Application of metabolism techniques using LC/MS and GC/MS profiling analysis of green tea leaves

By: T. OGURA, Y. SAKAMOTO

Instrument: Waters Micromass LCT Preimier Mass spectrometer LC/MS **and** Shimadzu GC/MS system

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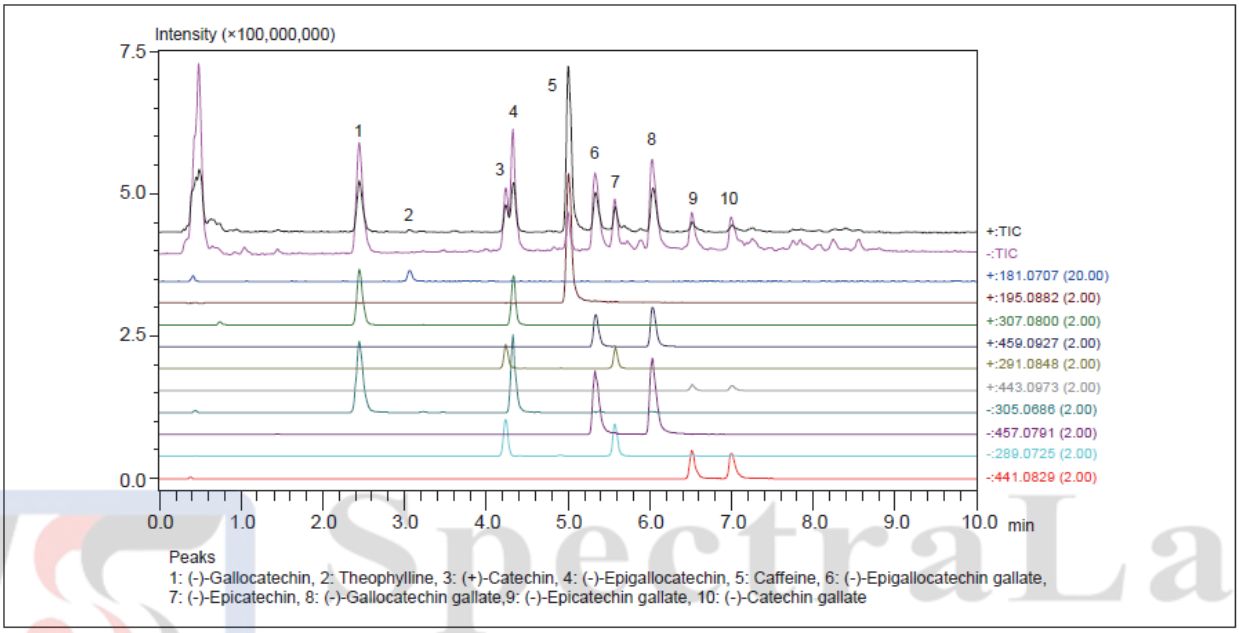
Table 1 LC/MS Analytical Conditions

Instrument	Prominence UFLC series, LCMS-IT-TOF
[LC Conditions]	
Column	Shim-pack XR-ODS (50 mm L. × 2.0 mm I.D., 2.2 μm)
Mobile phase A	0.1 % formic acid aqueous solution
Mobile phase B	Methanol
Gradient program	B concentration 2 % (0 min) - B 60 % (10 min) - B 98 % (10.01 – 14 min) - B 2 % (14.01 min) - (STOP) (19 min)
Flow rate	4 mL/min
Column temperature	40 °C
[MS Conditions]	
Ionization mode	ESI (+ / - switching)
Measurement range	*m/z* 100 - 1000
CDL temperature	200 °C
BH temperature	200 °C

Table 2 GC/MS Analytical Conditions

Instrument	GCMS-QP2010 Plus, AOC-20i + s (auto injector)
[GC Conditions]	
Column	Rtx®-5MS (30 m L. × 0.25 mm I.D. df = 0.25 mm, Restek Corp.)
Injection temperature	250 °C
Column temperature	80 °C (2 min) - (15 °C/min) - 320 °C (20 min)
Injection mode	Split
Carrier gas	He (Constant Linear Velocity)
Linear velocity	36.8 cm/sec
Split ratio	25 : 1
Injection volume	1 μL
[MS Conditions]	
Ion source temperature	200 °C
Interface temperature	250 °C
Measurement range	*m/z* 50 - 1000
Event time	0.2 sec
Scan speed	5000 μ/sec



Chromatogram of Caffeine, Theophylline, and Catechins in Commercially Available Green Tea Beverage

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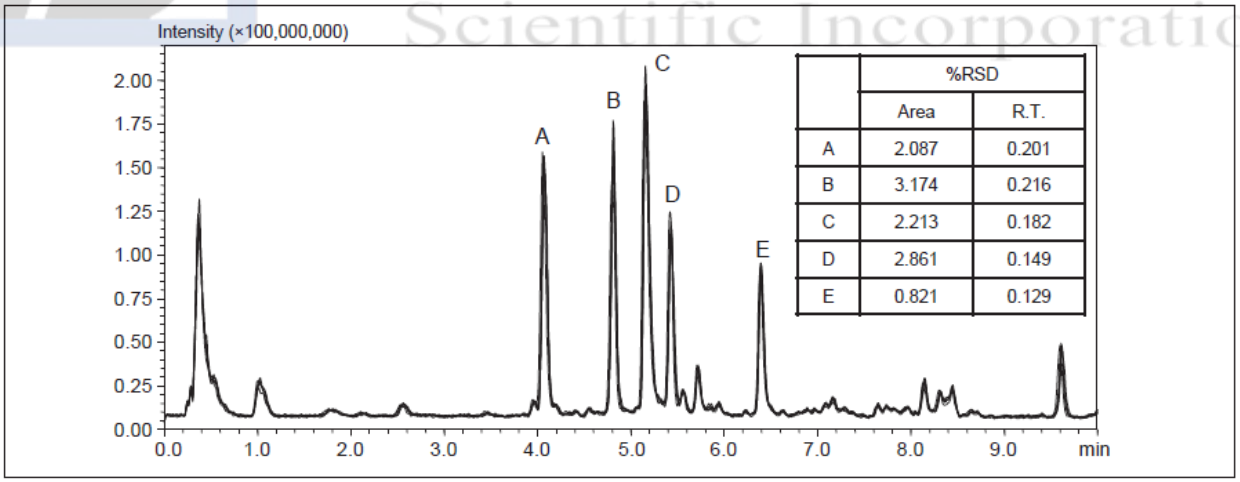

	%RSD	
	Area	R.T.
A	2.087	0.201
B	3.174	0.216
C	2.213	0.182
D	2.861	0.149
E	0.821	0.129

Overlaid Chromatograms of Green Tea Leaf Sample (Analysis Results at 1st, 20th, 40th, 60th, 80th Measurement)

References:

1) http://www2.shimadzu.com/applications/GCMS,LCMS/laancxxe011.pdf
2) Fukusaki, E.; Possibilities and Technological Obstacles in Metabolomics. Biotechnology 2006, 84, 231-234
3) Pongsuwan, W.; Fukusaki, E.; Bamba, T.; Yonetani, T.; Yamahara, T.; Kobayashi, A. Prediction of Japanese Green Tea Ranking by Gas Chromatography/Mass Spectrometry-Based Hydrophilic
Metabolite Fingerprinting. J. Agric. Food Chem. 2007, 55, 231-236.