

Application Data Sheet



GC-MS Gas Chromatograph Mass Spectrometer

Analysis of Metabolites in Rat Urine Using MRM via GC-MS/MS

GC-MS provides excellent chromatographic separation, and is capable of highly sensitive and stable measurements. Consequently, GC-MS is widely utilized when measuring low-molecular-weight metabolites in living organisms and performing metabolomic analysis to assess their fluctuations. When analyzing biological samples featuring a large number of matrix components, however, separation from the matrix can be difficult using GC-MS. An alternative is GC-MS/MS, which provides excellent separation performance via MS. In this Application Datasheet, an analysis of metabolites in rat urine is performed using GC-MS/MS. Results comparing this data with GC-MS data are also introduced.

Experimental

Rat urine was treated using the urease-treated direct drying method [1]. The samples were then subjected to trimethylsilylation prior to measurement.

Analysis Conditions

SIM was used as the GC-MS measurement mode and MRM was used for the GC-MS/MS measurements.

Table 1: Analysis Conditions

GC-MS Column	:GCMS-TQ8030 :DB-5 (Length 30 m, 0.25 mm I.D., df=1.0 μm)					
[GC] Injection Temp. Column Oven Temp. Injection Mode Sampling Time	:280 °C :100 °C (4 min :Splitless :1 min	ı) → (4 °C /min) → 32	[MS] Interface T Ion Source Tuning Mo	emp. Temp. de	:280 °C :200 °C :Standard	
Flow Control Mode Injection Volume	:Linear velocity :1 µL	y (39.0 cm/sec)	GC-MS Mo Acquisition SIM Event	ode Mode Time	:SIM :0.3 sec	
SIM monitoring m/	z			GC-MS/MS Acquisition	S Mode Mode	:MRM
Compound name RT (min) Quantitative Qualitative				ve		
Lactic acid-2TM	/IS 7.5	51 219	191			
Glycerol-3TMS	14.7	711 218	205			
Glutaric acid-2	TMS 18.8	827 261	158			
Adipic acid-2TM	/IS 22.0	078 275	185			
Suberic acid-21	TMS 27.	.76 303	217			
MRM monitoring <i>m/z</i> Quantitative Transition Qualitative Transition						
Compound nan	ne RT (min)) Precursor>Produc	t CE (V)	Precursor>Product	CE (V)	
Lactic acid-2TM	IS 7.51	219 > 149	8	219 > 191	5	
Glycerol-3TMS	14.711	218 > 159	6	218 > 113	14	
Glutaric acid-27	TMS 18.827	158 > 116	8	158 > 101	15	
Adipic acid-2TM	AS 22.078	275 > 141	8	275 > 111	10	
Suberic acid-21	MS 27.76	303 > 109	12	303 > 191	4	

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

Analysis Results

A comparison of SIM measurements in GC-MS mode and MRM measurements using the GC-MS/MS mode is shown in Fig. 1. Using the GC-MS SIM mode, the identification and quantification of Glycerol-3TMS and Suberic acid-2TMS compounds are difficult due to matrix effects. In contrast, with GC-MS/MS MRM measurements, the mass separation of matrix effects enabled both identification and quantification.

GC-MS/MS thus proved effective for the analysis of biological samples containing large quantities of impurities.



Fig. 1 Comparison of SIM (Left) and MRM (Right) Mass Chromatograms for Metabolites in Rat Urine



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