SHIMADZU

Application Data Sheet

No.60

GC-MS

Gas Chromatograph Mass Spectrometer

Analysis of Metabolites in Rat Urine Using Scan/MRM via GC-MS/MS (1)

The GCMS-TQ8030 is a GC-MS/MS system equipped with Scan/MRM mode to allow simultaneous Scan and MRM data measurements. If Scan/MRM mode is used for simultaneous multicomponent analysis, the number of components targeted for MRM measurement can be minimized since Scan is relatively unaffected by impurities, and also provides ample sensitivity for component measurement. As a result, the investigation of MRM analysis conditions can be kept to a minimum. If method files already exist in which compound information for use in Scan measurements is registered, then Scan/MRM measurements can be easily performed by adding MRM measurement analysis conditions to these method files.
This Application Datasheet introduces results from the measurement of metabolites extracted from rat urine, utilizing Scan/MRM mode with 5 component MRM measurements added to a Scan measurement method from the GC/MS Metabolites Spectral Database.

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. The analysis conditions are shown in Table 1. Measurements were performed with 5 component MRM conditions added to the method file for Scan measurements in which 179 components were registered from the GC/MS Metabolites Spectral Database.

Table 1: Analysis Conditions

GC-MS :GCMS-TQ8030
Column :DB-5 (Length 30 m, 0.25 mm I.D., df=1.0 µm)

[GC]
Injection Temp. :280 °C
Column Oven Temp. :100 °C (4 min) → (4 °C /min) → 320 °C (0 min)
Injection Mode :Splitless
Sampling Time :1 min
Flow Control Mode :Linear velocity (39.0 cm/sec)
Injection Volume :1 µL

[MS]
Interface Temp. :280 °C
Ion Source Temp. :200 °C
Tuning Mode :Standard

Acquisition Mode :Scan/MRM
Scan Mass Range :*m/z* 45 - 600
Scan Event Time :0.2 sec
Scan Speed :3,333 u/sec

MRM monitoring *m/z*

		Quantitative Transition		Qualitative Transition	
Compound name	RT (min)	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, and the total ion chromatogram from Scan is shown in Fig. 1. In addition, the Scan mass chromatograms are shown in Fig. 2, and the MRM mass chromatograms are shown in Fig. 3. Neither the Scan measurements nor the MRM measurements were affected by the impurities.

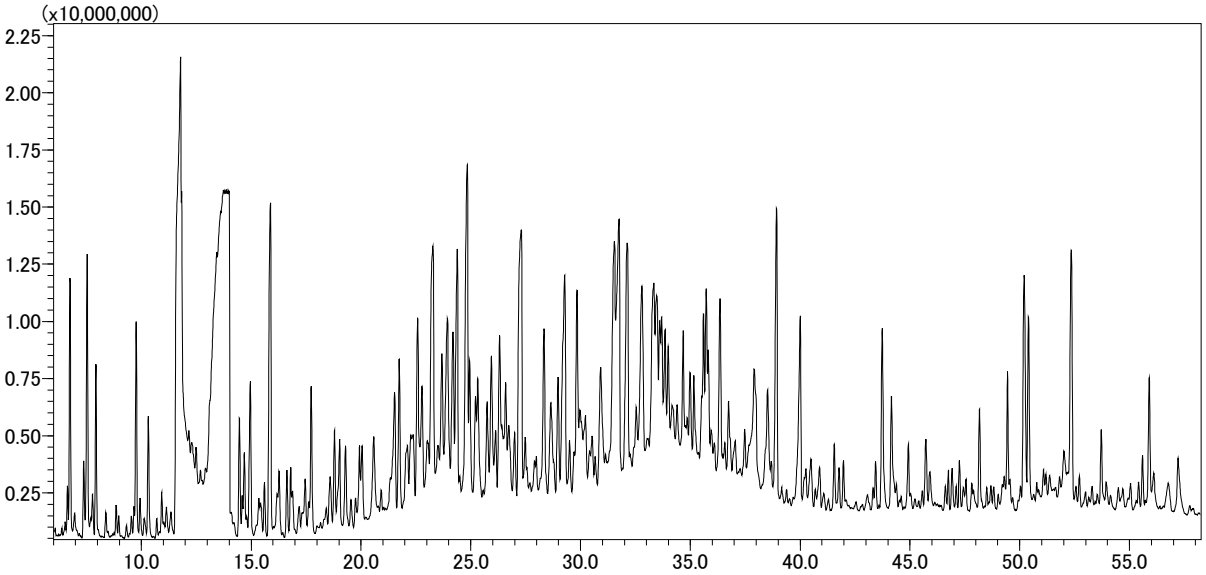

Fig. 1 Scan Total Ion Chromatograph of Metabolites in Rat Urine Measured with Scan/MRM

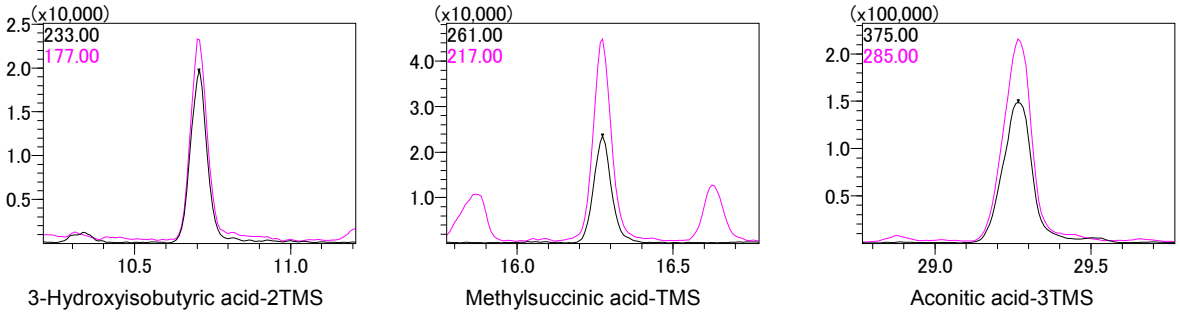

Fig. 2 Scan Mass Chromatogram Comparison of Metabolites in Rat Urine

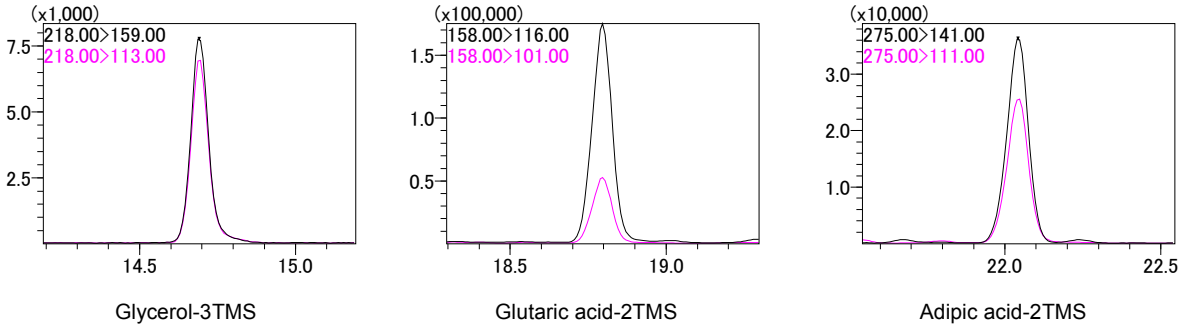

Fig. 3 MRM Mass Chromatogram Comparison of Metabolites in Rat Urine

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