

Workstation Software Combines Ease of Use and Versatility for Increased Productivity

A GC/MS workstation must incorporate many functions, from data acquisition to qualitative or quantitative data analysis to versatile reporting.

GCMSsolution incorporates these features and more to set a new standard for laboratory productivity.

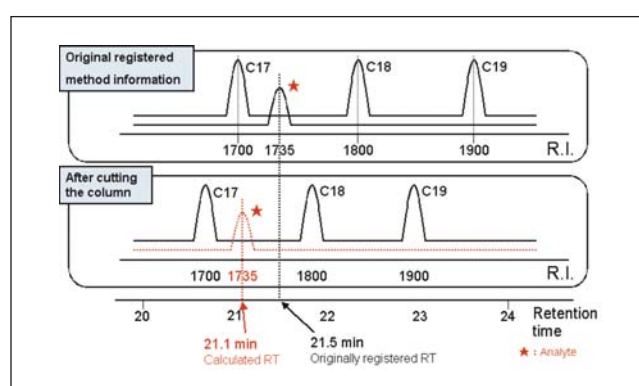
AART (Automatic Adjustment of Retention Time)

Retention times may change as a result of capillary columns being trimmed during maintenance or exchanged with a new one from a different lot. With AART, the retention times of multiple analytes can be easily and accurately adjusted as column age and length change. Method Compound Tables containing a large number of analytes can be easily updated or Methods may be transferred to other instruments easily by using this wizard.

This is accomplished by generating a linear retention index based on an alkane standard mix. Peak tables may then be updated as required without changing the instrument acquisition parameters.

AART Features

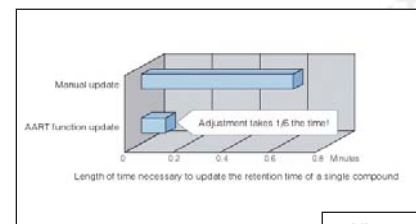
- Retention times of up to 1000 compounds can be updated with analysis of a single n-alkane solution.
- Correction is performed at multiple points from low to high boiling points, enabling accurate correction over a wide range of retention times. The carbon numbers of the alkane series are chosen based on the analytes. Indexing compounds other than alkanes may be used.
- Retention time updating based on analysis of n-alkanes is easily accomplished using the AART wizard function.
- Time correction of SIM acquisition parameters may be updated using AART.
- AART can easily be applied to an existing method by just adding the retention index information to the method.



Sharing a method between instruments is easy.

AART enables easy method transfer between instruments. Retention times may be updated with the analysis of an indexing standard. Then the system is ready for use. Various method packages are available with the compound list and calculations pre-entered.

Note: Excellent correction accuracy is maintained by using the same type of column and the same analytical conditions.



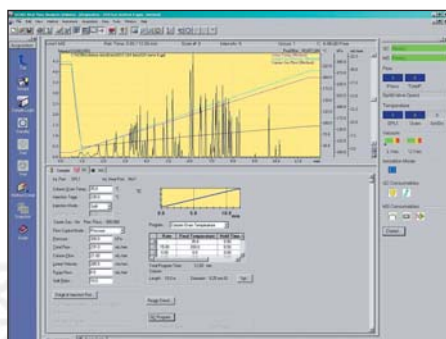
ID	Compound Name	Corrected Time	Actual Time	Error
1	Octadecane	8.530	8.530	0.000
2	Nonadecane	9.824	9.813	-0.001
3	Acenaphthene	7.640	7.626	-0.001
4	Acenaphthylene	7.655	7.653	-0.001
5	Acenaphthene	7.655	7.653	-0.001
6	2-Chlorobiphenyl	8.000	8.000	0.000
7	Fluorene	8.960	8.960	0.000
8	2,3-Dichlorobiphenyl	10.196	10.196	0.000
9	Hexachlorobiphenyl	10.200	10.204	0.004
10	Quinoline	10.200	10.200	0.000
11	Anthracene	10.225	10.204	-0.001
12	Phenanthrene	10.263	10.261	-0.001
13	Indene	10.265	10.265	0.000
14	Phenylacetylene	11.550	11.546	-0.001
15	Phenanthrene	11.550	11.553	0.003
16	Phenanthrene	11.550	11.553	0.003
17	2,4,6-Trichlorobiphenyl	11.877	11.875	-0.001
18	Acenaphthene	12.000	12.000	0.000
19	Hexachloro	12.000	12.013	0.013
20	2-Chlorobiphenyl	13.200	13.200	0.000
21	2,4,6-Trichlorobiphenyl	13.200	13.200	0.000
22	Alanine	13.200	13.200	0.000

Note: The retention times registered in the method are the times used for identification and verification of compounds based on the retention index data from the method and the results of the n-alkane standard analysis.

One-Window Technology

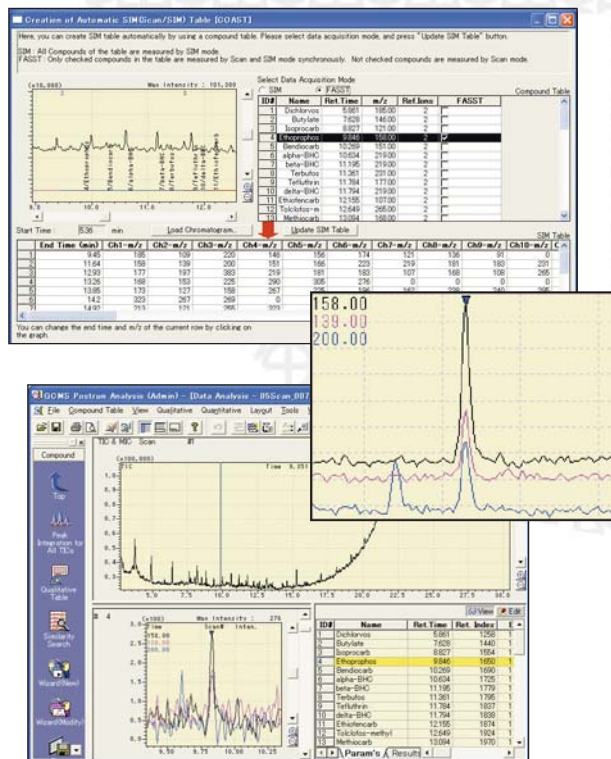
Working closely with customers, Shimadzu software engineers have created complete and user-friendly instrument control and processing software. With "one-window" design, users can simplify operation and put total control within the reach of the mouse.

"One-window" means that all data reduction information is now visible on one screen. Changing parameters for the viewed compound in the quantitation table simultaneously changes the display for the quantitative results, peak integration, spectrum, ion ratio, and peak locator on the TIC. Additionally, compound calibration, private library editing, chromatogram comparison, and reporting software are accessed from the same place. Use the right mouse button to enable manual integration, search for matches in any commercial library, or identify chromatographic peaks with the base peak m/z.



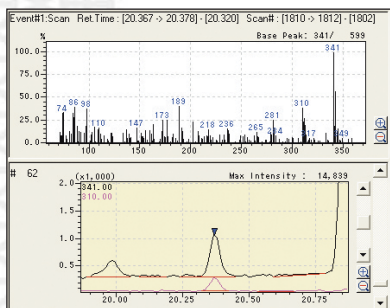
COAST (Creation of Automatic SIM [Scan/SIM] Table)

COAST is a wizard that allows the user to quickly set up a SIM/Scan data acquisition method. The user runs the wizard while viewing a chromatogram to quickly and easily create a SIM/Scan table. FASST measurements can be specified for the entire analysis or just in regions where sensitivity enhancement is desired. It is also possible to alternate acquisition modes between Scan, SIM, and FASST.



FASST (Fast Automated Scan/SIM Technique)

With FASST, both a scan chromatogram and a SIM chromatogram can be obtained by switching at high speed between scan and SIM modes for data acquisition. Even with sequential data acquisition in both modes, there is no degradation of sensitivity from the high-speed data acquisition technology employed in the GCMS-QP2010 series. The FASST measurement parameters are easily set using the GCMSsolution automatic setting function.



Similarity Search with Linear Retention Indices

It is not unusual for compounds of a similar class or molecular weight to produce identical spectra. Library searches will be refined to identify the actual isomer with the help of this retention time indexing feature.

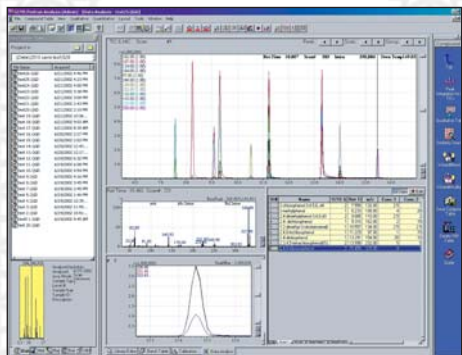
Intelligent Batch Sequencing

Improve the productivity of your laboratory by automating the corrective action plans established by most regulatory methods.

Batch sequence injections may be evaluated for a variety of QA/QC parameters, including sample upper/lower limits, precision, recovery, spiked samples, and blank samples. GCMSsolution uses pass/fail criteria to evaluate each injection and automatically executes the appropriate user-defined corrective actions, which include rerun, stop, pause, goto, and return commands. Intelligent Batch Sequencing allows the end user to save valuable time and minimize the loss of valuable samples.

Improved Method Development

Acquisition parameters for the GC oven, AFC flow and pressure profiles are displayed behind the TIC trace. Constant linear velocity optimizes separation with one-button operation. When utilizing mass pattern tuning by setting ion ratios in the software, GCMSsolution consistently produces accurate tuning results. On the “acquire” display, a reference chromatogram behind the acquisition trace speeds method development. Changes to all method parameters are made graphically. The ability to time-program the GC and MS is standard.



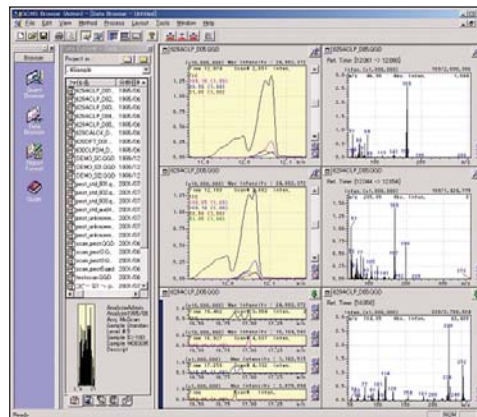
Powerful Quantitation

Post-run processing places all needed information for quantitation visually available and graphically accessible. The Data Explorer keeps the working project visible and a simple “click and drag” loads individual data files. A file can be searched visually on the Preview window below the file or icon list.

The chromatogram window presents TIC, extracted ion profiles, SIM profile, multiple ion chromatograms with integration, compound name labeling, and base peak m/z labels to allow easy peak identification. Data files can be overlaid for convenient comparison.

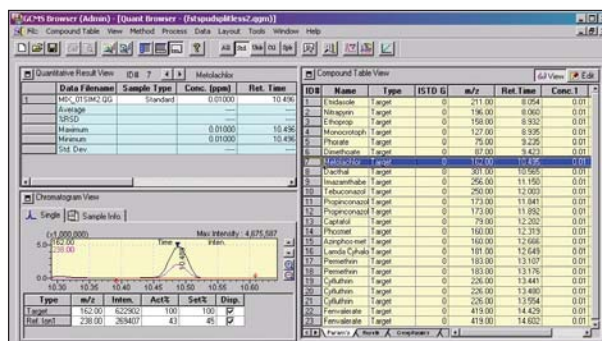
The spectrum shown is generated from the integrated peaks or from manual spectrum generation and background subtraction. Multiple background subtraction points can be used. Right-mouse clicking provides library search results from any commercial library or up to five total libraries in any search.

The compound table contains the identification information for ion ratios or full spectrum scan data. By using scan spectrum, GCMSsolution provides more accurate compound identification and the “Compound Finder” can locate a compound anywhere in the chromatogram, ensuring easy method transfer between instruments and when changing columns.



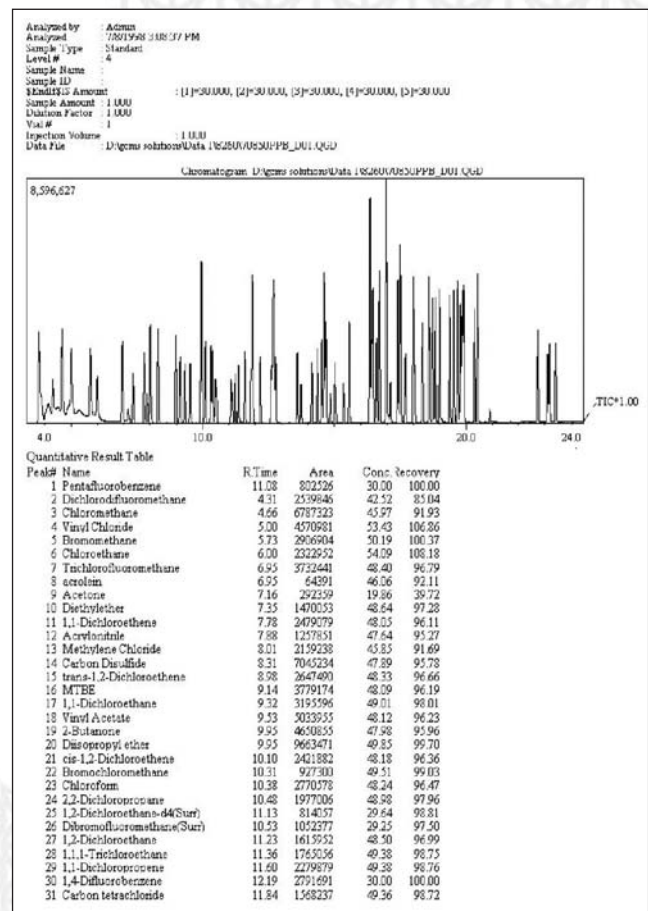
Quantitation Browser

Designed in the style of spreadsheets, and enhanced by QA/QC selected intelligence sequencing, the quantitation browser can process up to 1000 samples per batch, and 1000 batches in the sample queue, providing the ultimate in unattended operation.



Flexible, Customized Reporting

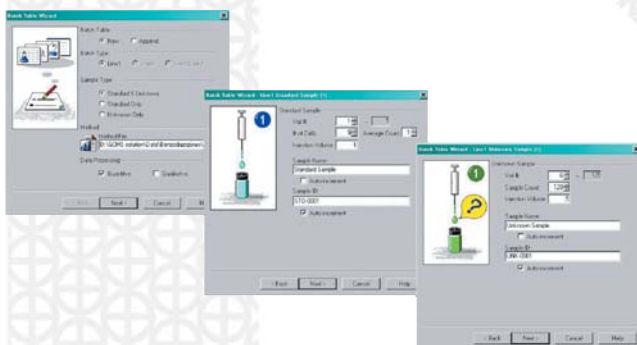
Report easily with visually customized formats. All chromatographic, spectral, qualification, and quantitation data can be placed anywhere on the page graphically. GCMSsolution reporting complies with USEPA, ASTM, and NIDA requirements for format and completeness, with surrogate and internal standard recovery standard. The report settings can be saved as a report format, allowing the same format to be used repeatedly.



Abundant Wizard Functions

Wizard functions lead users through creating methods, target compound tables, and batch analysis parameters to simplify the process of using the system. In addition, they facilitate the setting of SIM and other analytical conditions, such as integration parameters and calibration curve type. Specific wizards include:

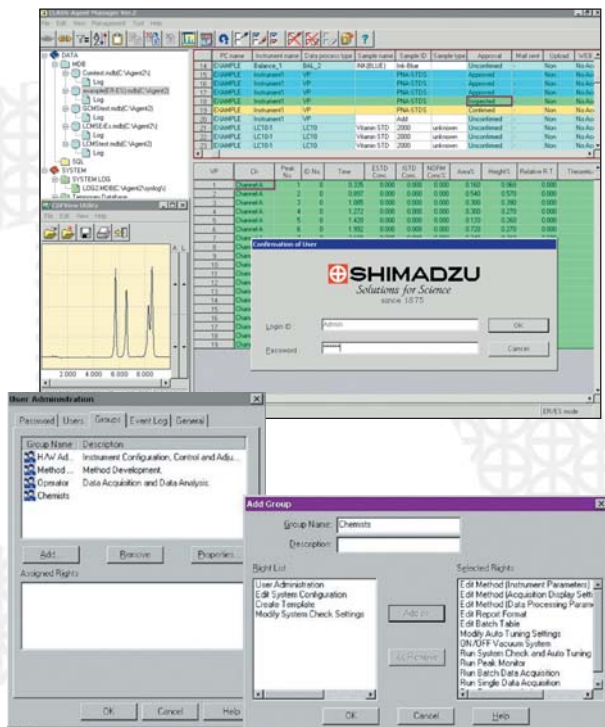
- Method Wizard—Speed your method development with easy setup of analysis parameters
- Compound Table Wizard—Compound tables are built with minimal effort by simply typing the name for each identified peak
- Batch Table Wizard—Upon creation, each line of a batch can have visual basic programmability for pre-run, post-run or decision-based operations, minimizing research time



Complete Compliance

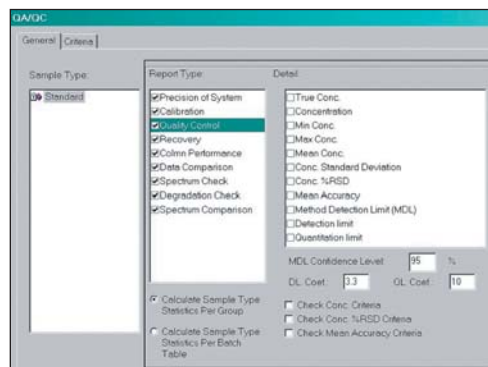
The heart of the compliance system is the versatility afforded by multilevel user access as assigned by the system administrator. GCMSsolution is fully equipped with security, audit trail, hardware/software verification and QA/QC functions for GLP/GMP compliance. Groups can share access to the functions of the software, or rights can be customized for each user as required. Dual-level password security and time limits for passwords ensure only authorized users will be able to access your data.

GCMSsolution provides the tools for 21 CFR Part 11 compliance in cooperation with CLASS-Agent, which enables data archiving for Shimadzu Instruments' control software packages. Audit trail records and all updates to the GCMSsolution files are maintained.



Superior Data Quality and Flexibility

GCMSsolution QA/QC software is the most comprehensive available. Verify quantitative precision, spectral integrity, column performance, and system degradation for all compounds. Verify spectra in accordance with USEPA methods for BFB or DFTPP compliance, and verify spectral matching for every target compound that the system measures. Perform testing for minimum and maximum RF, calibration accuracy, standard deviation from the calibration curve, and an MDL study using the QA/QC software.



System Checking

System checking software monitors the entire system for each analysis. Verify column integrity by standard methods or specified criteria. Verify MS performance by testing air leaks, ion ratio, isotopic resolution and baseline noise, and re-tune on failures. Correct any performance variance or stop the analysis during batch operation.

A batch of files can be quantitatively processed together, and quantitation results for all compounds in the batch can be validated. Data files, the re-quantitation window, and the compound table are linked, simplifying review and reprocessing.

