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Application News

High Performance Liquid Chromatograph Mass Spectrometer

Efficient Peak Integration for Metabolomics Data Using Peakintelligence™ - Application to Single Quadrupole LC-MS data -

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User Benefits

- The peak processing software Peakintelligence reduces the time and effort required for peak integration.
- With no need to specify parameter settings, it provides the same level of results as experienced users regardless of who performs peak integration.

■ Introduction

In recent years, with the remarkable development of mass spectrometry technology, the number of metabolites being analyzed has increased, and it is not uncommon to analyze more than 100 compounds at once. In the analysis of multi-component and multi-sample data such as metabolomics, it is necessary to visually confirm a large number of peaks, so peak picking takes a long time and is a heavy workload. Even an analysis with a small number of compounds can have a huge cumulative effort if it is repeated in a routine analysis. In addition, human errors and the habits of each person pose risks affecting analysis results, and a peak processing algorithm that can reduce these risks is desirable.

Peakintelligence is peak processing software with algorithms developed using artificial intelligence (AI) for liquid chromatograph mass spectrometers (LC/MS). This article describes an example of using Peakintelligence software to reduce the labor requirement and increase the efficiency of the peak integration process in metabolomics data of single quadrupole mass spectrometers.

Note: R&D for this product was carried out as a collaboration between Shimadzu Corporation and Fujitsu Ltd.

■ Problems with Previous Algorithms

Previous peak detection algorithms required reoptimizing a large number of detection parameter settings for each chromatogram(Fig. 1). If peaks were still not detected properly after that setting optimization, peak detection had to be corrected manually, which was taxing on personnel. Proficiency and standardization of such tasks were also major problems.

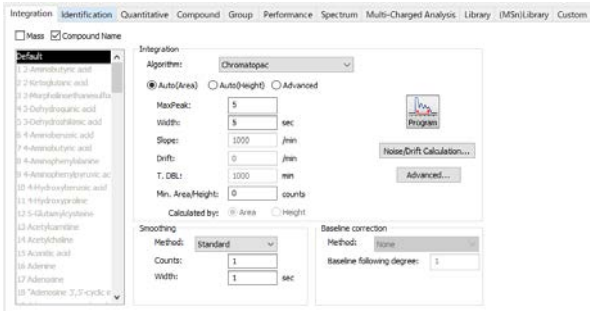

Fig. 1 Previous Peak Integration Parameter Setting Window

■ Peak Integration Algorithm in Peakintelligence

Peakintelligence software is based on new peak integration technology developed using "deep learning," which is a type of artificial intelligence (AI). AI refers to the overall concepts and technologies, whereas "machine learning" and "deep learning" are two types of techniques used for AI (Fig. 2). For machine learning, characteristics to be analyzed and learned must be identified by a person, whereas for deep learning, a machine (computer software) identifies the characteristics to be analyzed. That means large amounts of data can be learned without the variability caused by humans.

For Peakintelligence, about 13,000 chromatograms with peak integration checked by experts were used to prepare a dataset of chromatogram data and peak starting/ending point labels. Then the dataset was used for learning, hyperparameter tuning, and performance evaluation processes to create a pre-taught model, as shown in Fig. 3. That pre-taught model is installed in the data analysis computer and used for automatic LC/MS data analysis.

Note: Peakintelligence does not include functionality for learning from customer peak integration.

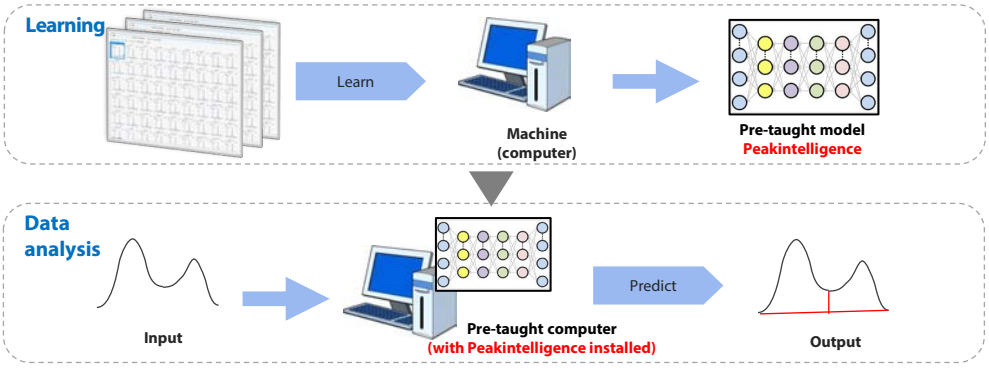

Fig. 2 Illustration of Peakintelligence Software

■ Parameterless Peak Integration

Because Peakintelligence is based on machine-learned peak integration performed by experts, it can achieve data analysis results equivalent to an expert. Unlike previous algorithms, it does not require preliminary parameter setting adjustments.

The parameter setting windows for the previous algorithm and for Peakintelligence are shown in Fig. 3. Peakintelligence peak integration is applied by simply selecting the algorithm in the [Integration] window. There are no complicated parameter settings. That eliminates operator-dependent variability in integration results.

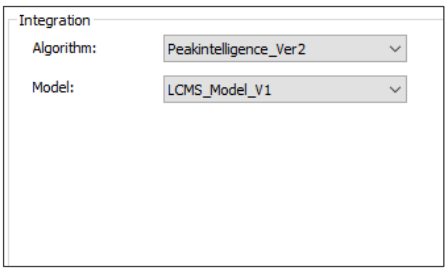

Fig. 3 Parameter Setting Window for Peakintelligence

Fig. 4 and 5 show peak integration examples of previous method(defolt setting) and Peakintelligence. Previous algorism sometimes incorrectly detected the noise as a peak (Fig. 4, left), processed unnecessary vertical splits (Fig. 4, center), or performed insufficient tailing processing (Fig. 4, right). In such cases, there need to be adjusted parametars to appropriate values. On the other hand, Peakintelligence detected correctly close to manual integration by human without setting parameters as shown in Fig. 5.

■ Reduction of Peak Integration Time

As an example, to compare peak integration results with the previous method (Chromatopac), 143 metabolites were analyzed in beer, as shown in Fig. 6. In the previous method, 19 components were incorrectly detected/identified and 12 components needed to be integrated manually. On the other hand with Peakintelligence, these numbers were 3 and 6 components, respectively. Assuming it takes 10 seconds to check each misdetected peak and perform manual peak integration, Peakintelligence would shorten the time required for peak integration of 143 components included in each data set from 5.2 minutes to 1.5 minutes, which is less than 1/3.

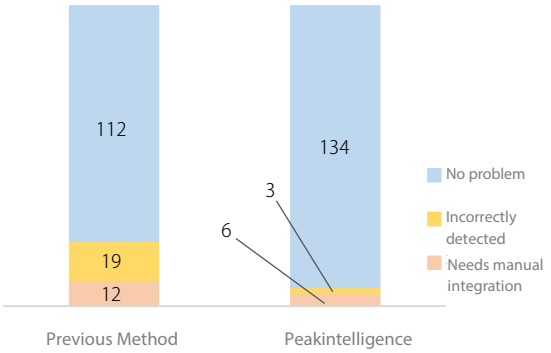

Fig. 6 Comparison of Peak Integration Results for 143 metabolites in Beer

■ Conclusion

Using Peakintelligence for peak integration in analysis of metabolomics by single quadrupole LC-MS eliminated the need for preliminary parameter setting adjustments and significantly reduced the number of incorrectly detected or identified peaks compared with the previous method. Consequently, Peakintelligence can be expected to shorten the time required for peak integration and reduce the burden on operators during peak picking. Because no parameter settings need to be configured, there is no risk of operator-dependent variability in the integration results, which helps eliminate dependence of the results on specific personnel.

Previous method

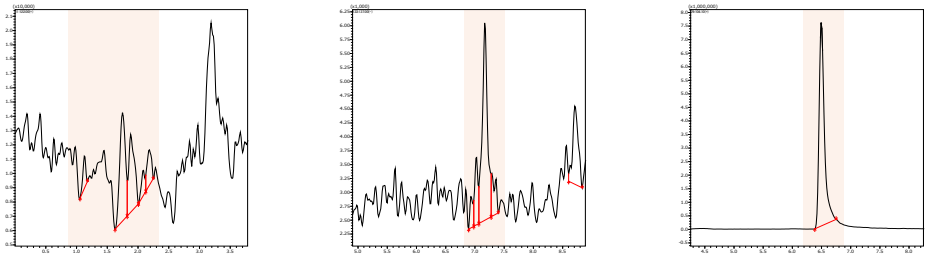

Fig. 4 Example of Peak Integration by Previous method

Peakintelligence

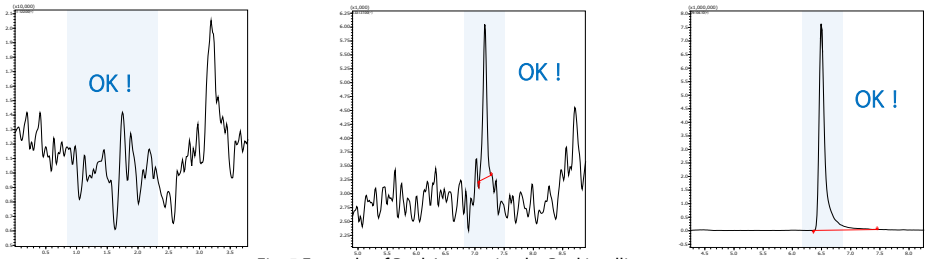

Fig. 5 Example of Peak Integration by Peakintelligence

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