Analytical Data System
LabSolutions
Integrated software for LC, GC, LC/MS, and LC/MS/MS, LabSolutions features enhanced software operability and provides solutions for a variety of tasks and issues in analytical laboratories through a highly reliable system environment.
An Integrated Operating Environment

Data Acquisition

Data Browser

Quant Browser

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Improved Efficiency of Analysis Tasks

Improving the efficiency of each analytical run as well as the overall analytical work flow is required to improve the efficiency of data acquisition. LabSolutions provides you with a number of functions for improving the efficiency of data acquisition including an enhanced instrument monitor function that quickly verifies the instrument conditioning status and an overlap injection function that shortens the analysis cycle. Furthermore, routine analysis can also be fully automated through the automatic determination of instrument condition or data acquisition status.

Advantages of LabSolutions in Data Analysis Operations

- Graphic display of baseline, pump pressure, oven temperature, etc. for visually checking instrument condition
- Linking with external software or simple editing functions for Batch Tables for continuous data acquisition
- Overlap injection function for ensuring an overall shorter data acquisition time on an LC system

Substantial Instrument Monitor Functions

LabSolutions’ chromatogram monitor allows instrument status (e.g. pump pressure and oven temperature), concentration gradient profiles, signals from detectors, etc. to be displayed. As a result, the instrument condition can be visually confirmed. Also, chromatograms of standard samples or past data can be displayed as reference chromatograms on the chromatogram monitor, and the status of acquired data, such as the elution time and peak shape of each compound, can be easily checked on the monitor sub-window at the same time as the analytical run.

Chromatogram Monitor

Detector signals, instrument status and other monitored information can be displayed. LCMS data can also be monitored simply by switching tab pages.

Data Acquisition Task Log Display

This feature allows you to verify data acquisition-related logs. Also, a popup appears when errors occur to provide information on how to remedy the problem.
Data Acquisition Made Even More Convenient by Batch Files

Various functions are provided for supporting the faster creation and editing of Batch Tables. These include a Wizard-driven Batch Table creation function and a function for automatically incrementing cell information, a data file name auto generation function, and spreadsheet import and copy-and-paste functions. Support functions are also provided to enable preliminary checking of specific samples and the simple execution of postrun analysis, such as a function for only executing only samples within a specified range, repeat execution of the same sample and priority run. Data acquisition can be set to match the progress of data acquisition tasks. Also available is an overlap injection function for shortening the overall analysis time. The overlap injection function can also be applied to existing auto-samplers such as the SIL-10ADvp and the Nexera UHPLC series.

Full Automation of Data Acquisition Tasks

Batch Tables in LabSolutions have a function for automating operations from instrument startup to shutdown. For example, in an LC analysis, operations matched to the workflow can be automated by setting auto-purge and confirmation of baseline stabilization when the mobile phases used in the previous and next analyses differ, and cancelling analysis and re-testing based on the results of the system suitability test.

<table>
<thead>
<tr>
<th>Instrument/PC Power ON</th>
</tr>
</thead>
<tbody>
<tr>
<td>Check operating status of analytical instrument (system check function)</td>
</tr>
<tr>
<td>Replacement of mobile phase and system flowpaths (auto-purge function)</td>
</tr>
<tr>
<td>Equilibration of column (baseline check function)</td>
</tr>
<tr>
<td>Measurement of standard and control samples (system suitability test (SST), creation of calibration curve)</td>
</tr>
<tr>
<td>Split setting of real-time batch (e.g. re-injection of sample, cancellation of analysis) based on SST results or linearity judgment of calibration curve</td>
</tr>
<tr>
<td>Measurement of unknown sample</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Instrument Shutdown Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Custom parameters</em> field</td>
</tr>
<tr>
<td><em>System suitability</em> field</td>
</tr>
<tr>
<td><em>Batch action</em> field</td>
</tr>
<tr>
<td><em>Baseline check</em> field</td>
</tr>
<tr>
<td><em>Auto-purge</em> field</td>
</tr>
<tr>
<td><em>System check</em> field</td>
</tr>
</tbody>
</table>

Batch Editing Support Functions

Batch Setup Sub-Window

Batch Table Editing Sub-Window
Effective Utilization of Analytical Instruments

To efficiently operate instruments, each one must be easily accessed as desired, and analysis schedules determined while the operating status of each instrument is confirmed. LabSolutions allows both LC and GC instruments to be operated at the same time and the analysis status of each instrument to be monitored. For LC/MS instruments, LabSolutions allows analysis instructions and results to be checked and reports output from Internet Explorer, and provides a free access environment.

Flexible Instrument Access

- Up to 16 systems can be registered on a single PC, and up to four systems can be controlled simultaneously.
- LC and GC systems can be controlled simultaneously.

Simultaneous Control of HPLC and GC Systems

With LabSolutions, LCs and GCs can be operated via the same interface, and up to four LC and/or GC systems can be controlled simultaneously on a single PC. Instrument information for up to 16 systems can be registered to a single PC, allowing the system to be switched between LC or GC systems connected to the network. Sharing the operating environment for analysis on the LC and GC systems reduces training time.

Instrument Operating Status Monitor

LabSolutions’ instrument operating status monitor allows the operator to check the operating status of connected systems and the scheduled analysis end times on each instrument. Even if multiple LC and GC systems are operating at the same time, the operating status can be known at a glance, which is useful for scheduling data acquisition to effectively minimize instrument downtime.
**Open Solution**

*(optional software)*

Open Solution is web-based software that permits observation of LC/MS analysis results and report printing from any networked PC. Open Solution fully exploits an open access environment in Internet Explorer to dramatically enhance the efficiency of analysis work.

**Open Access**

Open Solution allows analysis results to be checked or reports to be output from any networked PC installed with Internet Explorer. No special software or extra licences are needed.

**Start Analysis in Just 3 Steps**

Analysis can be started in a mere three steps. Step 1 is to first log into Open Solution. Step 2 involves setting the minimum required parameters, such as registering the sample and specifying the method for data acquisition, and then placing vials at specified positions. Finally, in Step 3, just click the start button.

**E-mail Notification at End of Analysis**

Analysis tasks can be performed more efficiently since analysis results can be instantly accessed. These analysis results can be easily checked and printed, and an analysis report can be output as a PDF file by the click of a button.

* Internet Explorer IE: Registered trademark of Microsoft Corporation
Confirmation of Data (Browser Functions)

The capability to quickly check data is an important facet to improving the efficiency of analysis work. In particular, in ultrafast analysis in which large volumes of data can be processed in a short time, the key point is how these large volumes of data can be batch-processed. LabSolutions browser functions make this possible. With "Quant Browser," the series of acquired data is loaded simultaneously and postrun analysis after optimization of data processing parameters is applied to all data merely by dragging-and-dropping a batch file.

Furthermore, checks from system suitability and the validity of calibration curves to pass/fail of sample measurement results can be automatically judged.

Also, with "Data Browser," PDA spectra and LC/MS spectra as well as multiple chromatograms can be easily compared and checked, which is useful when evaluating analytical conditions. LabSolutions provides you with various analysis functions that are effectively located in the software and facilitate data visibility and analysis operations.

Advantages of LabSolutions in Data Analysis

- Series of analysis data can be loaded rapidly simply by dragging-and-dropping a batch file.
- Large volumes of data can be instantly analyzed by the batch analysis function.
- System suitability and the validity of calibration curves can be automatically judged.
- PDA spectra and LC/MS spectra as well as multiple chromatograms can be easily checked in a single sub-window.

Quant Browser

Simple mouse operation allows measurement results to be checked easily via an individual batch schedule. This browser adopts an interface that groups the Quantitative Results Table, calibration curves, chromatograms, and the analysis parameters editing sub-window in a single window, which proves its worth in the analysis of data from numerous specimens.

Data Explorer

(1) Drag-and-drop the batch file to be analyzed on the Quant Browser sub-window.

(2) Filter and display standard samples (or control sample) or unknown samples.

(3) This is for checking the area values or the statistic calculation result values of the retention times of each peak displayed in the table.

(4) Chromatograms can be switched for confirmation by clicking the mouse on the Quantitative Results Table or by using the down cursor key on the keyboard.
Checking Analytical Results

System suitability or the validation of calibration curves is automatically checked by preset criteria, and the results are displayed in red in the check results field if an error occurs. Also, any abnormalities in the check results can be immediately checked by the upper and lower limit values of the sample quantitative values. These enable analytical results to be checked quickly after an analytical run ends.

### Manual Peak Integration of Displayed Chromatogram

Manual peak integration can be performed on individual data, if necessary. Peak detection points can be moved, peaks can be inserted or removed and other operations performed on only the displayed chromatogram. After identified peaks have been integrated, they immediately undergo quantitative calculation, and the result is displayed in the Quantitative Results Table.

### Data Browser

The data of multiple chromatograms can be easily compared by simply dragging-and-dropping a data file onto the Data Browser sub-window. This is useful for comparing chromatograms measured by different analytical conditions in method development, or for displaying LC/MS and PDA chromatograms and spectra.

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**Example of Automatic Checking of Analytical Results**

<table>
<thead>
<tr>
<th>ID# 1</th>
<th>[Methyl paraben]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>2.636</td>
<td>74.400</td>
</tr>
<tr>
<td>2.635</td>
<td>115.467</td>
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<tr>
<td>2.633</td>
<td>296.780</td>
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<tr>
<td>2.632</td>
<td>204.154</td>
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<tr>
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<tr>
<td>2.623</td>
<td>296.780</td>
</tr>
<tr>
<td>2.621</td>
<td>204.154</td>
</tr>
</tbody>
</table>

**Example of Data Display in Data Browser**
Numerous Types of Calculations Supported

As part of its standard specifications, LabSolutions is provided with functions for calculating parameters such as column performance and $S/N$ ratio, that are required for verifying the validity of chromatograms in method development and routine data acquisition. It also supports a reference standard function that enables quantitation of impurities, for example, for which a standard sample cannot be obtained and a factor function for standard sample acquired amounts, and provides substantial quantitative calculation functions such as a custom parameter function for achieving a variety of calculations. Moreover, with analysis on a GC system, a function for automatically correcting the retention time of the target component in relation to changes in the column state, for example, during replacement of the capillary column is available.

<table>
<thead>
<tr>
<th>Numerous Calculation Functions Provided by LabSolutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>▶ Automatic calculation of the $S/N$ ratio, quantitative limit and detection limit for each identified peak.</td>
</tr>
<tr>
<td>▶ Simultaneous output of column performance evaluation parameters based on multiple calculation methods (JP, USP, EP, etc.).</td>
</tr>
<tr>
<td>▶ Creation of calibration curves and quantitative calculation for compounds for which standard samples cannot be prepared.</td>
</tr>
<tr>
<td>▶ Custom calculation functions for quantitative results in the same data.</td>
</tr>
<tr>
<td>▶ AART (Automatic Adjustment of Retention Time) function for automatically batch-correcting the retention time of target components.</td>
</tr>
</tbody>
</table>

Simple Display of $S/N$ Ratio, Quantitative Limit and Detection Limit Output Results

In LabSolutions, the measurement results of the $S/N$ ratio, quantitative limit and detection limit for each identified peak can be easily displayed on screen and also output in reports by setting data processing parameters. Also enables simultaneous output of column performance evaluation parameters based on multiple calculation methods (JP, USP and EP) and output of the peak/valley ratio appended by the Japanese Pharmacopeia Fifteenth Edition Supplement I (General Test Methods).
Quantitative calculation results can be computed by applying calculation formulas using a desired factor to the area value, height value, concentration value, retention time, etc. of identified peaks. This is useful for calculating the existence ratio of related substances totaled against the main peak of the measurement data and calculating elution amounts in elution tests for drugs, for example. This custom parameter function can be set to any row of the Batch Table, and custom formulas are applied to the measurement data of rows that this function is enabled for.

Retention time of the target component must be corrected to match changes in the column’s state, for example, when the capillary column is replaced. The retention times of target components can be calculated and batch-corrected from retention index values of pre-registered target components and the retention time measurement values of n-alkane by using the AART (Automatic Adjustment of Retention Time) function.

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Custom Parameter Function for Quantitative Results

AART (Automatic Adjustment of Retention Time) Function for Automatically Batch-Correcting the Retention Time of Target Components

When standard substances, such as impurities, cannot be prepared for all components, a calibration curve is made using a standard substance having the same (or in a proportional relationship) relative sensitivity as the detector and the concentration (amount) of the other components (impurities, etc.) is quantitated. The calibration curve of preset compounds is created by entering the ID and sensitivity correction factor of the compounds that will reference the calibration curve information, and quantitative calculation is performed using that calibration curve.
PDA Data Analysis

With LabSolutions, data can be analyzed in various ways based on 3D data, with time, wavelength and absorbance as its three axes, obtained from the LC-PDA (photodiode array detector), and information useful both qualitatively and quantitatively for eluted components can be obtained instantly.

PDA Data Analysis by LabSolutions

- Analysis of profiles of all eluted peaks using 3D display and contour graphs
- Various purity analyses of individual eluted components
- Identification of each eluted component based on UV-VIS absorption spectra (library search)
- Multi-chromatogram analysis for quantitating each eluted component using the optimum wavelength
- Calculation processing of a UV-VIS spectrum of eluted components

Analysis of Profiles of All Eluted Peaks Using 3D Display and Contour Graphs

The 3D display takes the time, wavelength and absorbance of the UV-VIS absorption spectrum as its axes. In this display, the viewing angle can be changed as desired, allowing profiles to be viewed in detail. And, in the contour graph display, wavelengths with high absorbance, namely, wavelengths with high sensitivity, can be found for each eluted component. Additionally, components, such as impurities, which could not be seen by 2D chromatograms, can be discovered from the elution profile of individual components.

Contour Graph Display

3D Display

Various Purity Analyses of Individual Eluted Components

LabSolutions enables purity to be analyzed, for example, by checking the deviation of RT in multi-wavelength chromatograms or analyzing purity curves that are obtained by converting changes in the pattern of the UV-VIS spectrum for each eluted peak. Purity values can also be analyzed in a variety of ways by using calculation means, such as the 3-point and N-point methods.

Purity Curve

Peak Profile
Identification of Each Eluted Component Based on the UV-VIS Absorption Spectrum (Library Search)

Components in the UV-VIS spectrum of the peak top of each eluted component can be identified by searching in the UV-VIS spectrum library prepared in advance. Searching is performed by calculating the similarity of patterns in the UV-VIS spectrum. During a search, identification threshold values can also be calculated automatically by pre-evaluating noise and other uncertain factors.

Multi-Chromatogram Analysis for Quantitating Each Eluted Component Using the Optimum Wavelength

Sometimes the maximum wavelength of the UV-VIS spectrum differs for each eluted component. With LabSolutions, quantitative calculation based on multi-chromatograms is possible and quantitation using the optimum wavelength (maximum absorption wavelength) for each eluted peak can be performed, which means that quantitation can be performed at high sensitivity on all eluted peaks. Also, the optimum wavelength of each component can be easily set based on the contour graph display.

Calculation Processing of the UV-VIS Spectrum of Eluted Components

Various operations can be performed on the UV-VIS spectrum of each eluted component: detection of minimum and maximum absorption wavelengths, calculation of the derivative spectrum or subtraction of the spectrum, arithmetic operations such as smoothing, and overlaying of spectra between multiple data. This allows highly reliable qualitative information to be obtained for each eluted component.
Creation of Reports

LabSolutions supports the creation of custom reports, from individual analytical reports to summary reports, in the same operating environment. A wide range of reports is supported thanks to substantial report items and a highly flexible layout. Also, even in continuous data acquisition, report formats matched to each individual sample can be set. LabSolutions contributes to the use of fewer paper-based resources in laboratories and promotes eco-friendly countermeasures since it is provided with PDF output functions as standard.

With CLASS-Agent Report, reports can be generated based on Excel. In addition, data acquisition results are automatically reflected in templates and manual entry or confirmation involving manual entry is not needed, which means that the time required to create reports can be considerably shortened. Reports can be generated seamlessly with system operation since templates and calculation result sheets are managed in a database.

A Wide Selection of Report Creation Functions

- PDF file-based analytical reports promote less use of paper resources in laboratories (PDF output function provided as standard).
- Reports created as desired with multi-stage display of chromatograms, peak comment callouts, etc.
- Report creation tasks drastically reduced by custom calculations made using measurement results generated by Agent Report.

PDF File Output of Analytical Reports

LabSolutions is provided with a PDF output function as standard in addition to regular printer output to promote the use of less paper. PDF files of analytical reports are also automatically loaded to a database where they are batch-managed.
Substantial Summary Report Output Functions

LabSolutions supports the creation of custom reports, from individual analytical reports to summary reports, in the same operating environment. A wide range of reports is supported thanks to substantial report items and a highly flexible layout. Also, even in continuous data acquisition, report formats matched to each individual sample can be set.

Examples of Summary Reports for Standard Sample Chromatograms and Quantitative Results for Samples

Considerable Reductions in Custom Calculation and Report Creation Tasks

With the optional CLASS-Agent Report software, pre-registered Excel format templates are registered to a database, and calculations are automatically performed and reports automatically generated by merely selecting the data of the desired report and template when creating reports. As a result, Excel templates managed on the database are used, and Excel sheets containing results are automatically stored and managed. So, the integrity of the audit trail, security and data can be kept intact without the user having to touch the data at all. The laborious task of creating reports for measurement results in Excel can be lightened, thus preventing errors caused by manually re-entering result values. Custom calculations and the results of various quantitation methods and elution tests can also be output based on Excel templates.

*Excel: Registered trademark of Microsoft Corporation
Substantial Lineup of Functions for Compliance with GxP and ER/ES Regulations

Instruments used in laboratories must conform to requirements such as computerized system validation as defined in GxP and FDA 21 CFR Part 11 as well as in other authorities’ guidelines relating to electronic recording/electronic signatures (ER/ES). LabSolutions is provided with security policies and system policies, user rights and user administration functions, audit trail and other functions that enable effective system operation and compliance with these regulatory requirements.

### LabSolutions Compatibility with Regulatory Requirements

- Effective and stringent access control by assignment of operation rights to users
- High security through password policies and lockout functions for user accounts
- Log browser and information display functions for ascertaining system condition and access status
- Audit trail and program and raw data checks for ensuring data and system reliability

### Effective User Management

LabSolutions’ user administration comprises the setting of rights groups and assignment of rights to users just as in Windows. Access rights required for each user can be set simply by setting various rights groups. Rights groups matched to required tasks are set to each user. Functions such as these achieve effective user administration matched to laboratory operations from managerial tasks to data acquisition operations.

### Firm Security

Functions for setting an audit trail to ensure data reliability and for mailing events occurring on the system can be set. Various settings, such as setting the length, expiration date and complexity of passwords for user accounts, setting the lockout function to prevent illegal access, and registering settings for the deletion and alteration of registered users, can be made to enable highly secure system operation. Settings for overwriting data files and other information and settings relating to items to output in reports also are supported.
Log Browser for Ascertaining System Operation Status

The Log Browser allows the user to easily ascertain system status from system operation and administration to system usage status and error status. Functions for searching for log details, user names, instrument names, etc. also are provided so that the necessary information can be quickly checked.

Audit Trail for Achieving Change History Management

The change history of method files is managed by the audit trail. Application of the audit trail to all methods can also be set in the security policy settings. This prevents inconsistencies in compliance with regulations. A history of postrun analysis after data acquisition can also be managed by applying the audit trail to data files.

Alteration Checks for Ensuring System Reliability

The integrity of the programs that comprise the system and the raw data acquired by instruments can be checked. This ensures the reliability of the system and data in use. The results of these alteration checks can be managed as printouts.

Information Display for Ascertaining System Condition

The information of the PC on which the system is running (e.g. PC OS information and security information, network configuration, CPU specifications) can be quickly ascertained.
**Full Regulation Compatibility**

For compliance with regulations, system management and operation procedures must be documented, and the system operated in accordance with these procedures. Operating requirements are also mandatory for functions other than those held by products in use. Shimadzu provides detailed, total support throughout the entire life cycle of the system from consultation before its installation to post-introduction periodic inspection and then system upgrading (retirement). Shimadzu has also set up a complete support system in order to respond quickly to domestic and overseas trends, such as new requirements made by regulatory authorities and customer requests.

<table>
<thead>
<tr>
<th>Total Compliance with Regulations</th>
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<tbody>
<tr>
<td>- Full support from the evaluation of new systems to operation management and system retirement</td>
</tr>
<tr>
<td>- Implementation of DQ/IQ/OQ validation by qualified personnel</td>
</tr>
<tr>
<td>- Documentation structure support based on document templates prepared in advance for compliance with regulations</td>
</tr>
</tbody>
</table>

**System Life Cycle and Tasks to Be Implemented**

![System Life Cycle Diagram]

- **Introduction Plans**
  - Validation plans
  - Definition of user requests
  - Supplier evaluations

- **System Introduction**
  - Validation report
  - Performance Qualification (PQ)
  - Functional specifications
  - Operational Qualification (OQ)
  - Configuration establishment specifications
  - Installation Qualification (IQ)

- **System Operational Management**
  - Configuration establishment
  - Periodic inspections
  - Renewal plans

- **Retirement**

**Sample Architectural Documentation**

[**System Developmental Documents**]
- Validation Plans
- Definition of User Requests
- Supplier Assessment Plans and Reports
- Functional Specifications
- Configuration Establishment Specifications
- DQ Plans and Reports
- IQ/OQ/PQ Plans and Reports
- Validation Reports, etc.

[**System Operational Management Documents**]
- Operational Management Standards
- Documentation Management Procedures
- Configuration Management and Change Management Procedures
- System Management Procedures
- Security Management Procedures
- Backup and Recovery Procedures
- Archiving Procedures
- Troubleshooting Procedures
- Education and Training Implementation Procedures etc.
Management of Laboratory Information

CLASS-Agent Network System

CLASS-Agent enables data management, electronic signatures and other operations to be performed on measurement results obtained from various analytical instruments such as HPLC, GC, LCMS, UV, FTIR, TOC, thermal analyzers, X-ray diffractometers, particle size analyzers, balances, and products made by other manufacturers. Data is automatically stored on the database, and the desired data can be easily searched later on. Also, methods and schedule information used for data acquisition, measurement date/time, operator, chromatograph, analytical report image files (PDF files), and other information can be stored at the same time, thus enabling complete compliance with FDA 21 CFR Part 11. Network support also allows the data of all instruments to be batch-managed on a server PC, which means the data can be easily browsed from client PCs.

System Building Using CLASS-Agent

- Integrated management of various analytical instrument data on a database over a network
- Complete compliance with FDA 21 CFR Part 11
- Display/utilization of chromatogram and spectrum information, and numerical value information of data acquisition results

Agent Manager

Data stored and managed on a database by Agent Manager can be searched for, viewed, and appended with an electronic signature. Analysis results are displayed in the optimum format for each analytical instrument.

Integrated Management of Data Over Network

The data of analytical instruments connected on the network can be managed in an integrated manner in a database. And, the data stored on the database can be browsed from a client PC in a separate room, etc.