

GC/MS – Data Analysis

## Shimadzu GC/MS Data Compatibility with Next-Generation Deconvolution Software

### Written by:

Chua Chun Kiang

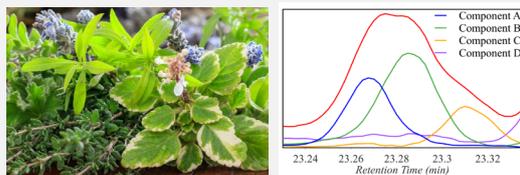
Chia Shao Hua

Udi Jumhawan

Jackie Jackie

### Abstract

Gas chromatography/mass spectrometry (GC/MS) is an indispensable tool in analytical sciences, yet its data analysis solution remains underexplored. The development of multivariate curve resolution (MCR) approach as a next-generation deconvolution tool for GC/MS data has hugely benefitted the community. Deconvolution using MCR approach promises a reduction of false identification, simplifies the analytical workflow and enables novices to generate accurate results. In this Technology Brief, Shimadzu GC/MS data is evaluated on its compatibility for deconvolution analysis using a commercially available MCR-based software. In addition, high scan speed data generated by Shimadzu Advanced Scanning Speed Protocol (ASSP™) technology will be evaluated for suitability for deconvolution analysis. The adoption of such a next-generation deconvolution approach for data analysis could simplify the workflow of fast GC/MS and comprehensive GCxGC/MS.



### Keywords:

*Multivariate Curve Resolution,  
Deconvolution, High Scan Speed  
Mass Spectrometry*

*Shimadzu GC/MS data compatibility with deconvolution software is investigated using natural herb as sample analysis*

### Highlights

- Shimadzu GC/MS data can be deconvoluted with multivariate curve resolution approach to provide confident compound identification
- Data generated with Shimadzu ASSP™ technology at high scan speed of 20,000 u/sec can be effectively deconvoluted with multivariate curve resolution approach
- Multivariate curve resolution approach can assist in reducing false positives and negatives identification

### Technologies Featured

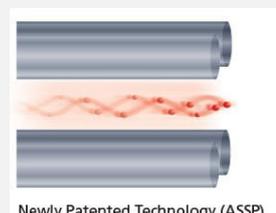
#### GCMS-TQ8050 NX



#### GCMS-QP2020 NX



#### Advanced Scanning Speed Protocol (ASSP™)



Newly Patented Technology (ASSP)

## 1. INTRODUCTION

The analysis of complex samples by GC/MS is often difficult due to the lack of chromatographic separation. Hence, the integration of computational approaches has long been applied to deconvolve components that could not be chromatographically resolved.

AMDIS is a well-known software that deconvolves co-eluting components based on the chromatogram waveform. Differently, the multivariate curve resolution (MCR) approach is tailored to solve the mixture analysis problem by using dimensionality reduction and bilinear models. The development of the MCR approach for GC/MS data analysis has picked up pace in recent years and numerous software are already commercially available.

In this article, we investigate the compatibility of Shimadzu GC/MS data with one of the MCR-based software available in the market, called SmartDalton™ (ChemoPower Technology, Singapore). Also, the compatibility of the MCR approach in analyzing high scan-rate data will be evaluated.

## 2. EXPERIMENT

### 2.1 Experiment Setup

The natural herb sample was donated. The sample was analyzed with Shimadzu GCMS-QP2020 system, with the SH-Rtx-5MS column (30 m long, 0.25 mm i.d. and 0.25  $\mu\text{m}$  film thickness). The carrier gas was helium with a flow rate of 1.5 mL/min. The analysis was performed in full-scan mode from  $m/z$  35-500. The injection temperature was 250°C with splitless mode. The oven temperature was ramped from 50°C to 200°C over 26 min and held at 200°C for 5 min.

Standard solutions of ethyl acetate, heptane, butanoic acid, octanoic acid, nonenal, bromophenol, and eugenol were prepared in equal ratio without diluent. The mixture was analyzed with Shimadzu GCMS-TQ8050 system, with the SH-Rtx-5Sil MS column (30 m long, 0.25 mm i.d. and 0.25  $\mu\text{m}$  film thickness). The carrier gas was helium with a flow rate of 0.6 mL/min. The analysis was performed in full-scan mode from  $m/z$  29-500. The injection temperature was 280°C with split ratio of 1500. The oven temperature was set to 320°C and maintained at isothermal.

### 2.2 Software and Processing

Experimental data from Shimadzu GCMSsolution were exported to common data format (.CDF). The CDF data were imported into SmartDalton™ software. The deconvoluted mass spectra were matched against an in-house library and the NIST 2020 library using NIST MS Search 2.4 software.

## 3. RESULTS AND DISCUSSION

### 3.1. Resolve Closely Co-eluting Components

One of the most important features of deconvolution software is to resolve co-eluting components with minimal false positives or negatives. Figure 1a shows a portion of the total ion chromatogram (TIC) profile from a natural herb sample. A quick visual inspection of peak X could immediately foretell that numerous components co-elute within this region. However, it is difficult to ascertain the number of co-eluting components with high confidence without a deconvolution software. Subsequent analysis of peak X with SmartDalton™ software unexpectedly showed the presence of three co-eluting components, mainly components A, B, and C (Figure 1b).

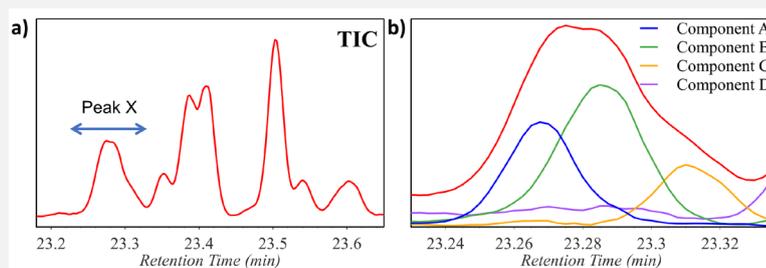


Figure 1. (a) A portion of TIC from herb sample with region of interest – peak X  
(b) Deconvolution result of peak X

Being an MCR approach, the software also provided the corresponding profile of chromatographic background signals as component D. To improve the confidence of analysis, SmartDalton™ software provides a surface plot of raw GC/MS data (Figure 1c) to function as a quality control tool and aids users in detecting false positives or negatives results. The close resemblance of the surface plot profile to the deconvolution result affirmed the accuracy of the MCR approach and hence the compatibility of Shimadzu GC/MS data for use with such a next-generation deconvolution approach.

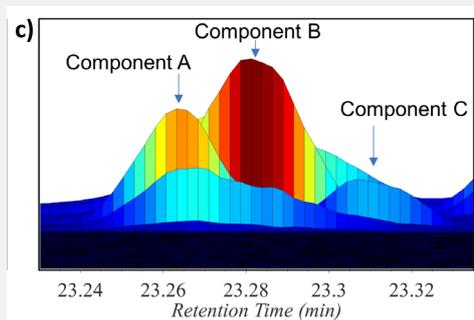


Figure 1. (c) Surface plot of raw data of peak X

Subsequently, the accuracy of the MCR approach on the deconvolution of a severely co-eluting scenario was evaluated. A mixture containing seven compounds, mainly ethyl acetate, heptane, butanoic acid, octanoic acid, nonenal, bromophenol, and eugenol were purposely co-eluted within a chromatographic elution time of 6 seconds. The mass peaks corresponding to each compound are shown in Figure 2. Upon analysis with SmartDalton™, the deconvoluted components were successfully matched against library spectra with average forward and reverse match scores of above 800. Although heptane reported lower match scores, the results were considered adequate given the severely co-eluting scenario as well as the fact that heptane and ethyl acetates share similar fragment ions.

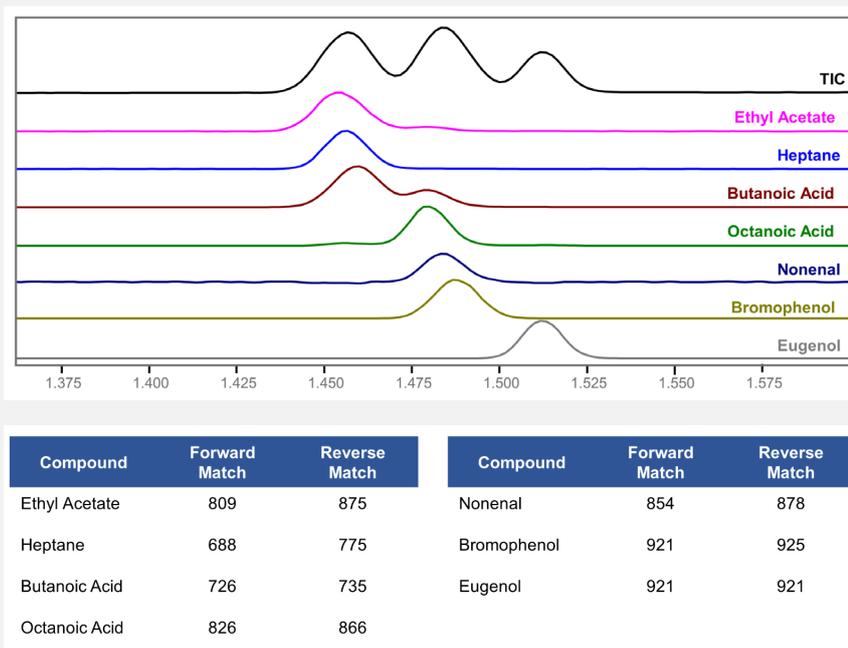


Figure 2. The extracted ion chromatograms of a coeluting mixture of 7 compounds. The table indicated the library forward and reverse match scores of deconvoluted mass spectra for the compounds

### 3.2. Resolve High Scan Rate Data

The rapid development of fast GC/MS and comprehensive GCxGC/MS techniques requires a robust mass spectrometer capable of high-speed scanning control. Shimadzu's Advanced Scanning Speed Protocol (ASSP™) technology is currently able to deliver scan speed up to 20,000 u/sec while maintaining sensitivity and mass spectral integrity. In contrast, a regular mass spectrometer tends to lose sensitivity and mass spectral integrity, i.e., capture a lower amount of fragment ions, at high scan speed. This inevitably causes a less successful library match.

Next, the compatibility of high-scan speed data with SmartDalton™ is evaluated. In fact, data collected at a higher scan speed naturally contains a higher amount of data points, which may not be accurately analyzed by conventional deconvolution software. Figure 3 shows a region of TIC profile of a similar sample collected at scan speeds of 3,333 u/sec and 20,000 u/sec. Even at the maximum scan speed of 20,000 u/sec, the TIC profile was similar to that of a lower scan speed. As seen in Figure 3b, the TIC profiles were successfully deconvoluted into three components, with two components being chemical components and one being a background component. More importantly, the deconvoluted mass spectra of component B from both data were almost identical without loss of essential fragment ions. Remarkably, the library forward and match scores for component B from both data were almost identical. This meant that the MCR-based deconvolution approach is suitable for the analysis of data collected at high scan speed, which will inevitably benefit fast GC/MS and comprehensive GCxGC/MS techniques.

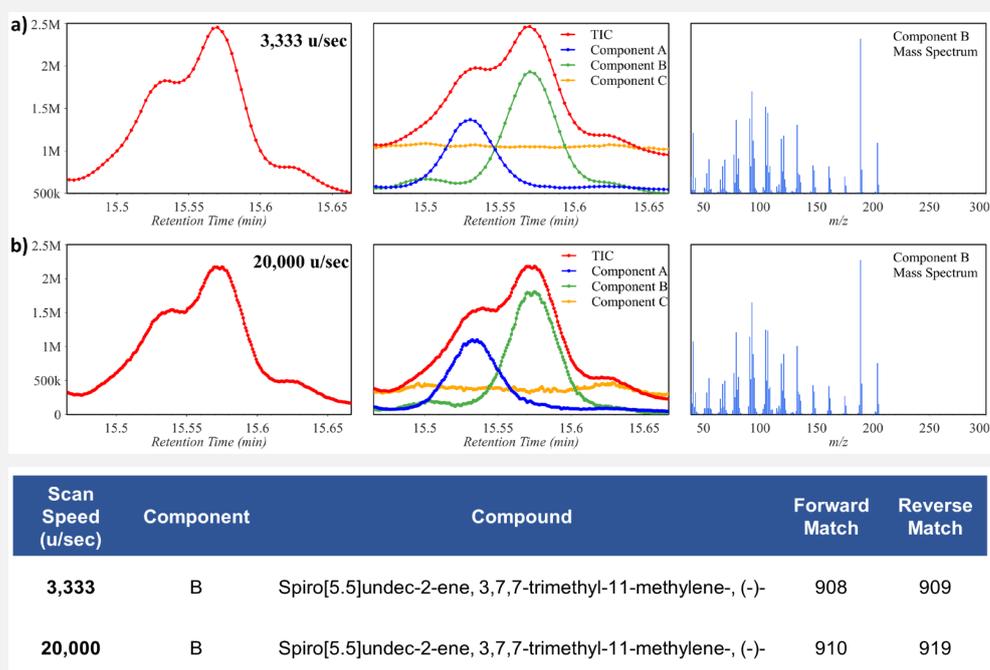


Figure 3. Comparison of deconvolution results between data collected at scan speed of (a) 3,333 and (b) 20,000 u/sec. The table indicated the library match scores for component B of both data

### 4. CONCLUSION

Next-generation deconvolution software based on multivariate curve resolution (MCR) approach, such as SmartDalton™, is capable of processing data collected with Shimadzu GC/MS effectively. The MCR approach can be beneficial to users who would like to extract more information from their data without compromising on accuracy. Also, usage of the MCR approach with high-scan speed data generated by Shimadzu ASSP™ technology could accelerate the adoption of fast GC/MS and comprehensive GCxGC/MS techniques.

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## Ultra-High Sensitivity Triple-Quadrupole GC/MS



GCMS-TQ8050 NX delivers the highest sensitivity for trace-level detection of analytes, on top of being able to handle all types of analysis possible with a triple-quadrupole GC/MS. Equipped with not only revolutionary OFF-AXIS ion optics for high ion transmission and outstanding noise elimination, but the GCMS-TQ8050 NX also features a highly efficient detector capable of performing unprecedented quantitative analysis of ultra-trace amounts.

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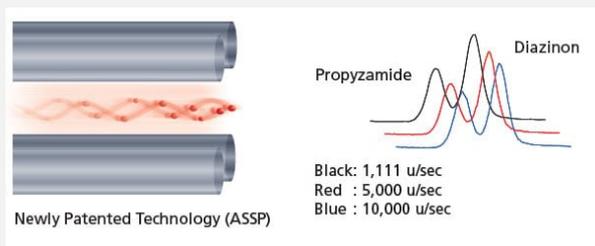
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GCMS-QP2020 NX is the most cost-effective workhorse for sensitive and high-speed analysis of volatiles. This high-end quadrupole GC/MS excels in both ease-of-use and robustness. It boasts the best performance in its class and is a must-have analytical instrument in diverse application areas including routine analysis, environmental pollution monitoring, forensics and material sciences.



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## Advanced Scanning Speed Protocol (ASSP™)



With ASSP™, the rod bias voltage is dynamically optimized during ultrahigh-speed data acquisition, thereby minimizing the drop in sensitivity that would otherwise occur above 10,000 u/sec. With the capability to achieve scan speed of 20,000 u/sec, product ion scans or simultaneous scan and MRM measurement can be performed with high sensitivity and accuracy.

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