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Application News

Efficient Data Analysis with Peakintelligence™ —Application for Analyzing Per- and Polyfluoroalkyl Substances (PFAS)—

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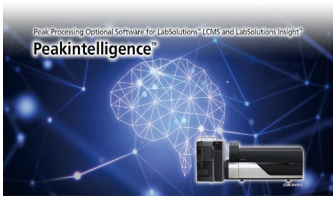
User Benefits

- Peakintelligence peak integration software substantially reduces the time and effort required for data analysis in PFAS analysis.
- Since it does not require parameter settings, Peakintelligence allows even inexperienced users to perform peak integration and achieve results on par with experienced workers.

■ Introduction

Per- and polyfluoroalkyl substances (PFAS) are lyophobic, heat resistant, and chemically resistant compounds used extensively as coatings, surface treatment agents, emulsifiers, and fire-extinguishing agents. Concerns about PFAS and their persistence in the environment, accumulation in living organisms, toxicity to living organisms, and ability to travel long distances have recently led to fact-finding studies on PFAS and the introduction of regulations. As of October 2023, only three PFAS are subject to regulatory restrictions in Japan (PFOS, PFOA, and PFHxS), but more are subject to restrictions in the USA and Europe. Throughout the world, an increasing number of PFAS are expected to require analysis. These changes will create more analytical data that will have to be processed, creating a need for more efficient methods of data analysis.

Peakintelligence is a peak integration software equipped with peak-finding algorithms that have been developed with the help of artificial intelligence (AI). This Application News describes a case example in which it was used to process chromatogram data of PFAS analysis and reduce the effort required and increase the efficiency of the analysis.



- Peakintelligence is a product developed through joint research between Shimadzu and Fujitsu.

■ Limitations of Previous Algorithms

Previous peak integration algorithms required the user to adjust and fine-tune numerous detection and integration parameters based on the chromatogram (Fig. 1). When the algorithms failed to detect and integrate peaks correctly, manual corrections were needed, which increased the workload for users. The skill level required to carry out this work and the challenge of standardizing this process also posed major issues when applying these algorithms.

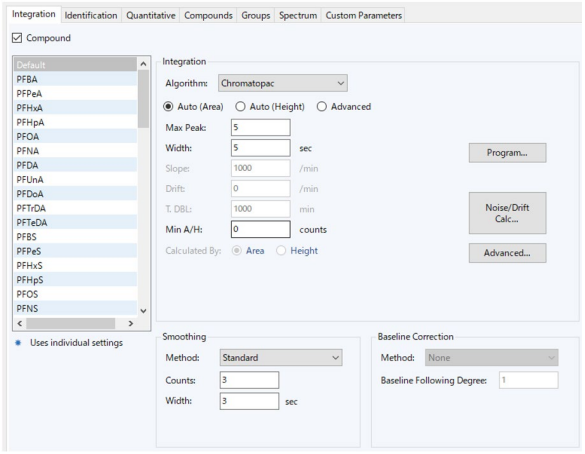


Fig. 1 Parameter Setting Window for Previous Peak Integration Algorithm

■ Peakintelligence Peak Integration Algorithms

Peakintelligence is a new peak integration technology that has been developed using deep learning, a type of AI. AI is the name used for the general concept and technology, while machine learning and deep learning are the techniques on which AI is built. Machine learning trains models with target attributes that must first be extracted by a person, but deep learning trains models with target attributes that are extracted mechanically by software on a computer. For this reason, deep learning can train models with large volumes of data and without the variability caused by person involvement.

The trained model used by Peakintelligence was created from approximately 13,000 chromatograms and with peak detection and integration verified by experienced specialists. A training dataset was prepared by labeling the chromatogram data and peak start and end points, tuning the training and hyperparameters, and assessing model performance (Fig. 2). Installing this trained model on a laboratory PC gives the user the ability to analyze LC-MS data automatically with minimal effort.

- Peakintelligence does not have the functionality to perform additional learning using newly acquired data.

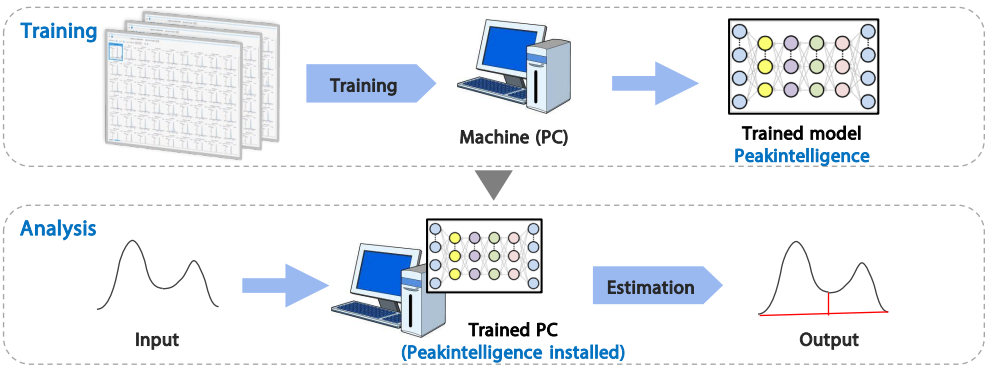


Fig. 2 Illustrative Overview of Peakintelligence

■ Excellent Peak Integration with No Parameter Adjustment

Because Peakintelligence is machine-trained with chromatograms processed by experienced specialists, it can analyze peaks to the same standard as experienced analysts. Unlike previous algorithms, It also requires no prior adjustment of parameters (Fig. 3). Users do not need to set multiple complex parameters. They can process chromatograms with Peakintelligence by simply specifying an algorithm and model. This ability also reduces variability arising from misconfigured parameters and other forms of human error.

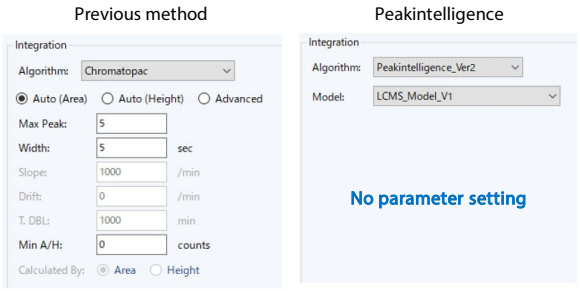


Fig. 3 Parameter Setting Window for Previous Algorithm and Peakintelligence

■ Reduced Data Analysis Times

Industrial wastewater was analyzed for 72 PFAS (31 internal standard substances) and Peakintelligence was used to process the resulting chromatograms. As shown in Fig. 4, it successfully detected and integrated peaks with a poor S/N.

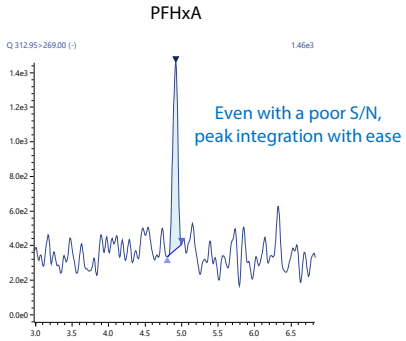


Fig. 4 Example Peak Integration by Peakintelligence

As shown in Fig. 5, the previous method falsely detected baseline noise and undulations, while Peakintelligence detected peaks accurately with no false detections. Processing peaks by the previous method resulted in false detections in 26 of the 72 components, while Peakintelligence showed no false detections for any component (Fig. 6). When a peak is falsely detected, the peak must be removed manually, which increases the analysis time. Peakintelligence required only 45 seconds to analyze a single piece of data compared to 2 minutes for the previous method. Scaled up to 100 pieces of data, Peakintelligence reduces the analysis time from 3.3 hours to around just 1.3 hours, offering substantial savings in labor and time.

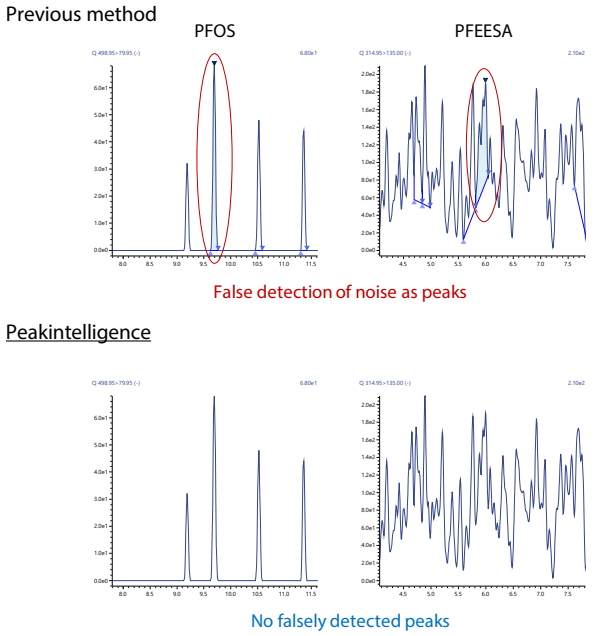


Fig. 5 Comparison of Peak Integration by Previous Method and Peakintelligence

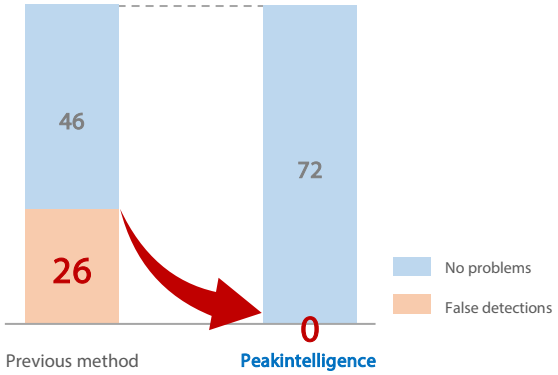


Fig. 6 Comparing Peak Integration Results for 72 PFAS in Industrial Wastewater

■ Conclusion

Using Peakintelligence to process peaks in PFAS analysis substantially reduced the number of false detections and falsely identified peaks. It also significantly reduced the number of peaks that required manual processing, and it did not need pre-analysis adjustment of parameters. These improvements enable substantial reductions in the time and effort required to perform data analysis. Avoiding parameter settings by the user also eliminates variability in the results between users, which helps eliminate dependency on specific personnel. As the number of PFAS requiring analysis increases throughout the world, a more efficient method of analyzing peaks will be needed; Peakintelligence is an effective solution for this need.

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