Shuichi Kawana et al., Metabolomics 2013, 2:7
http://dx.doi.org/10.4172/2153-0769.S1.014

OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference and Exhibition on
Metabolomics & Systems Biology
April 08-10, 2013 Hilton Chicago/Northbrook, USA

Non-target and target analysis of metabolites using Scan/MRM of GC-MS/MS

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Gas chromatography/mass spectrometry (GC-MS) and a gas chromatography-tandem mass spectrometry (GC-MS-MS) are highly suitable techniques for metabolomics analysis due to the high separation power, reproducible retention times and sensitive selective mass detection. If GC-MS provides insufficient separation of some target metabolites, GC-MS/MS has been used to improve mass spectrometric separation. However, multiple reaction monitoring (MRM) mode of GC-MS/MS can be applied only to target compound analysis. Therefore, two measurements are required for non-target metabolite (scan) and target metabolites (MRM).

We evaluated a simultaneous scan and MRM data acquisition mode (Scan/MRM) by analysis of urinary organic acids. GCMS-TQ8030 (Shimadzu, Japan) was used as GC-MS and GC-MS/MS. Urinary samples were treated following the direct unease method and were subjected to trimethylsilyl (TMS) derivatization prior to analysis.

In the scan data obtained by Scan/MRM, 307 peaks were detected, 147 showed less than 20%RSD for repeatabilities of the peak area of mass chromatogram, and 99 were identified at high hit score by mass spectrum library search. In the MRM data, %RSD of the repeatabilities was improved from 10.77-50.94 to 0.89-9.55% to evaluated 12 components which could not separated by scan mode.

These results demonstrate that Scan/MRM mode is effective in tentative detection of non-target metabolites and precise determination of target metabolites by only one measurement.

Biography

Shuichi Kawana has completed his Ph.D. at the age of 36 years from Department of Pediatrics, Shimane University School of Medicine. He works at Shimadzu cooperation and is in charge of GC-MS. He has published more than 4 papers in reputed journals.

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