AI-based peak determination for pesticide analysis

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1. Introduction

The global problem of water pollution is jeopardizing the collective health. It occurs when harmful substances like chemicals or microorganisms contaminate oceans, lakes, streams, rivers or any other body of water, degrade water quality and render it toxic for humans, animals or the environment. In order to measure the multitude of pesticides and toxins in water, the multi-component simultaneous analysis of GCMS is used. Among the tasks for chromatographers, peak integration is the one that has some difficulty to fit in. Most of the public methods or official analytical documents rarely define a strict rule for peak integration.

Therefore, peak integration may be a process that has a risk for missing sufficient analytical objectivity. Peakintelligence™ for GCMS is an option software for LabSolutions Insight™ GCMS, which is trying to resemble the way of peak integration by professionals. This is totally independent of subjectivity, because there are no parameters for peak integration.

2. Methods and Materials

2.1 Injected Sample and System

Mixed standard solutions with concentrations of 0.003, 0.005, 0.01, 0.025, 0.05, 0.1 and 0.5 mg/L were prepared by diluting standard agricultural chemical samples containing 140 types of agricultural chemicals in water. The internal standard samples used at this time were anthracene-d10, 9-bromoanthracene and chrysene-d12. Repeated verification of analytical accuracy was carried out at a concentration of 0.005 mg/L. A GCMS-QP2050 was used with an AOC-30i as autoinjector (Figure 1). Table 1 shows the conditions used in this analysis.

Figure 1: GCMS-QP 2050, AOC-30i/20s U

Table 1: Analysis conditions of the GCMS-QP2050

System	
GCMS model	GCMS-QP2050
Autosampler	AOC-30i
Column	SH-I-5Sil MS (30 m x 0.25 mm ID x 0.25µm); P/N 221-75940-30
Insert	Topaz Liner Splitless Single Taper; P/N 227-35008-01
GC conditions	
Injection mode	Splitless
Injection volume	2 µL
Carrier gas	He
Carrier gas control	Constant velocity (44.5 cm/s)
Column temperature	80 °C (2 min) → 20 °C/min → 180 °C → 5 °C/min → 300 °C (3 min)
MS conditions	
Ion source temp.	230 °C
Interface temp.	250 °C
Data acquisition mode	SIM

2.2 Peakintelligence for GCMS

The multi-analyte quantitation software LabSolutions Insight was used in the data analysis, and Peakintelligence for GCMS was used as the algorithm for peak waveform processing. Peakintelligence is a new AI peak integration algorithm that uses machine learning to simulate the peak integration of experience operators. Peak integration using Peakintelligence does not require parameter setting by the operator and can achieve peak integration results equal to that of experienced operators (Figure 2).

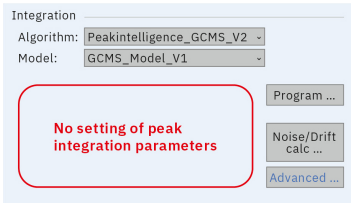

Figure 2: LabSolutions Insight software integration with Peakintelligence for GCMS

3. Results

The SIM chromatograms (Figure 4) at 0.005 mg/L and calibration curves of representative pesticides. Even at this low concentration, sensitivity with a sufficient margin of performance and satisfactory linearity of the calibration curves were achieved by using the GCMS-QP2050. Figure 3 shows the repeatability (%RSD, n=5) of the area ratio of the target pesticides in this analysis. Good results within 5% were obtained for the repeatability of all compounds with an average of 2.21%.

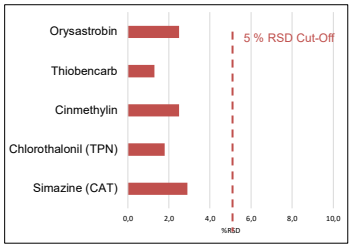

Figure 3: Repeatability of Area Ratio (%RSD, n = 5) of selected compound from 139 in total.

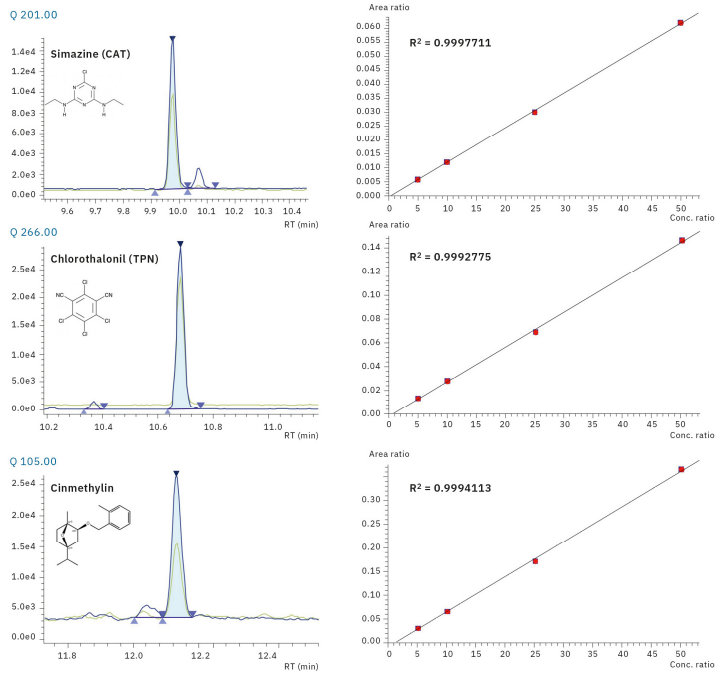

Figure 4: SIM Chromatograms (0.005 mg/L) and Calibration Curves of Agricultural Chemicals in Water

4. Comparison of peak integration by Peakintelligence for GCMS

The results of peak integration by the AI-based software Peakintelligence for GCMS and conventional peak integration algorithm Shimadzu Chromatopac were compared (Figure 5). In conventional peak integration, there were cases in which integration was incorrect, for example, in the low concentration region and when small neighboring peaks exist. In contrast, proper peak integration was possible with Peakintelligence even with these chromatograms. Thus, peak integration by Peakintelligence not only reduces the time required for correction of peak integration but also makes it possible to obtain highly reliable quantitative analysis results by eliminating individual differences between operators.

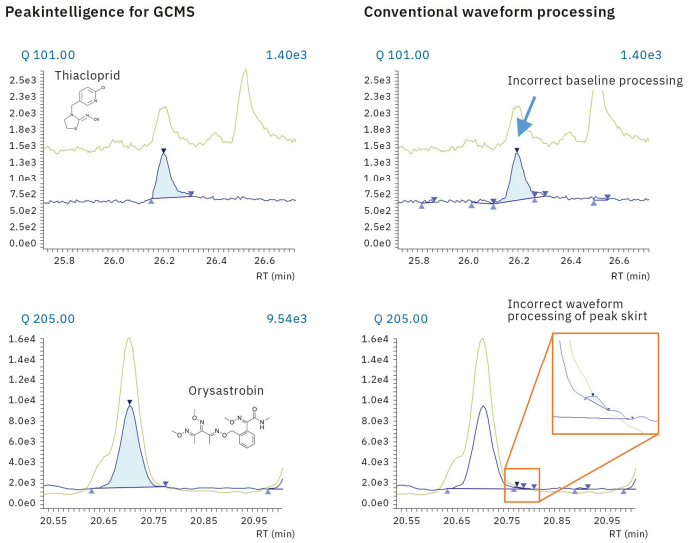

Figure 5: Comparison of Waveform Processing Results by Peakintelligence for GCMS and Conventional Waveform Processing

5. Improved results thanks to great sensitivity and Peakintelligence

The GCMS-QP2050 achieved excellent sensitivity and quantitative analysis accuracy in a multi-component simultaneous analysis of pesticides in water. In peak integration, highly accurate results were obtained, and processing time was substantially reduced by using the AI-based software Peakintelligence for GCMS. It may also be noted that the GCMS-QP2050 demonstrates high performance when hydrogen is used as the carrier. In that case, selection of a turbomolecular pump (TMP), which enables a higher evacuation rate, is recommended. The GCMS-QP2050 with its superior performance in multi-component simultaneous analysis and higher efficiency hereby contributes to identifying pesticides in water and creates the basis for purification and a cleaner and safer environment.