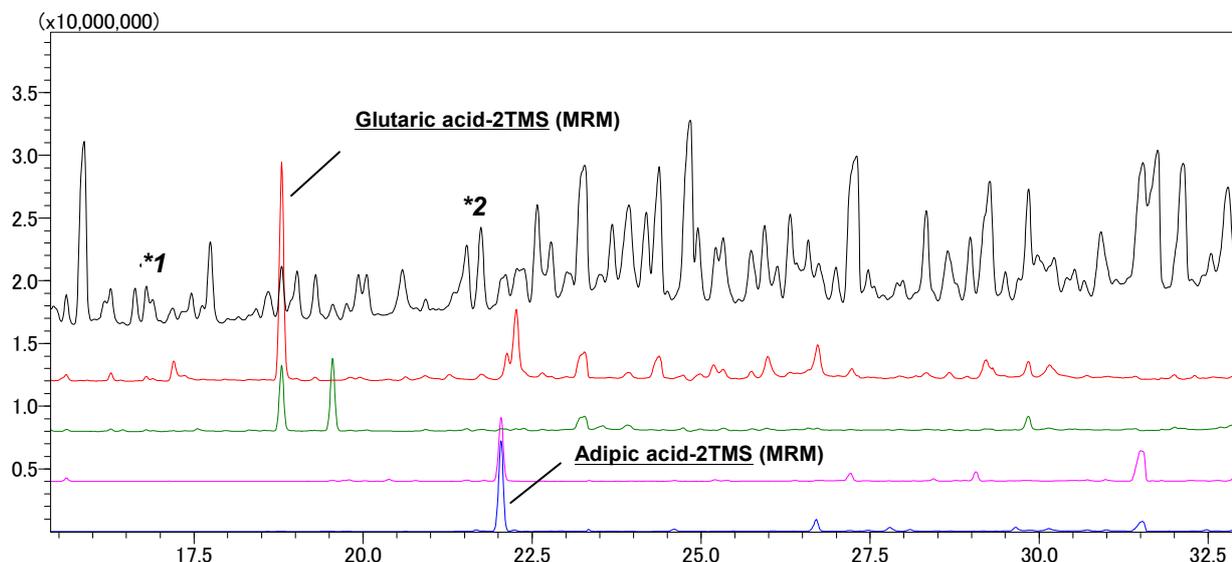


Fig. 1 Scan Total Ion Chromatogram from Scan/MRM Measurement of Metabolites in Rat Urine
Black: Scan Total Ion Chromatogram, Red: MRM Transition 158 > 116, Green: MRM Transition 158 > 101, Purple: MRM Transition 275 > 141, Blue: MRM Transition 275 > 111

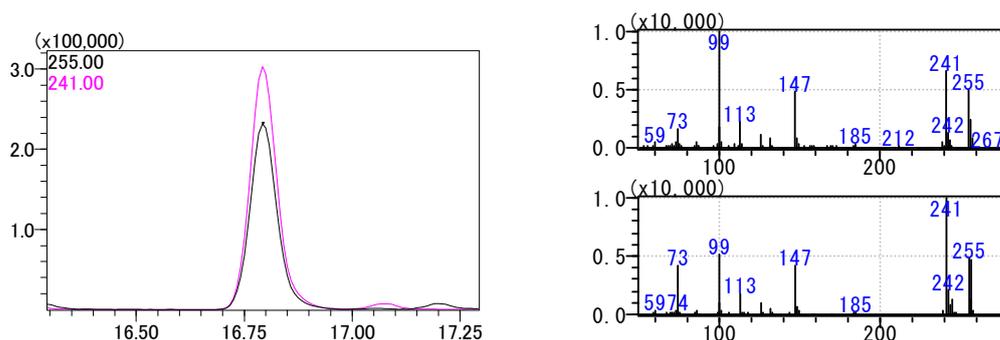


Fig. 2: Scan Mass Chromatogram and Mass Spectra for Uracil-2TMS(*1)
(Upper: Measurement spectrum, Lower: Library spectrum)

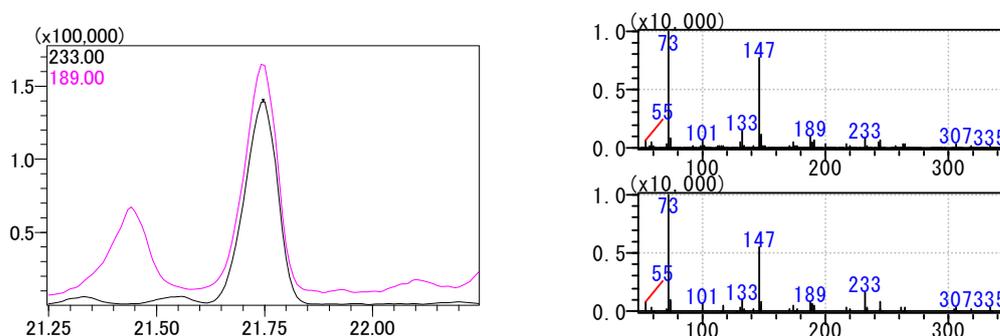


Fig. 3: Scan Mass Chromatogram and Mass Spectra for Malic Acid-3TMS(*2)
(Upper: Measurement spectrum, Lower: Library spectrum)