

Comprehensive Two-dimensional Gas Chromatograph Quadruple Mass Spectrometer for Plant Metabolite Analysis

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Introduction

Applications of plant metabolomics

- Identification of metabolic engineering targets
- Understanding of stress response
- Genetically modified food certification
- Human nutrition



Characteristics of plant metabolite analysis

Several thousands of target compounds such as organic acids, amino acids, sugars etc. Different concentration levels for each compound

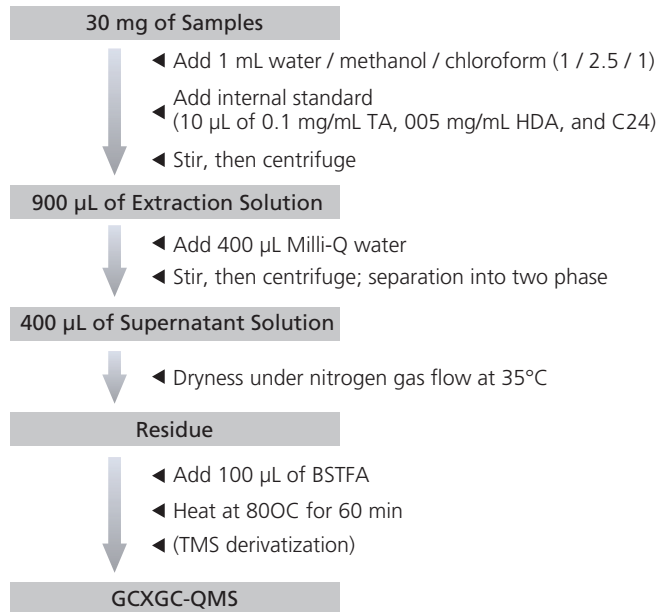
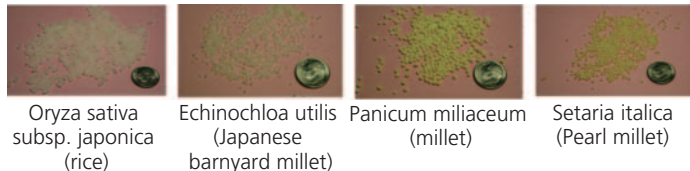


Ultra-high separation efficiency and wider dynamic range required

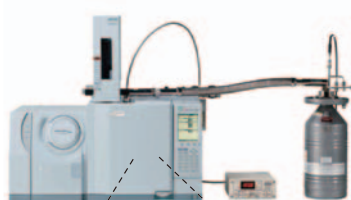


GCxGC-QMS

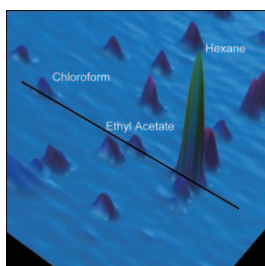
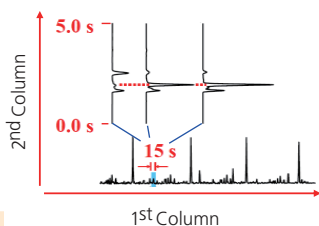
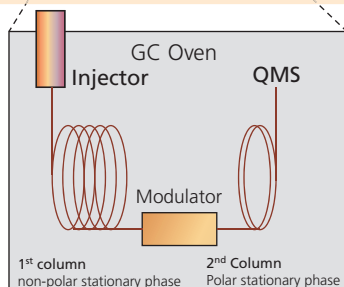
Sample Preparation



Experimental System Configuration of GCxGC-QMS



GC-MS: GCMS-QP2010 Ultra (Shimadzu Corp.)
GC*GC modulator: ZX1-GCxGC modulator (Zoex Corp.)



Analysis Conditions

GCxGC

Column: 1st DB-5 30 m x 0.25 mm I.D., df = 1.0 μ m
2nd BPX-50 2.5 m x 0.1 mm I.D., df = 0.1 μ m
Injection: split (1:50)
Injection volume: 1 μ L
Injection temp.: 280°C
Column temp.: 100°C (4min) \rightarrow 2°C /min \rightarrow 320°C (10 min)
Carrier gas: He (Constant = 150 kPa)
Modulation time: 6 sec

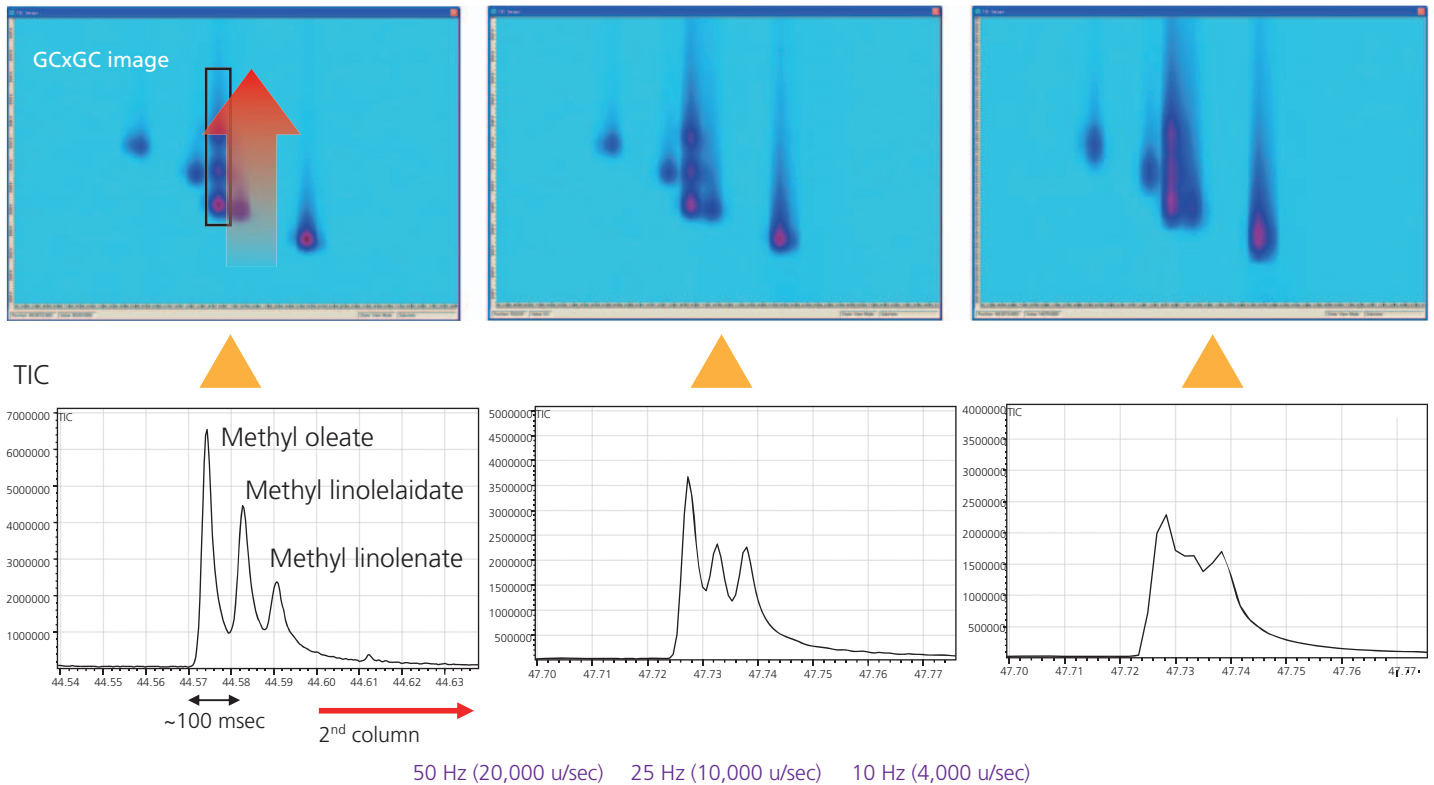
MS

Interface temp.: 280°C
Ion-source temp.: 200°C
Ionization mode: EI
MS mode: scan (m/z 50-500)
Event time: 0.03 sec
20,000 u/sec

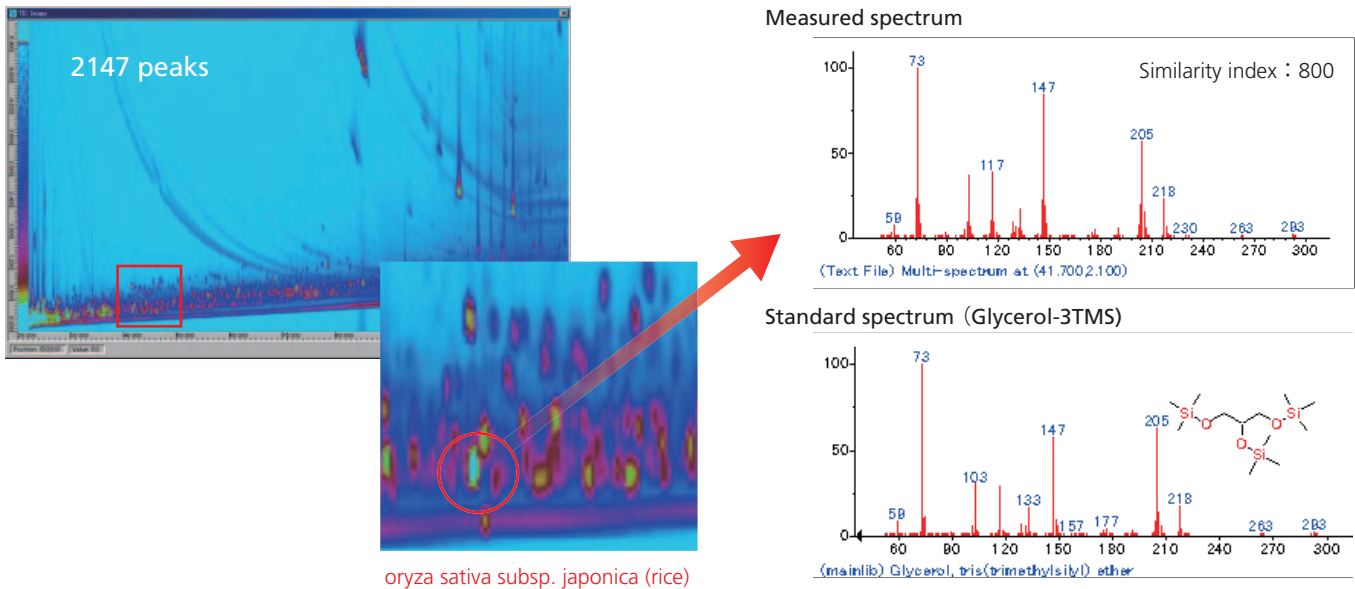
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Results

Scan Interval and Chromatographic Peak Shape

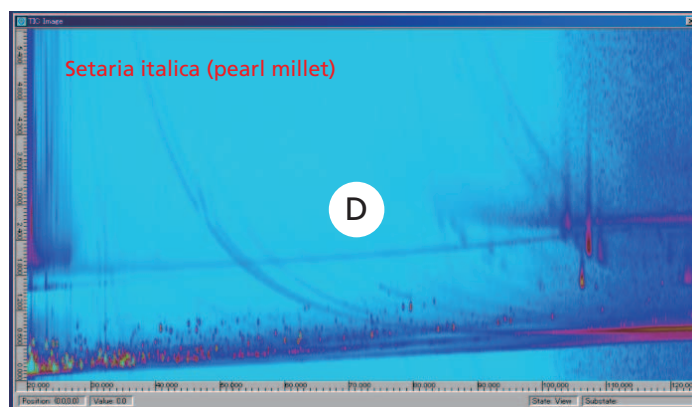
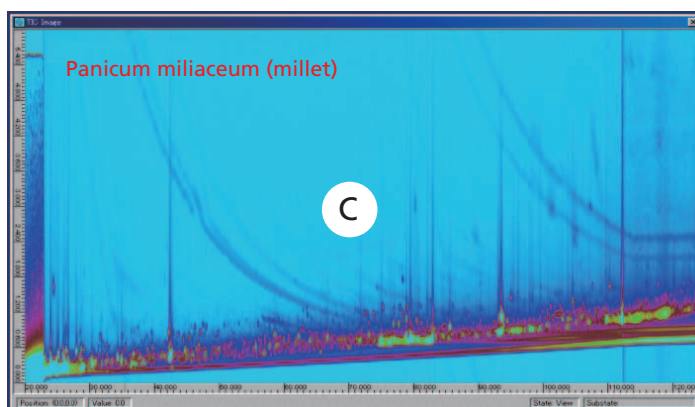
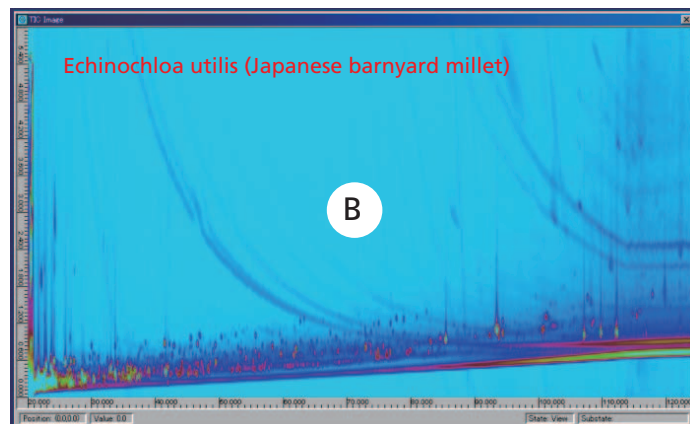
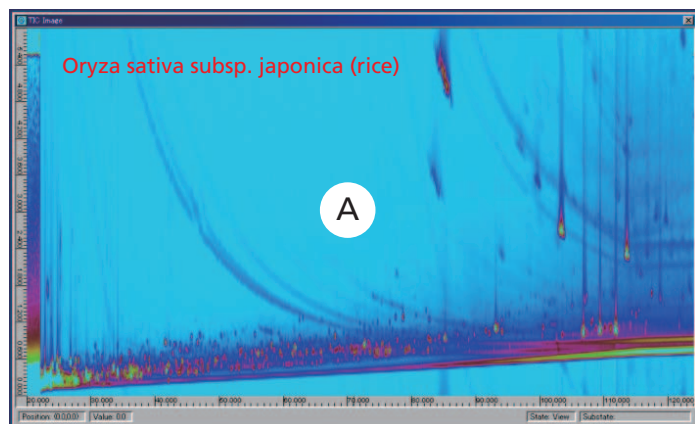


Analysis Results of *oryza sativa* subsp. *japonica*



Although this component was not be separated by 1st column, it was separated by GCxGC.

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Similarity Index	Number of Chromatographic Peaks			
	A	B	C	D
> 800	50	19	80	7
700 - 799	609	368	649	377
600 - 699	1329	1377	1101	1704
500 - 599	158	186	128	245
< 499	1	0	3	0
Total	2147	1950	1961	2333
>600 (%)	92.6	90.4	93.3	89.4

Summary

- A fast scanning quadruple mass spectrometer (QMS) was shown to have a sufficient scan speed to fully characterize the ultra narrow peaks generated by the GC X GC system.
- Using this system, cereal samples (*oryza sativa* subsp. *japonica* (rice), *echinochloa utilis* (Japanese barnyard millet), *panicum miliaceum* (millet), and *setaria italica* (pearl millet)) were analyzed.
- The number of detected chromatographic peaks ranged from 1950 to 2333.
- These results demonstrated the GCxGC-QMS can be effectively used to detect several thousand plant metabolites in a wide concentration range.



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