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GC-MS GCMS-TQ™ 8040 NX

Application News

GC/MS Metabolomics with Automated Sample Preparation and Measurement followed by AI-assisted Data Analysis and Discussion

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User Benefits

- Peakintelligence™ improves the accuracy of automatic waveform processing.
- The SPL-M100*1 can analyze odor by dynamic HS and metabolomics pretreatment by solid-phase derivatization.
- SPL-M100 automatically completes the next sample preparation (in 15 minutes) while the previous sample is measured by GC, achieving high-throughput analysis in virtually 0 minutes of sample preparation.

■ Introduction

Herbal medicine is a traditional drug therapy developed in ancient China. These chemicals use natural plant and animal-derived ingredients to condition the body. However, as a challenge in Chinese medicine, the taste is bitter and difficult to drink, and various methods have been tried to adjust the taste.

A gas chromatograph mass spectrometer is used to analyze these taste components, which can comprehensively analyze even small amounts of components with high accuracy. However, sample preparations to extract and derivatize these components (hydrophilic metabolites) require much effort, TMS derivatives lack stability over time (appropriate correction methods are required), and data analysis takes time.

This application illustrates an analysis of three commercially available Chinese herbal medicines (n=5) measured with a gas chromatograph mass spectrometer, GCMS-TQ8040 NX, equipped with an online preprocessing automatic device, SPL-M100 (AiSTI Science Inc.) (Fig. 1)[1]. Since simultaneous measurement of TMS derivatization of more than 400 components, such as organic acids and amino acids by GC-MS, can be completed in 23 minutes, while sample preparation by SPL-M100 can be completed in about 15 minutes, the system is designed to automatically prepare the next sample while GC-MS measures the previous sample. For data analysis, we used AI signal processing called Peakintelligence, which performs AI signal processing, to perform more precise peak integrations. Using the time gained from the automation and AI assistance, we performed statistical analysis using the Multi-Omics Analysis Package (Garuda). We used Chatcata (Xi'an Startia Soft Co., Ltd.), a secure generative AI that learns proprietary information (confidential information such as your company's internal documents, etc.) and provides answers (Fig. 2).

Fig. 1 GCMS-TQ™8040 NX with SPL-M100

■ Experimental

Three commercially available powdered herbal medicines (n=5) were used for analysis. Sample preparation was performed using the standard protocol of SPL-M100, and GC-MS simultaneously measured amino acids, nucleic acids, fatty acids, and organic acids with more than 400 components using Multiple Reaction Monitoring (MRM) as the data collection mode with an analysis time of 23 minutes (Table 1).

Table 1 Analytical conditions

GC-MS	
Oven Temp.	: 100 °C (4.5 mins) → (15 °C/min) → 330 °C (1 min) Total 23.0 mins
Carrier Gas	: Helium
Injection volume	: 30 µL

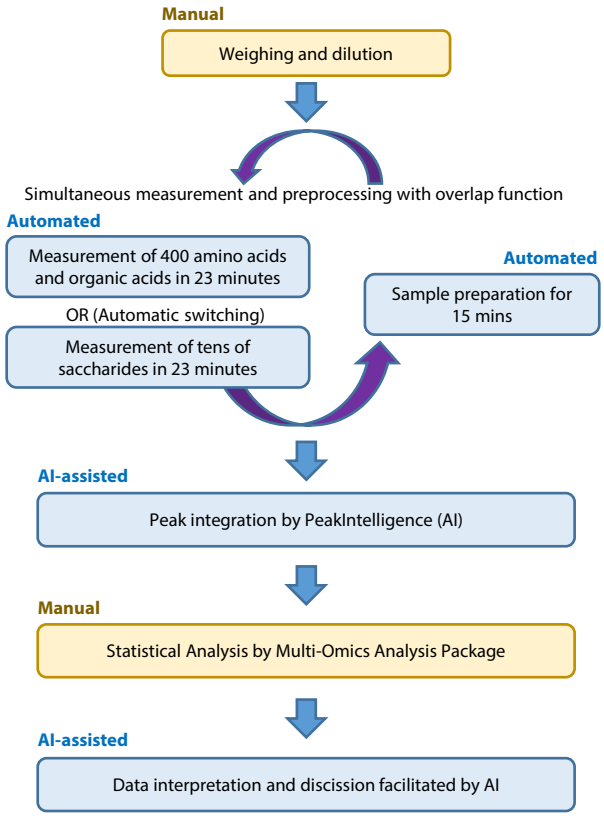

Fig. 2 Workflow from sample weighing to discussion

*1 Please consult Ryoichi Sasano at sasano@aisti.co.jp for SPL-M100 availability in your region/country.

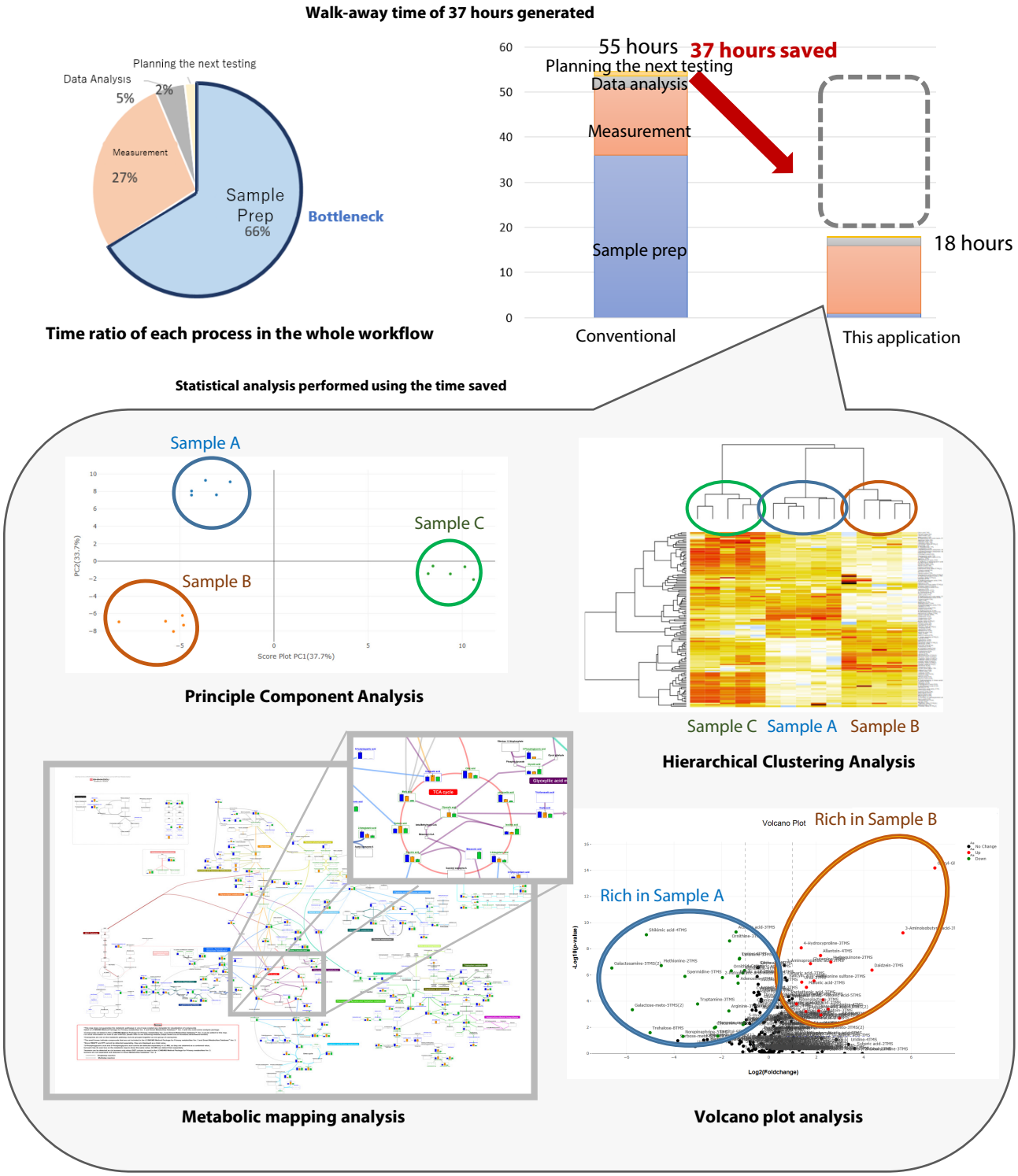

Fig. 3 Statistical analysis performed using the time generated from automation and AI assistance (Multi-Omics Analysis Package)

The advantages of automating sample preparation, which is the rate-limiting step of the conventional method, include not only a reduction in work hours (1.5 days/sample → 15 minutes/sample, 144 times reduction. There is also an improvement in reproducibility because the time between derivatization and injection is fixed for all samples, and there is no need to consider a method to correct the change in TMS derivatization over time by automatically performing derivatization immediately before injection (Fig. 3). In addition, this method is effective against the problem that derivatization becomes unstable and the instrument becomes contaminated when a sample containing a large amount of sugar (e.g., a sweet soft drink) is treated by the conventional method because it has a protocol for cleaning contaminants derived from samples containing sugar.

When the conventional method is put into operation in the laboratory, purchasing a freeze dryer, a centrifuge, a centrifugal concentrator, a warming shaker, and a fume hood is necessary. Thus, it is beneficial to use only the SPL-M100 to complete the sample preparation and to save space by mounting it on top of the GC.

When measuring 30 samples, the conventional method takes 55 hours, but this method takes 18 hours, reducing man-hours by 37 hours. You can perform statistical analysis with a Multi-Omics Analysis Package in the time the automation provides. The multi-omics analysis package is data visualization and statistical software that includes principal component analysis, hierarchical clustering analysis, box plot analysis, volcano plot analysis, and metabolic pathway analysis.

■ Results

About 250 components were detected by measuring 3 kinds of commercial Chinese medicine (n=5). Statistical analysis was performed using a multi-omics analysis package to detect specific components in each Chinese medicine. Using PeakIntelligence*2, we confirmed that we could perform a more accurate analysis by not picking up unwanted peaks and using accurate peak integration (Fig. 4). The analysis effort was reduced from 2.5 hours to 1.75 hours. In addition, we used a generative AI that learned our materials for discussion to eliminate the personalization of discussion work (Fig. 5). When we asked about the benefits of Hypoxanthine, specifically detected in certain Chinese herbal medicines, we received an answer that it is related to the energy metabolism pathway as a purine base. Therefore, we developed an experimental plan to confirm the metabolism pathway of the purine base, leading to the next action.

*2 Peakintelligence cannot learn the user's peak integration. In addition, PC and LabSolutions GCMS for analysis are required separately from GCMSSolution for instrument control. We also offer a 100-day demo license to pre-test the benefits of Peakintelligence on real lab-acquired data.

■ Summary

Three commercially available herbal medicines (n=5) were measured with a gas chromatograph mass spectrometer, GCMS-TQ8040 NX, equipped with an online automatic sample preparation device, SPL-M100. TMS derivatives with more than 400 components, including organic acids and amino acids, were analyzed in 23 minutes.

Automated sample preparation reduced the work hours from 55 hours to 18 hours compared to the conventional method. Using the Multi-Omics Analysis Package (Garuda), we could visualize and analyze the data using principal component analysis, hierarchical cluster analysis, and volcano plots and detect specific metabolites in each sample. Using generative AI that has learned our internal documents, we could reduce the time spent on result interpretation and discussion and quickly plan the next measurement.

<References>

1) メタボローム分析用オンラインSPE-GCシステム SPL-M100 [Online SPE-GC System for Metabolome Analysis SPL-M100], AiSTI SCIENCE Co. Ltd, accessed on Dec 5th, 2023

<Related Applications>

1. Time-saving data processing for pesticide residues with Peakintelligence™ for GCMS, Application News No. 01-00585-EN

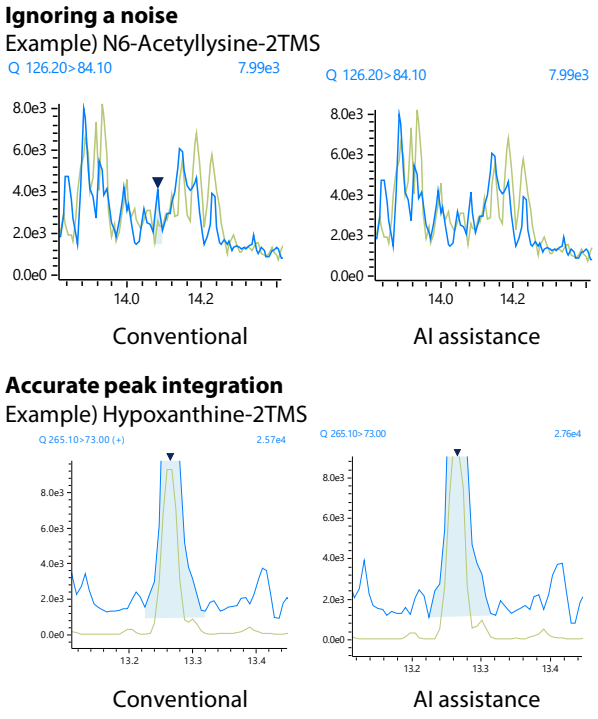

Fig. 4 PeakIntelligence (Peak integration by AI)

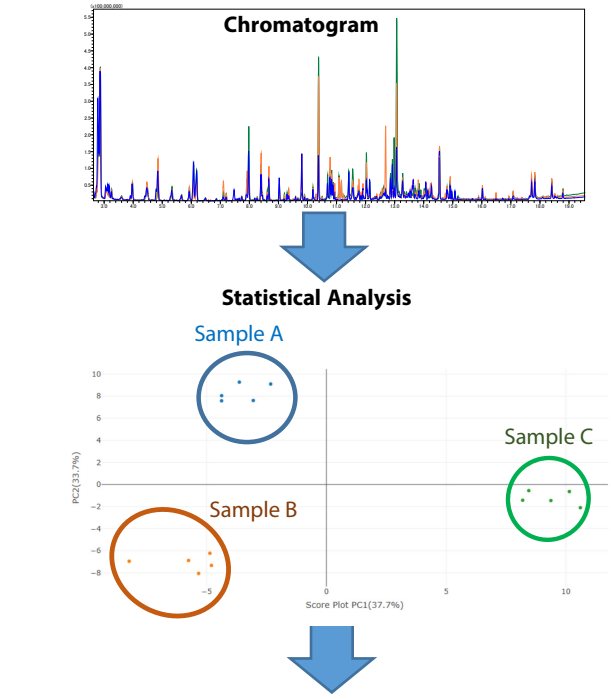

Fig. 5 Result interpretation by a generative AI that has learned internal documents

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01-00719-EN First Edition: Mar. 2024