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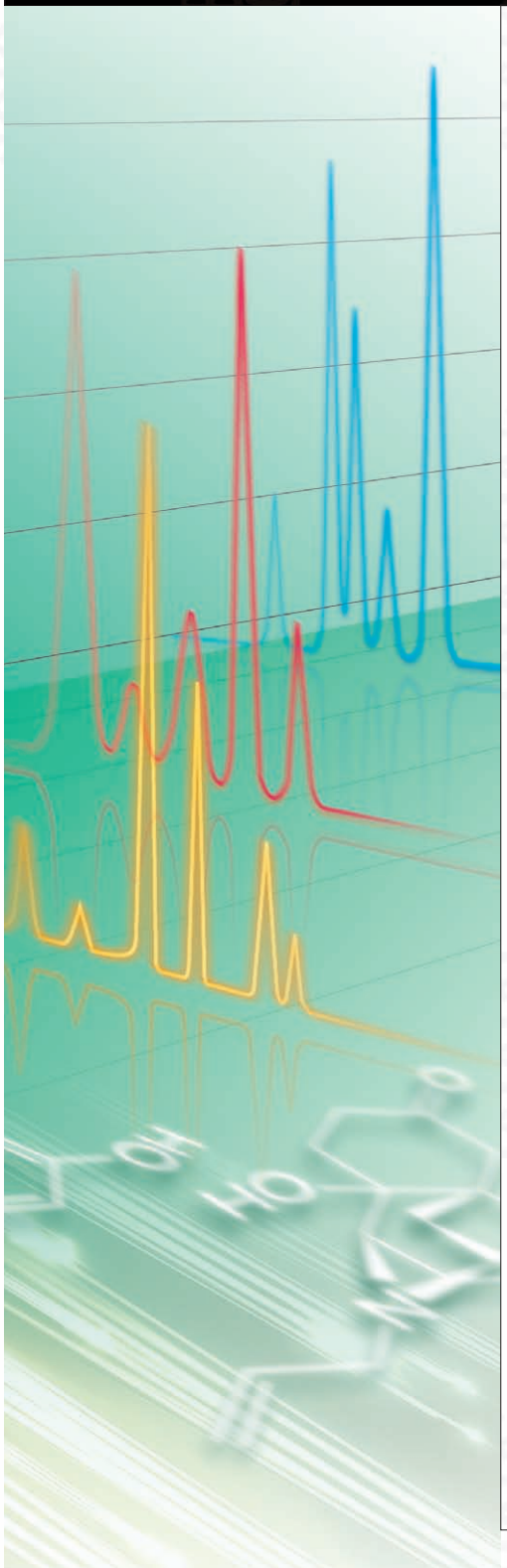
Using LabSolutions Browser Function for Improved Efficiency & Data Analysis

Technical Report vol.37



1. Introduction

The task of verifying acquired measurement data including the chromatogram and quantitation results can be daunting and troublesome, particularly for new operators in the lab. Even simple operations can be confusing, such as opening the measurement data for standard samples and unknown samples, operating the table with the quantitation results displayed, verifying abnormal peaks in the chromatogram, checking abnormal values in the quantitation results, changing the analysis parameters, and conducting re-analysis of the data, to name a few. LabSolutions greatly facilitates operations for novices as well as experts by effectively arranging the various analysis functions on the window, providing good visibility of data and facilitating analysis operations. Here we describe the data analysis operations using the browser functions of LabSolutions.

2. Flow of Data Analysis

A typical data analysis flow is shown in Fig. 1. First, LC or GC standard sample or control sample data acquired using single analysis or batch analysis are analyzed, then all the chromatograms, retention times, and peak area values are checked, and the operator confirms visually whether or not the system is operating normally and that the calibration curve is generated correctly. If correct results are not obtained at this time, the data analysis parameters are edited and measurement data is re-analyzed. This is repeated until the correct results are obtained, and then the calibration curve is re-generated. Next, after checking the unknown sample chromatogram and quantitation results, a report of the results is output as a report document. If the chromatogram contains a target peak that hasn't undergone peak integration correctly, in the same manner as handling the standard sample measurement results, the data analysis parameters are edited, manual peak integration (manipulation) is conducted, and the measurement data is re-analyzed. If these series of data analysis operations, for example chromatogram display and quantitation results verification, etc., could be performed in a single window, data analysis efficiency by the operator could be dramatically improved.

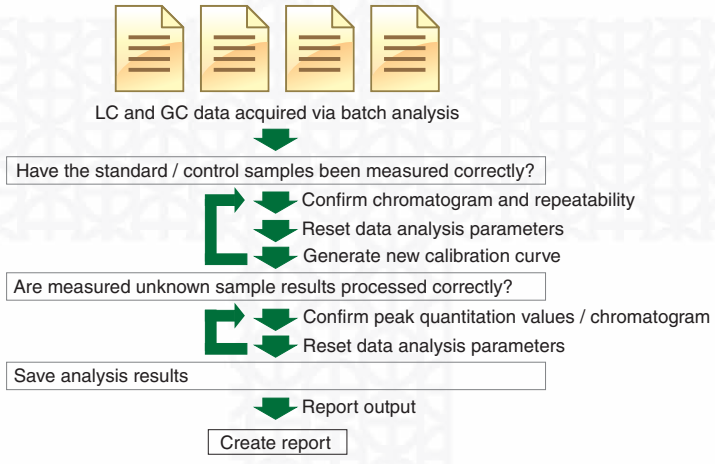


Fig. 1 Data Analysis Flow

3. Data Analysis Using the Quant Browser

The LabSolutions quant browser window is shown in Fig. 2. The measured data quantitative result table and chromatogram display, data processing parameters editing window, and the calibration curve information display window are all contained in the quant browser window. With all of these functions provided in this single window, all the information and analysis operations required for data analysis are readily accessible. To analyze measurement data, first, the relevant batch file is dragged and dropped via mouse operation from LabSolutions' Data Explorer into the quant browser window. The chromatograms and quantitation results of the respective standard samples or control samples, and the unknown samples that were measured using the batch file are automatically loaded into the quant browser window.

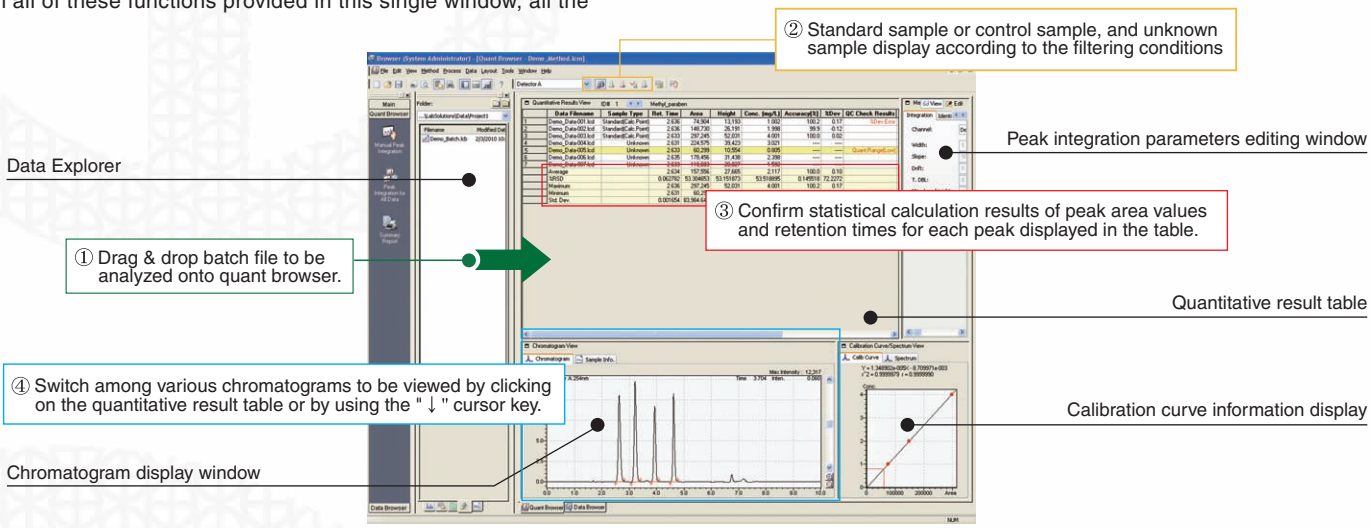


Fig. 2 Quant Browser Window

3-1. Viewing the Chromatogram, Calibration Curve, and Quantitation Values

The measurement results (column performance evaluation results including peak area value, height, retention time, quantitation value, theoretical plate number, symmetry coefficient, etc.) for each compound data item in the selected batch file are shown in the quantitative result table in the quant browser window. Further, in the quantitative result table, the standard sample or control sample are displayed selectively according to type, and the statistical calculation results, including the average value and CV value for each compound, are displayed for the specified data in the batch file. Thus, the work flow for conducting system suitability test (SST) prior to analyzing an unknown sample allows smooth verification of autosampler injection repeatability and retention time repeatability.

The operations for verifying chromatographic data acquired in batch analysis are also conducted using the quant browser, thereby facilitating the work flow. Using the mouse to click on each data item in the quantitative result table, or pressing the " ↓ " cursor key on the keyboard, allows switching among the chromatograms displayed in the chromatogram display window for efficient viewing of the measurement data. In this way, the quant browser allows viewing of the chromatogram for each data item without requiring excessive mouse-clicks.

Calibration curve information is also easy to check in the quant browser. Since the calibration curve for each compound is displayed in the calibration curve information window along with the quantitation results and chromatogram, calibration curve points for the standard sample and the linearity can be viewed in the quant browser. Further, if the unknown sample data has been selected in the quantitative result table, orientation intersecting lines corresponding to that compound area value and concentration are displayed in the calibration curve graph.

3-2. Changing Peak Integration Parameters of Detected Peaks

When peak integration has not been performed correctly for a target peak in the measured data chromatogram, the peak integration parameters can be changed in the quant browser to replace the peak integration results with the correct peak integration.

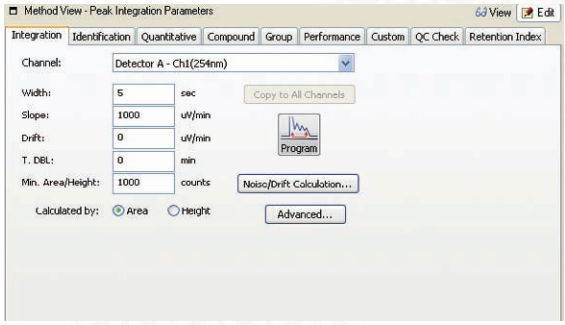


Fig. 3 Peak Integration Parameters Window

The detection peak integration parameters can be changed using two different approaches, one by using the peak integration parameters editing window, and the other by manual peak integration which applies only to a specific chromatogram.

To edit the analysis parameters using the peak integration parameters editing window (Fig. 3), first confirm that the [Edit] button at the top of the window is enabled to switch to the editing mode. Then, each of the parameter values for the Width, Slope and

Drift, etc., and the peak integration time program are edited. After editing, clicking the [View] button at the top of the window automatically executes peak integration for all of the data displayed in the quant browser using the newly set analysis parameters, and the re-analysis results are displayed in the quantitative result table. In the Edit mode, not only can the peak integration parameters be edited, but at the same time, it is also possible to edit the noise / drift, quantitation limit value and detection limit value calculations, as well as the compound table and column performance evaluation parameters, including the theoretical plate number and symmetry coefficient.

In addition, to conduct manual peak integration (manipulation) with respect to the currently displayed chromatogram, just select [Manual pIntegration Bar] on the right-click menu accessed by right-clicking on the chromatogram display window. The manual integration bar (Fig. 4) can be used for such peak integration as shifting peak detection points, and insertion / deletion of peaks, etc. Peaks that are identified using peak integration are immediately quantitated, and those results are displayed in the quantitative result table.

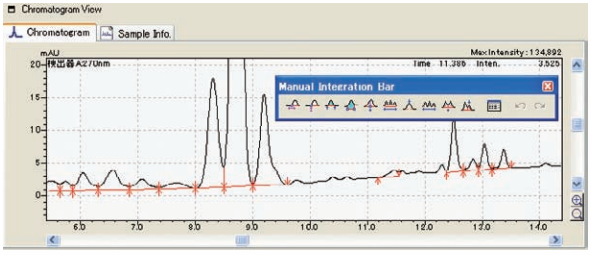


Fig. 4 Manual Integration Bar

3-3. Judgment by Quantitation Result Criteria

In the quant browser, it is possible to judge deviation % and accuracy % for the standard sample used to generate the calibration curve based on the upper / lower limit criteria values, and to judge whether or not the concentrations (quantitation values) of the compounds in the measured unknown sample are within the calibration range. The judgment results can be displayed in the [Judgment Result] field in the quantitative result table, and further, if an abnormal value is detected, the judgment result corresponding that data is displayed in red, making it very easy to pick out abnormal values among multiple data in a batch file (see Fig. 5).

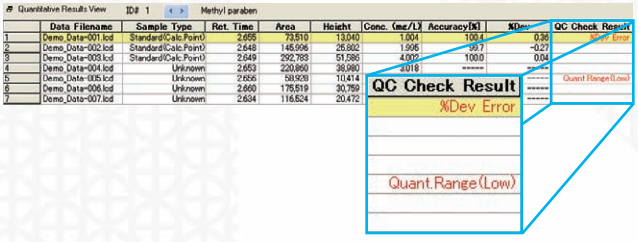


Fig. 5 [Judgment Result] Field in Quantitative Result Table

To evaluate the measurement results using the criteria values, the sample settings for Std, control, Spike and Unknown to be used for judgment of deviation % and accuracy % and the upper and lower limit input settings are set by inputting values in the [QC Check] tab page of the peak integration parameters window (Fig. 6). After setting the parameters, clicking the [View] button in the window automatically executes re-analysis processing, and the judgment results are displayed in the [Judgment Result] field.

In addition to judgment based on the above criteria values, in the [QC Check] tab page it is also possible to set whether or not to judge if the concentration value of each compound is below the detection limit and the quantitation limit value. By enabling this setting, it is also easy to check for detection of peaks with concentrations (quantitation values) that are below the quantitation limit.

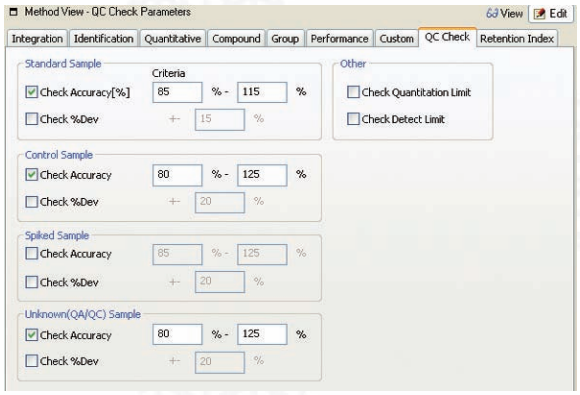


Fig. 6 Judgment Criteria Settings (QC Check Tab Page)

3-4. Summary Printout of Quantitation Results

The quant browser has not only been enhanced with more powerful data analysis functions, but also with robust print functions.

Three types of reports are now supported, including a summary report for the compounds displayed in the quantitative result table window. Output reports include method reports, Calibration reports, and Peak reports which can be set and executed from the batch table, and a separate report of the selected data chromatogram and quantitation results. To print a report, on the main menu in the quant browser, select [File] and then any one of [Print Table], [Data Report for Current Data] or [Print Quant.Report for Current Data]. Then, just selecting [Print] on that same menu will execute output of the selected report (Fig. 7). It is also possible to change the report format at this time. Using the same procedure as described above, select the [Edit] menu for the report format, and edit the output items and content in the displayed report editing window.

In addition to the printing of reports on paper using the report printout function, LabSolutions supports report output in the PDF file format as standard, contributing to environmentally-friendly paperless analysis operations in the lab.

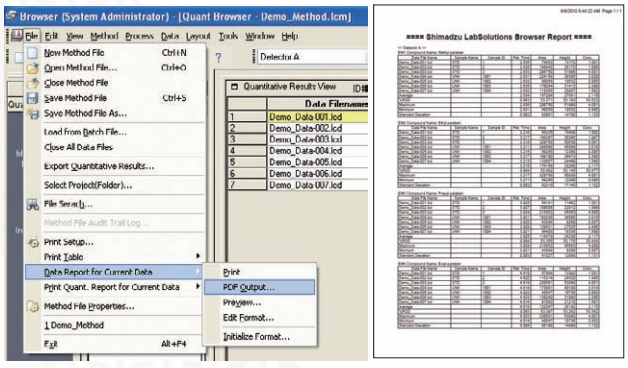


Fig. 7 Quant Browser Printout Functions and Summary Report Output Example

4. Display of Measurement Results in Data Browser

Analysis of measured data in LabSolutions is conducted using the quant browser together with the data browser (Fig. 8). The chromatograms and spectra, sample information and peak table, etc. for multiple data can be viewed in one window using the data browser, allowing convenient comparison of measurement results between data, demonstrating the power of this software. To display data in the data browser, just drag and drop a batch data file from the data explorer into the data browser window. Measurement results information is displayed in each data cell of the data browser window according to the output criteria specified. The layout of measurement data to be displayed in data cells (number of rows, and columns, data cell displayed content setting, settings for displaying the same data in multiple cells, etc.) can be customized as desired, and that layout can be saved for future use.

In addition, even peak integration can be conducted for chromatograms in the data browser window. By selecting the [Data Processing Parameters] icon or the [Manual Peak Processing Integration] icon in the LabSolutions assistant Barbar, the most appropriate peak integration parameters can be applied for each displayed chromatogram, just as in the quant browser.

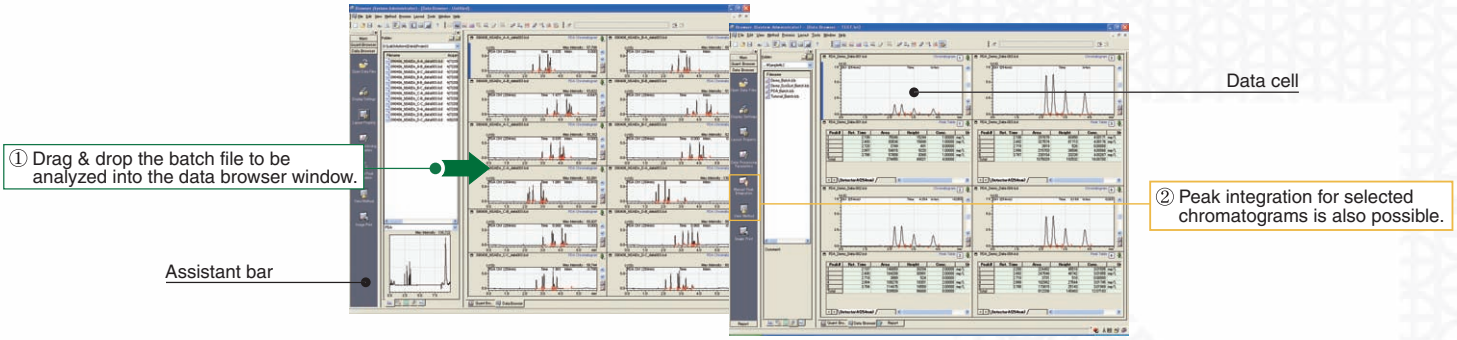


Fig. 8 Data Browser Window

5. Conclusion

The LabSolutions browser functions are conveniently accessible to permit an efficient data analysis flow, including verification of quantitation results for multiple data, evaluation of chromatogram peak separation and shapes, viewing of calibration curve information, editing of peak integration parameters, and re-analysis. Displaying the various types of information included in the measurement data is easily accomplished by just dragging and dropping the desired file into a browser window, allowing data analysis to be performed easily even by operators unfamiliar with the software operations.

These browser functions support a variety of application in the lab. For example, when conducting analysis of data from multiple specimens, a single batch file containing the data of these specimens can be loaded as is into the quant browser, and then, at a single glance, abnormal values detected via previously set data processing evaluation criteria, can be picked right out of the multiple sets of highly visible measured data. In addition, take for example data files generated using a method development system in which measurements were conducted while switching between multiple mobile phases. The data files can be viewed and compared with great flexibility to allow effective and efficient decision-making. When viewing the peak separation and peak shapes in multiple chromatograms and analyzing data generated using a PDA detector, both chromatograms and spectra can be displayed simultaneously, allowing smooth verification of peaks using the spectra from multiple sets of data.

Thus, the browser functions of LabSolutions can be used as a powerful tool for various lab applications to dramatically improve analysis efficiency.

First Edition: October, 2010

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Printed in Japan 3295-09004-10ANS