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Application News

Gas Chromatograph Mass Spectrometer GCMS-TQ™8040 NX

Time-saving data processing for pesticide residues with Peakintelligence™ for GCMS

T. Sakai, S. Kanazawa

User Benefit

- Peakintelligence for GCMS, which is an option software for LabSolutions Insight™ DB GCMS, can perform rapid and accurate peak integration for the peaks.
- Peakintelligence for GCMS avoids person-dependency due to parameter-free user interface.

■ Introduction

Among a series of the tasks for chromatographers, peak integration is the one that has some difficulty to find it appropriate or not. Most of the public methods or official analytical documents rarely define a strict rule for peak integration. They mostly imply that the peak integration should be performed by a person who has adequate experience and analytical morality. Therefore, peak integration may be a process that has a risk for missing sufficient analytical objectivity.

Adding to that, in multi-components simultaneous analysis that is more and more popular in recent days, analysts are often suffering from taking care of countless peaks. Although most of chromatographic software have an automatic peak detection function, the parameter optimization sometimes causes analysts exhaustion as well as manual peak integration itself.

Peakintelligence for GCMS is an option software for LabSolutions Insight DB GCMS, which is trying to resemble the way of peak integration by professionals. This is totally person-dependency-free because there are no parameters for peak integration.

In this report, this software was utilized for GC-MS/MS pesticide data processing and compared it to the conventional peak integration. The result was fruitful and more accurate peak integration was achieved.

Operating Environment

OS	Windows® 10 Professional
Software	LabSolutions Insight DB GCMS (Ver.3.9 or later) LabSolutions Insight™ CS (Ver. 3.9 SP1 or later)

* Operates on LabSolutions™ DB GCMS (Ver.6.116 or later) or LabSolutions™ CS (Ver. 6.115 or later)
* Peakintelligence for GCMS is available on LabSolutions Insight processing mode.

■ Failures in Automatic Peak Integration

The conventional automatic peak integration works without any parameter optimization for peaks that has sufficient height. (Fig. 1)

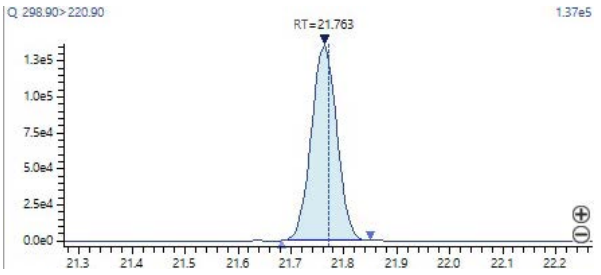

Fig. 1 Peak integration result for a peak which has sufficient height

On the other hand, peak integration result like Fig. 2 is sometimes seen in especially for small peaks. Although the problem is not critical, the integration starting point should be earlier.

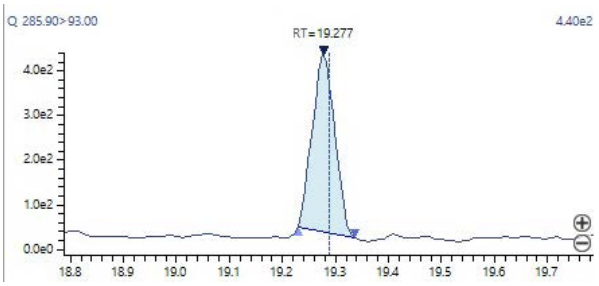

Fig. 2 Peak integration result for a small peak

This is because the parameter which defines the starting point of a peak is not fully optimized especially when the peaks are considerably small.

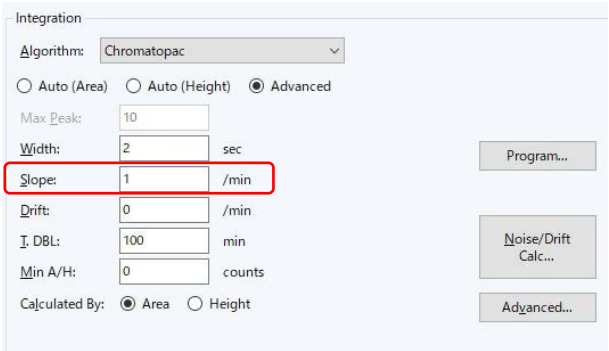

Fig. 3 Peak integration parameters in Chromatpack

However, modifying this parameter for the smaller peaks makes overall peak integration confused because noise level oscillation were detected as peaks, which leads misidentification like shown in Fig. 4

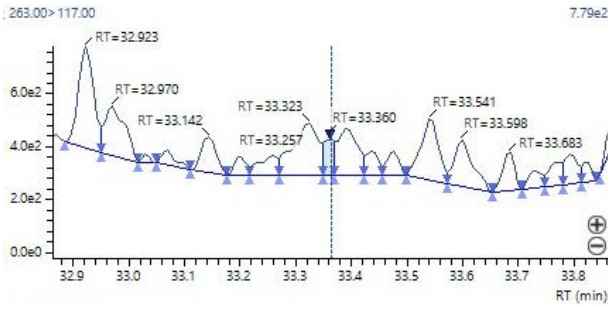

Fig. 4 Integration result when the Slope parameter is low

Thus, integration parameters are useful for automatic integration when they are carefully optimized. However, it sometimes takes a considerable time for optimization itself.

■ Parameter-free automatic peak integration

Peakintelligence for GCMS gets rid of all the parameter settings, using AI algorithm. (Fig. 5)

Arbitrary result difference between analysts will mostly disappear with this parameter-free user interface.

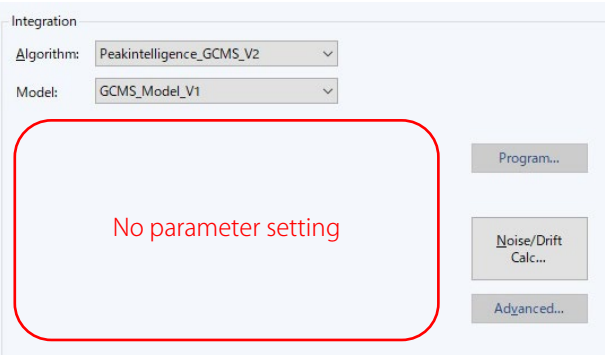

Fig. 5 Parameter setting window in Peakintelligence for GCMS. Peakintelligence for GCMS is not for learning the way of integration.

■ Comparison to the conventional method

The conventional method for peak integration and Peakintelligence for GCMS were compared.

As previously described, it's difficult to define the integration appropriate or not. Hence, some well-experienced analytical engineers judge the integration result, and calculate the ratio of "appropriate" and "inappropriate". The data were from our GC/MS Residual Pesticides Database that focuses on 471 pesticides. Each data has two chromatograms that are quantification ion and reference ion for each compound and two data from these data set that contains 1884 chromatograms were evaluated. The result is shown in Table 1.

Table 1 The result of peak integration (1884 chromatograms)

	Percentage of "appropriately" integrated peaks
Chromatopack (default setting)	89.61%
Peakintelligence for GCMS	98.27%

Although nearly 90% chromatograms were "appropriately" integrated even in Chromatopack, far better result was obtained in Peakintelligence for GCMS.

■ Time comparison to the conventional method

The time consuming for integration processing was compared to the conventional method. Inappropriate peak integration like shown in Fig. 2 must be manually corrected by analysts. In this case, 204 chromatograms in Chromatopack and 34 chromatograms in Peakintelligence for GCMS were inappropriately integrated, respectively. The less inappropriately integrated chromatograms were obtained, the less time takes for data processing

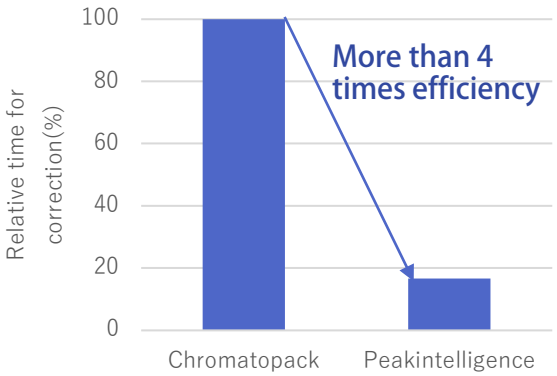

Fig. 6 Schematic image of time efficiency for peak integration

■ Summary

Arbitrary result difference among analysts can be technically excluded with Peakintelligence for GCMS. Adding to this, it reduces time for data processing and achieves more efficiency.

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