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Application News

LC/MS

Efficient Peak Integration for Analyzing Residual Pesticides in Foods Using Peakintelligence™ LC/MS Peak Processing Software

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User Benefits

- Reduces the time and trouble required for peak integration.
- With no need to specify parameter settings, it provides identical results regardless of who performs peak integration.

■ Introduction

As food imports and exports increase, the number of regulated pesticide types and the maximum residue limits (MRL) in various foods have been increasing as well. Consequently, food safety testing and research institutions need to supply accurate information more quickly.

Data analysis for multiple components or multiple analytes requires visually checking a large number of peaks, which is a very time-consuming and labor-intensive process. Furthermore, due to risks of human errors or the habits of individuals affecting analytical results, there is a need for peak integration methods that minimize such risks.

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 requirements and increase the efficiency of the peak integration process involved in analyzing residual pesticides.

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

■ Peak Integration in Simultaneous Analysis of Residual Pesticides in Foods

The number of pesticides monitored for simultaneous analysis of residual pesticides in foods can vary significantly depending on the type of food, but typically it involves monitoring several hundred components to make sure none of them exceed specified reference values. With many pesticides not detected, personnel must visually check chromatograms to make sure no pesticides are misidentified or incorrectly detected. Given that the process is repeated multiple times for each component in each sample, the total number of iterations is enormous and is very taxing on personnel.

■ Problems with Previous Algorithms

Previous peak detection algorithms required reoptimizing a large number of detection parameter settings for each chromatogram. 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.

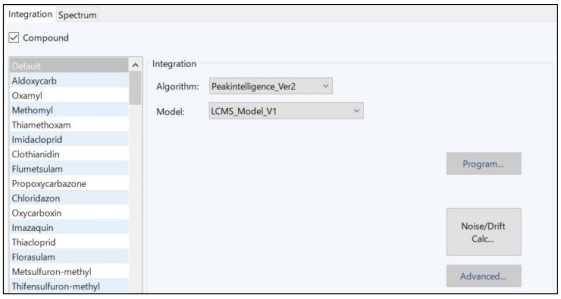

Fig. 1 Previous Peak Integration Parameter Setting Window

■ 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.

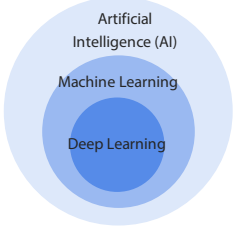

Fig. 2 Illustration of Deep Learning

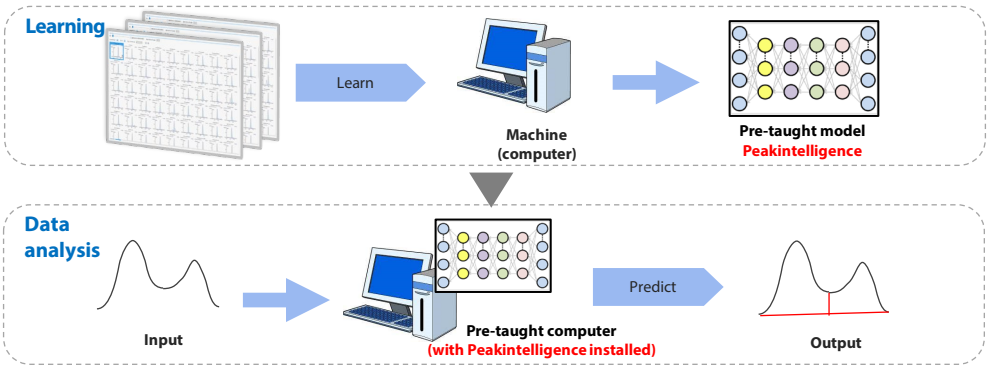

Fig. 3 Illustration of Peakintelligence Software

■ 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. 4. 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.

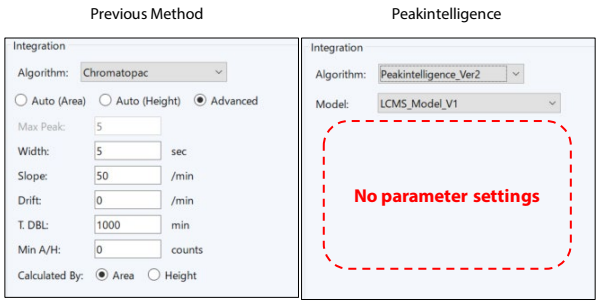

Fig. 4 Parameter Setting Windows for Previous Algorithm and Peakintelligence

Fig. 5 shows some peak integration examples. It shows that peaks with a low S/N ratio and peaks unseparated from contaminant or isomer peaks are properly detected in peak integration results.

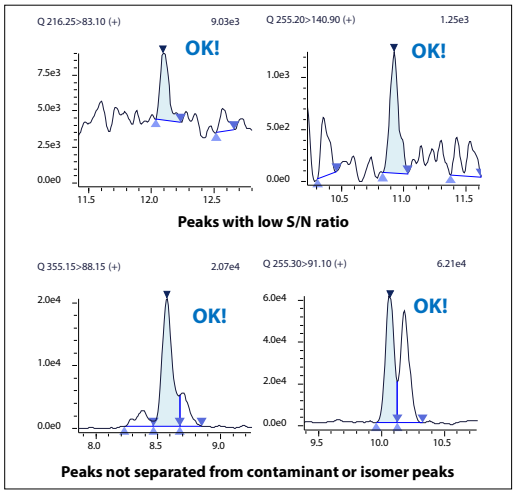

Fig. 5 Example of Peak Integration by Peakintelligence

■ Fewer Incorrectly Detected Peaks Shortens Peak Integration Time

As an example, to compare peak integration results with the previous method (Chromatopac), 157 pesticides were analyzed in soybean extract solution with no pesticides added, as shown in Fig. 6. The previous method incorrectly detected and identified 85 components due to baseline noise or undulations, but Peakintelligence incorrectly detected/identified only 28 components, which represents a decrease to 33 % of the previous method. 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 157 components included in each data set from 14 minutes to 4.6 minutes.

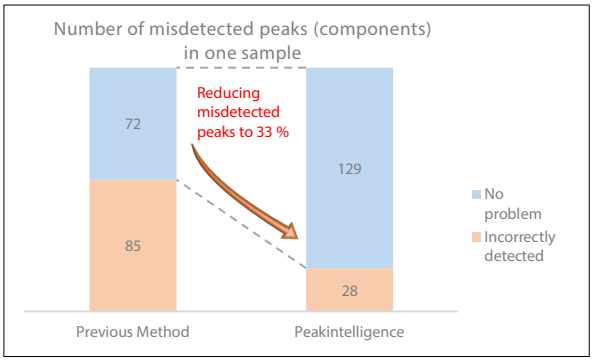

Fig. 6 Comparison of Peak Integration Results for 157 Components in Soybean Extract

■ Conclusion

Using Peakintelligence for peak integration during analysis of residual pesticides eliminated the need for preliminary parameter setting adjustments and reduced the number of incorrectly detected or identified peaks (components) to 33 % of the number incorrectly detected or identified by 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 integration results, which helps eliminate dependence on specific personnel.

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