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GC-MS GCMS-QP™2050

Application News

Simultaneous Analysis of Pesticides in Water Using GCMS-QP2050 and AI Peak Integration

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User Benefits

- The GCMS-QP2050 entry model offers excellent cost performance, and boasts high sensitivity and high quantitative analysis performance in simultaneous analysis of pesticides in water.
- Peakintelligence™ for GCMS, which enables peak integration by artificial intelligence (AI), allows anyone to obtain the same results as experienced GC-MS operators, and can substantially reduce the time spent in data analysis.

■ Introduction

Regulation of chemical substances, including environmental water and drinking water, is being strengthened worldwide in order to protect human health and the health of animals and plants. As part of this trend, agricultural chemicals are one important class of chemical substances that should be monitored, as they are widely used worldwide to control weeds and insect pests and have the risk of eluting into the soil and water resources. Since a wide range of pesticides are used, GC-MS is utilized in measurements of pesticides in water, taking advantage of its superior performance in multi-component simultaneous analysis.

On the other hand, accompanying changes in the business environment, the performance and functions required in analytical instruments are also changing. Higher efficiency in response a shortage of operators and reduction of training costs are examples of these needs. The GCMS-QP2050 represents a new generation of GC-MS with a completely new ion optical system, and boasts high sensitivity, quantitative analysis performance, and durability. High productivity and reliability were also ensured by various support functions that support the work of operators.

This Application News article introduces an example of an analysis of agricultural chemicals in water utilizing the GCMS-QP2050 entry model, which offers excellent cost performance, and AI peak integration.

Fig. 1 Appearance of Instruments (GCMS-QP™2050, AOC-30i/20s U)

■ Samples and Analysis Conditions

Mixed standard solutions with concentration 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 the concentration of 0.005 mg/L (Cadusafos and Piperophos: 0.003 mg/L, Trichlorfon (DEP): 0.025 mg/L). A GCMS-QP2050 (entry-level model) was used as the GC-MS, and an AOC-30i was used as the autoinjector (Fig. 1). Table 1 shows the analysis conditions used in this analysis.

Table 1 Analysis Conditions

[Instrument configuration]	
GC-MS	: GCMS-QP2050 Entry
Column	: SH-I-5MS (30 m × 0.25 mm, 0.25 µm i.d.) (P/N: 221-75940-30)
Insert	: Topaz Liner Splitless Single Taper Gooseneck w/Wool (P/N: 23336)
[GC]	
Injection temp.	: 250 °C
Injection volume	: 2 µL
Injection mode	: Splitless (high pressure injection: 250 kPa)
Carrier gas	: Helium
Flow control	: Constant linear velocity (44.5 cm/s)
Oven temp.	: 80 °C (2 min) – (20 °C/min) – 180 °C – 5 °C/min – 300 °C (3 min)
[MS]	
TMP evacuation rate	: 60 L/s
IF temp.	: 250 °C
Ion source temp.	: 230 °C
Ionization mode	: EI
Acquisition mode	: SIM

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 (Fig. 2).

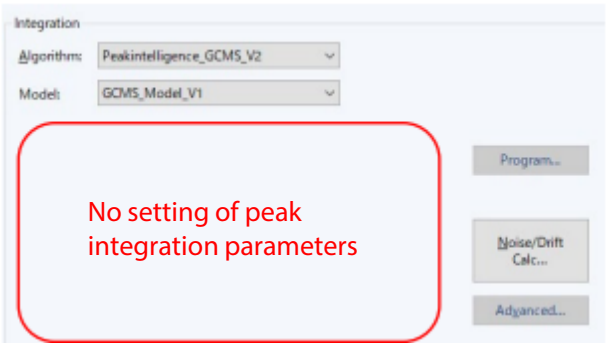
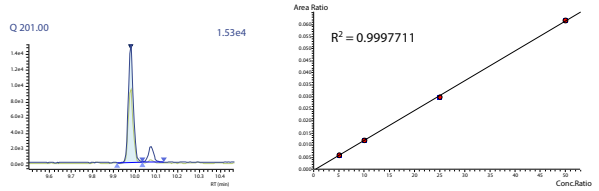


Fig. 2 Waveform Processing Screen of Peakintelligence for GCMS

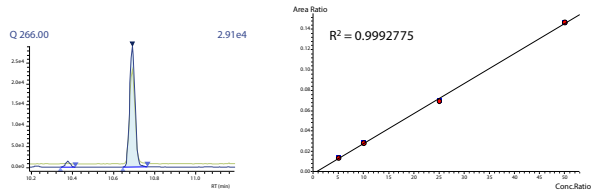
■ Results of Quantitative Analysis

Fig. 3 shows the SIM chromatograms 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. Table 2 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.

Simazine (CAT)



Chlorothalonil (TPN)



Cinmethylin

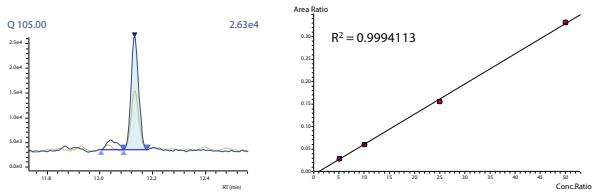
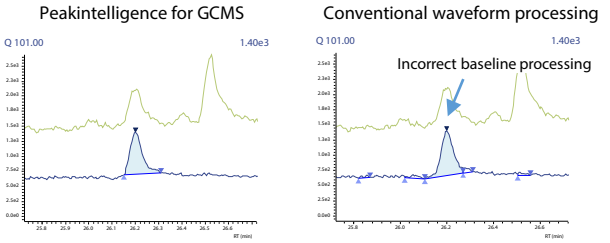


Fig. 3 SIM Chromatograms (0.005 mg/L) and Calibration Curves of Agricultural Chemicals in Water

■ Peak Integration by Peakintelligence for GCMS

The results of peak integration by the AI-based software Peakintelligence for GCMS and conventional peak integration by Shimadzu Chromatopac were compared (Fig. 4). 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.

Thiacloprid (0.005 mg/L)



Orysastrobin (0.025 mg/L)

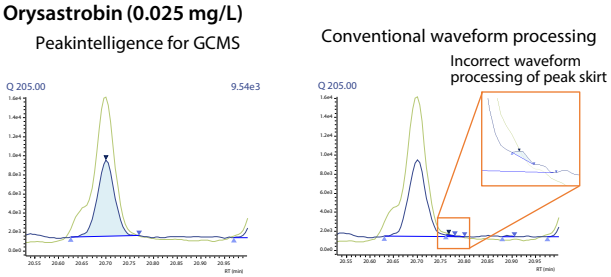


Fig. 4 Comparison of Waveform Processing Results by Peakintelligence for GCMS and Conventional Waveform Processing

■ Conclusion

Excellent sensitivity and quantitative analysis accuracy were obtained in a multi-component simultaneous analysis of pesticides in water using the GCMS-QP2050 entry model. 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 GCMS-QP2050 demonstrates high performance when hydrogen is used as the carrier. When a hydrogen carrier is to be used, selection of a turbomolecular pump (TMP), which enables high evacuation rate, is recommended.

Table 2 Repeatability of Area Ratio (%RSD, n = 5)

Compound name	%RSD	Compound name	%RSD	Compound name	%RSD	Compound name	%RSD	Compound name	%RSD	Compound name	%RSD
Dichlorvos (DDVP)	1.8	Tolclofos-methyl Oxon	1.8	Esprocarb	2.3	Captan	2.3	Buprofezin	2.1	Indanofan	2.7
Dichlobenil (DBN)	1.5	Benfuresate	0.8	Malathon (Malathion)	2.4	Dimepiperate	1.8	Isoxathion	2.1	Bifenox	1.7
Etridiazole (Echlomezol)	2.4	Fenitrothion Oxon	3.0	Chlorpyrifos Oxon	2.9	Procymidone	1.9	Cyproconazole	1.5	Anilofos	3.3
Trichlorfon (DEP)	3.3	Dichlofenthion (ECP)	2.3	Quinoclamine (ACN)	1.8	Butamifos Oxon	1.7	MPP Sulfoxide	2.2	Orysastrobin	2.5
Chloroneb	1.3	Propanil (DCPA)	2.8	Metolachlor	0.8	Triflumizole	2.4	(Z)-Pyriminobac-methyl	2.9	Furametpyr	2.6
Isoprocarb (MIPC)	2.0	Terbucarb (MBPMC)	1.0	Chlorpyrifos	2.9	Methidathion (DMTP)	3.2	Endosulfan β	2.0	(5Z)-Orysastrobin	2.9
Molinate	1.3	Metribuzin	2.8	Thiobencarb	1.3	Propaphos	2.0	MPP Sulfone	3.3	Iprodione Metabolite	2.5
Fenobucarb (BPMC)	1.6	Bromobutide	2.7	(Z)-Dimethylvinphos	1.6	Tetrachlorvinphos (CVMP)	3.6	Mepronil	2.5	Phosalone	2.3
Propoxur (PHC)	1.3	Chlorpyrifosmethyl	2.6	Cyanazine	2.0	Paclobutrazol	1.0	Chlornitrofen (CNP)	2.5	Pyriproxyfen	1.6
Trifluralin	3.2	Malaoxon	2.3	Fenthion (MPP)	2.8	Butachlor	1.9	Ediphenfos	1.9	Mefenacet	0.4
Benfluralin (Bethrodine)	3.2	Simeconazole	2.8	Chlorthal-dimethyl (TCTP)	1.3	Endosulfan α	1.9	Endosulfate	1.9	Cyhalofop-butyl	3.6
Cadusafos	2.5	Tolclofos-methyl	2.1	Isofenphos Oxon	3.3	Butamifos	2.7	Propiconazole -1	2.6	Pyraclofos	1.7
Pencycuron	1.7	Alachlor	1.9	Tetraconazole	2.7	Napropamide	0.6	(E)-Pyriminobac-methyl	2.6	Etobenzanid	1.3
Dimethoate	2.6	Simetryn	1.6	Fthalide	1.9	Flutolanil	2.6	Propiconazole -2	3.2	Cafenstrole	1.8
Simazine (CAT)	2.9	Ametryn	2.4	Fosthiazate -1	2.8	(E)-Metominostrobin	1.9	EPN Oxon	2.8	Boscalid	2.1
Atrazine	1.8	Metalaxyl	1.7	Fosthiazate -2	1.9	Prothiofos	1.8	Thenylchlor	3.3	Etofenprox	1.0
Diazinon Oxon	2.7	Prometryn	2.6	Thiamethoxam	2.6	Isoprothiolane (IPT)	1.4	Tebuconazole	0.8	Thiacloprid	1.2
Cyanophos (CYAP)	2.4	Cinmethylin	2.5	Pendimethalin	2.3	Isoxathion Oxon	2.5	Pyributicarb	1.7	Difenoconazole -1	2.6
Propyzamide	1.8	MPP Oxon	3.4	Cyprodinil	2.7	Pretilachlor	1.7	Acetamiprid	1.7	Difenoconazole -2	2.4
Diazinon	1.7	Dithiopyr	1.2	Dimethametryn	2.1	Uniconazole-P	2.0	Pyridaphenthion	2.0	Pyrazoxyfen	3.4
Pyroquilon	2.0	Pirimiphos-methyl	2.4	Isofenphos	1.8	MPP Oxon Sulfoxide	2.0	Iprodione	2.2		
Chlorothalonil (TPN)	1.8	Fenitrothion (MEP)	2.3	Methyldymron	1.5	Thifluzamide	3.4	EPN	2.8		
Disulfoton (Ethylthiomethon)	4.4	Bromacil	2.8	Prothiofos Oxon	1.7	MPP Oxon Sulfone	1.9	Cumyluron	2.9		
Iprobenfos (IBP)	3.3	(E)-Dimethylvinphos	2.6	Phenthoate (PAP)	2.1	CNP-amino	2.4	Piperophos	2.2		

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