C146-E460C

SHIMADZU
Excellence in Science

Peak Integration Software for LabSolutions Insight

Peakintelligence for GCMS

Peakintelligence™ for GCMS™

Parameter-Free Peak Integration

Frees the user from configuring the parameter settings,
and reduces the time spent on peak integration.

90 % Reproduction of Peak Integration Results by Experienced Users

Achieves high-quality peak integration results,
the same as experienced users.

Shortens the Time Spent on Corrections via Manual Peak Integration

Reduces the time spent confirming and correcting the peak integration results,
thereby reducing the total data processing time.

ANALYTICAL INTELLIGENCE

Equipped with a New AI Peak Integration Algorithm

In mass spectrometry, large amounts of data are routinely acquired from batch analyses with multiple samples and multiple compounds. In recent years, due to improved instrument functionality, both the speed at which data is acquired and the amount of data has increased. At the same time, data processing takes a tremendous amount of time, especially peak integration, because users need to confirm and correct the peak integration results visually and manually. For this reason, it is necessary to improve the efficiency of data processing tasks to deal with the increasing amount of data. Equipped with a new AI peak integration algorithm, Peakintelligence for GCMS significantly shortens the time spent on peak integration in the GC/MS or GC/MS/MS quantitative processing workflow.*1

An AI algorithm trained with peak integration know-how provides peak integration on par with that of an experienced user without configuring / adjusting parameters. In total, the time spent on data processing can be reduced by approximately 75 %.

*1 Patent pending

ANALYTICAL INTELLIGENCE

- Automated support functions utilizing digital technologies, such as M2M, IoT, and Artificial Intelligence (AI), that enable higher productivity and maximum reliability.
- Allows a system to monitor and diagnose itself, handle any issues during data acquisition without user input, and automatically behave as if it were operated by an expert.
- Supports the acquisition of high-quality, reproducible data regardless of an operator's skill level for both routine and demanding applications.

Applications to Metabolite Data

Metabolite analysis measures hundreds of compounds. Confirming the peak integration results and correcting with manual peak integration are bottlenecks in the quantitative processing workflow. Peakintelligence for GCMS achieves peak integration on par with experienced users without configuring the parameter settings, leading to an improved, more efficient workflow.

Product Package

The software is compatible with Smart Metabolites Database™ Ver. 2.
Combining it with the Multi-omics Analysis Package heightens the efficiency of metabolite data analysis tasks.

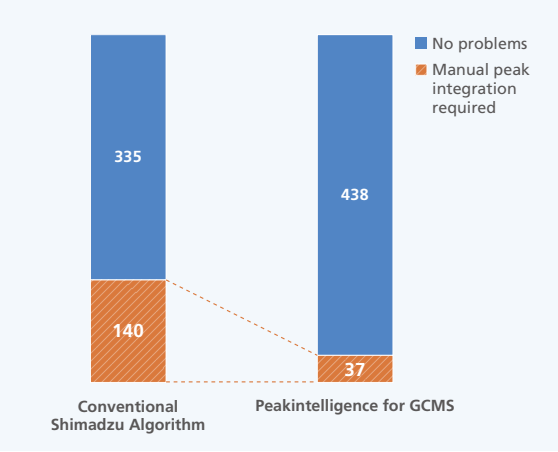
Smart Metabolites Database™ Ver. 2 | Peakintelligence™ for GCMS | Multi-omics Analysis Package

Shortens the Time Spent on Data Processing

In the quantitative processing workflow, users confirm automatic peak integration results visually, and if the results are not correct, they need to correct results via manual peak integration.
Peakintelligence for GCMS reduces the number of compounds requiring correction of peak integration results compared to the our conventional algorithm, and the time spent on correction via manual peak integration is shortened by **approximately 75 %**. (Assuming metabolite data for one sample containing 475 compounds.)

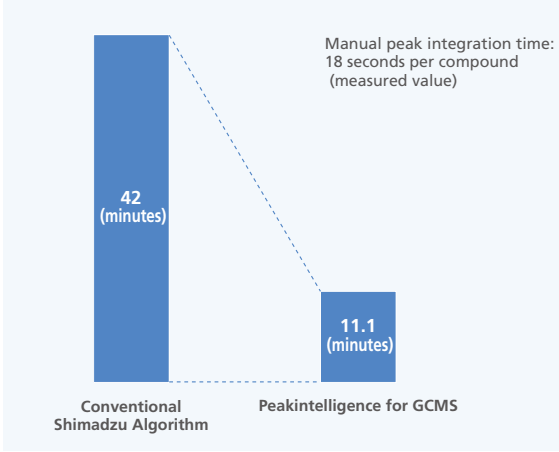
Number of Compounds with Peak Integration Results Requiring Correction

Note: Results from in-house test data



Time Spent on Data Processing

Note: Results from in-house test data

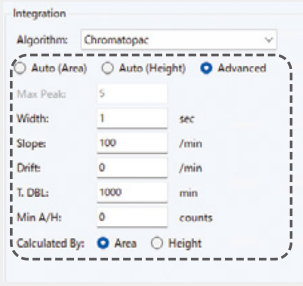


- This product was evaluated using MRM data from an analysis using Smart Metabolites Database Ver. 2.
- Due to the characteristics of the technology used, the reason for the processing results may not be explained.

Peak Integration Examples

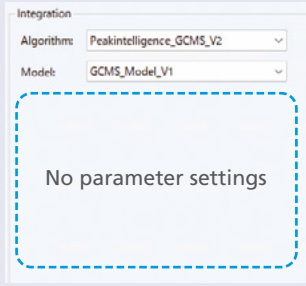
Peakintelligence for GCMS accurately processes data without configuring the parameter settings, even if baseline processing is difficult and multiple peaks overlap. In addition, false detections are suppressed and small peaks are correctly detected, resulting in stable quantitation.

Conventional Shimadzu Algorithm

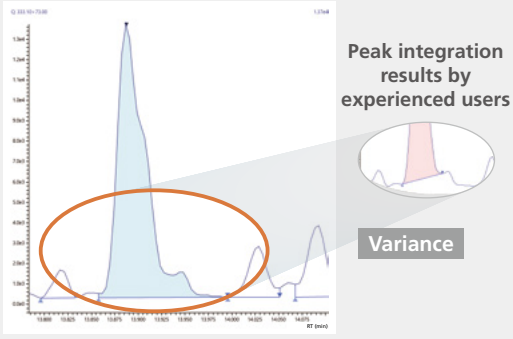


Parameter settings are required.

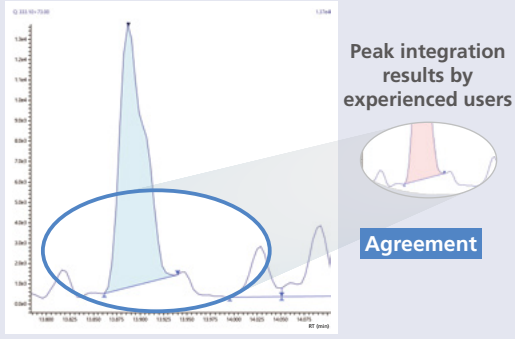
Peakintelligence for GCMS



Galacturonic acid-meto-5TMS (2) in a Banana Sample

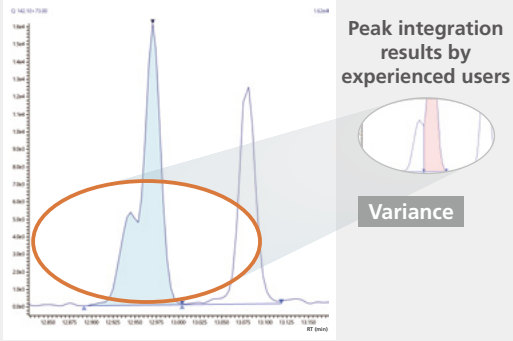


- Parameter configuration and adjustment know-how is required to process the baseline properly.
- If the settings are inappropriate, corrections via manual peak integration are required.

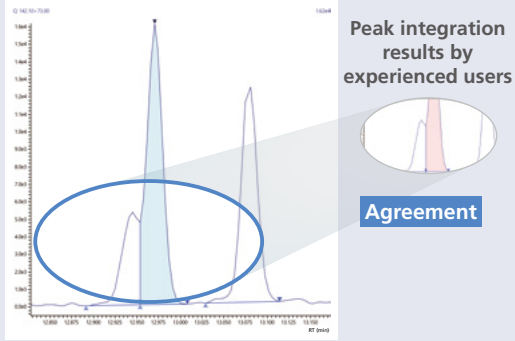


Peak integration results on par with experienced users are achieved without configuring the parameter settings.

Ornithine-4TMS in a Soy Bean Sample



Corrections are required via manual peak integration.



Anyone can perform peak integration on par with experienced users.

Applications to Residual Pesticides Data

Residual pesticides analysis requires the simultaneous analysis of hundreds of regulated pesticides. This makes it difficult to configure and adjust the peak integration parameters and requires a lot of time for correction with manual peak integration. In addition, if the peak areas are corrected via manual peak integration, data falsification may be suspected.
Peakintelligence for GCMS can process large amounts of data quickly and accurately without configuring the parameter settings. This reduces individual differences in the quantitative results and reduces the risk of suspected data falsification.

Time-saving data processing for pesticide residues with Peakintelligence for GCMS.
Application

Product Package

The software is compatible with Quick-DB GCMS Residual Pesticides Database Ver. 2.1 (LabSolutions™), a screening database, and Smart Pesticides Database™ Ver. 2.1 (LabSolutions), a database for quantitative analysis.

GCMS Residual Pesticides Database Ver. 2.1

Smart Pesticides Database™ Ver. 2.1

Peakintelligence™ for GCMS

Applications to Residual Pesticide SIM Data

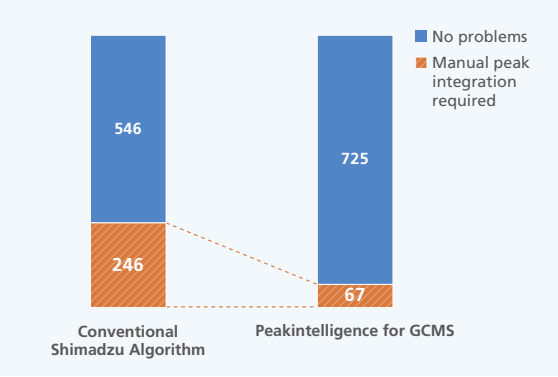
This software can accommodate not only MRM data but also SIM data.

Shortens the Time Spent on Data Processing

In the quantitative processing workflow, users confirm automatic peak integration results visually, and if the results are not correct, they need to correct results via manual peak integration.
Peakintelligence for GCMS reduces the number of compounds requiring correction of peak integration results compared to the our conventional algorithm, and the time spent on correction via manual peak integration is shortened by **approximately 75 %**. (Assuming residual pesticide data for four samples containing approximately 200 compounds.)

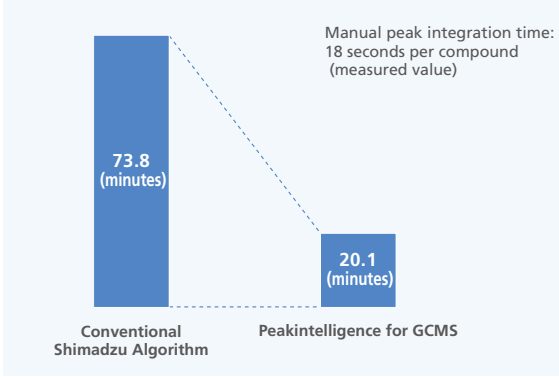
Number of Compounds with Peak Integration Results Requiring Correction

Note: Results from in-house test data



Time Spent on Manual Peak Integration

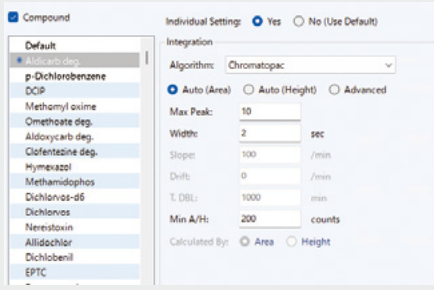
Note: Results from in-house test data



- This software has been evaluated using MRM data and SIM data from analyses with Quick-DB GCMS Residual Pesticides Database Ver. 2.1, a screening database, and Smart Pesticides Database Ver. 2.1, a database for quantitative analysis.
- Due to the characteristics of the technology used, the reason for the processing results may not be explained.

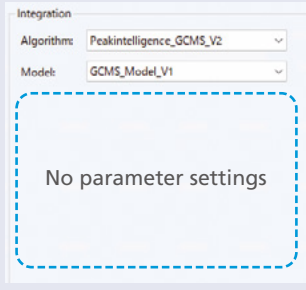
Peak Integration Examples

Conventional Shimadzu Algorithm



The simultaneous analysis of hundreds of regulated compounds.
Adjusting the peak integration parameters for each compound is a tremendous task.

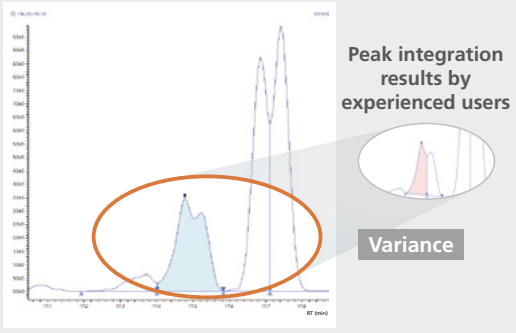
Peakintelligence for GCMS



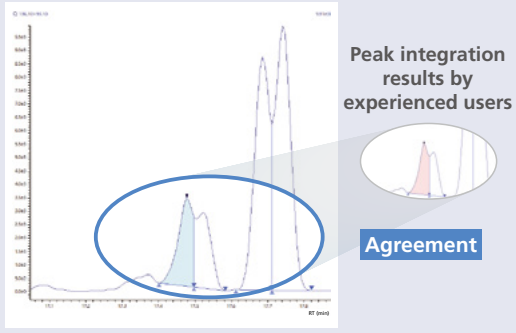
Accurate peak integration is achieved without configuring the parameter settings.

STEP 1: Create a calibration curve with standard samples and confirm the peak integration results.

Allethrin-1 in a Standard Sample



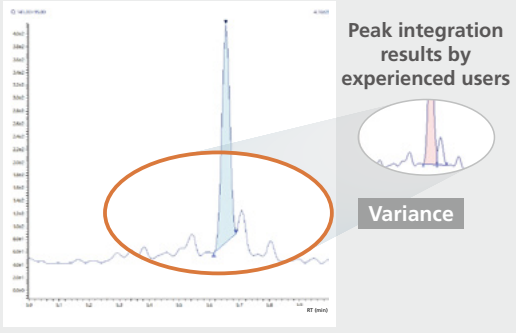
If peaks cannot be separated correctly, corrections via manual peak integration are required.



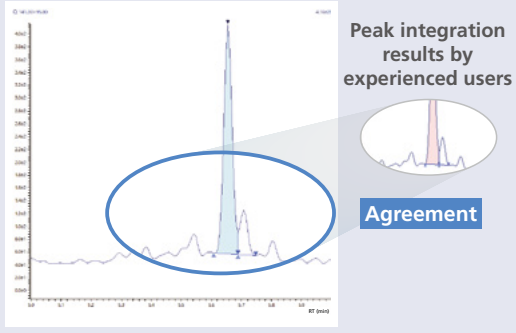
- Achieves peak integration on par with experienced users.
- Corrections via manual peak integration are not required.

STEP 2: Quantitate the actual samples using the calibration curve created.

Methamidophos in a Strawberry Sample



A complicated peak shape due to impurities.
Individual differences occur in quantitative results due to correction by manual peak integration.



- Anyone can perform peak integration on par with experienced users, which reduces individual differences in quantitative results.
- Configuring the parameter settings and performing corrections by manual peak integration are not required, reducing the risk of suspected data falsification.

License Types

- Starter pack
- 1-year license

Peakintelligence, LabSolutions Insight, the Analytical Intelligence logo, Smart Metabolites Database and Smart Pesticides Database are trademarks of Shimadzu Corporation or its affiliated companies in Japan and/or other countries.

Shimadzu Corporation
www.shimadzu.com/an/

For Research Use Only. Not for use in diagnostic procedures.
This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.
Company names, products/service names and logos used in this publication are trademarks and trade names of Shimadzu Corporation, its subsidiaries or its affiliates, whether or not they are used with trademark symbol "TM" or "®".
Third-party trademarks and trade names may be used in this publication to refer to either the entities or their products/services, whether or not they are used with trademark symbol "TM" or "®".
Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The contents of this publication are provided to you "as is" without warranty of any kind, and are subject to change without notice. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication.

© Shimadzu Corporation, 2024 / First Edition: July 2022, 3655-01402-PDFIT, C146-E460C