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LabSolutions Insight™

Instruction Manual

Operation Guide

Read the instruction manual thoroughly before you use the product.
Keep this instruction manual for future reference.

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Introduction

Read this Instruction Manual thoroughly before using the product.

Thank you for purchasing this product.

This manual describes the installation, operation, usage cautions and accessories for this product. Read this manual thoroughly before using the product and operate the product in accordance with the instructions in this manual.

Also, keep this manual for future reference.

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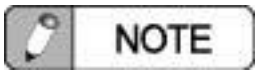
About This Manual

Throughout the text in this manual, warnings and other information essential when using this product, such as cautionary or prohibited items, appear classified as per the following:

Mark	Description
	Indicates a potentially hazardous situation which, if not avoided, could result in serious injury or possibly death.
	Indicates a potentially hazardous situation which, if not avoided, may result in minor to moderate injury or equipment damage.
	Emphasizes additional information that is provided to ensure the proper use of this product.
	Provides useful information about operation of this system. Please read the description when required.
 **Reference**	Indicates reference sections and pages.

For customers using the DVD distributed version:

This is a DVD disk. Do not play this on an audio CD player, as the high volume may damage your hearing or the audio speakers.

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1. Period: Please contact your Shimadzu representative for information about the period of this warranty.

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   4) Computer viruses leading to device failures and damage to data and software, including the product's basic software
   5) Power failures, including power outages and sudden voltage drops, leading to device failures and damage to data and software, including the product's basic software
   6) Turning OFF the product without following the proper shutdown procedure leading to device failures and damage to data and software, including the product's basic software
   7) Reasons unrelated to the product itself
   8) Product use in harsh environments, such as those subject to high temperatures or humidity levels, corrosive gases, or strong vibrations
   9) Fires, earthquakes, or any other act of nature, contamination by radioactive or hazardous substances, or any other force majeure event, including wars, riots, and crimes
   10) Product movement or transportation after installation
   11) Consumable items

   Note: Recording media such as floppy disks, CD-ROMs and DVD-ROMs are considered consumable items.

- If there is a document such as a warranty provided with the product, or there is a separate contract agreed upon that includes warranty conditions, the provisions of those documents shall apply.

Contents

Preface

About this manual

This manual contains detailed instructions on installing, configuring and using the LabSolutions Insight software.

This User Guide assumes that the reader has a reasonable knowledge of the Windows operating system, and how to use the standard Windows features, such as menus, checkboxes, drop-down lists and scroll bars. Please refer to your Windows support material (Help or the manual) for information on such matters.

About LabSolutions Insight

1.6.2

LabSolutions Insight (Insight) is a piece of software intended for displaying and manipulating multi-component mass spectrometry data. The software aims to flag target compounds that are outside of user-predefined tolerances and filter out unwanted data so that the observer can focus on important data.

The flags enable the operator to quickly assess the quality of the results and take any corrective action that may be possible, such as, but not limited to, re-integration or re-identification of a compound's peak and rejection of an outlying standard sample response.

The reporting limits enable the operator to produce reports that contain only those compounds that are within the specified limits, which is common in applications such as water quality analysis where a large number of compounds are screened but usually only a few may be significant.

The QC Chart shows the deviation of RT, Area and so on between each sample.

The analysis results and the method parameters used at each step of the workflow can be saved in a single file (the processing file). Using this file, it is possible to switch between various sets of analysis parameters to compare analysis results.

Insight handles GCMSsolution data (GCMS-QP series and GCMS-TQ series) and LabSolutions LCMS (LC-MS/MS 2020, 2050, 8030, 8040, 8045, 8050, 8060(NX), 9030, 9050) data.

Users are expected to analyse their samples using the GCMSsolution or LabSolutions workflow and use the Insight browser software for results review and re-processing of those compounds that have been automatically flagged. Later, a report may be produced from the Insight browser that outputs only those compounds that are within the reporting limits set.

When **LabSolutions Insight** is installed 4 icons will appear on the desktop and start-up menu:

Application Configuration

Report Configuration

LabSolutions Insight LCMS

LabSolutions Insight GCMS

Each application will be explained in detail in the following sections.

General Information

Computer Hardware

Insight makes use of data and programs stored on computer hard disk drives. Computer hardware including the hard disk drive is subject to daily wear and tear that can eventually result in hardware malfunction or dysfunction. It is strongly recommended that all contents stored on hard disk drives be backed up regularly according to site and or industry standards.

Please follow instructions provided by the computer hardware manufacturer or vendor on performing appropriate maintenance and updates.

User Name and Password

Access to Insight is restricted using the GCMSsolution user list for GCMS data and LabSolutions user list for LCMS data. When GCMSsolution or LabSolutions LCMS ins not installed, the user list configured in Application Configuration will be used. Please register all users requiring access to the Insight system on the GCMSsolution user management database, Insight user management system or LabSolutions user management database with appropriate passwords

Reviewing Results

In order to prevent erroneous results being reported and approved, please

-confirm that the intended data file is being used

-confirm that the expected compound is identified based on information such as the retention time and MS spectra.

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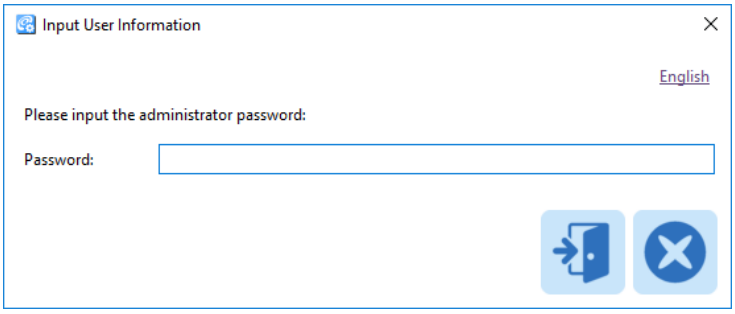
1 Application Configuration

The Application Configuration is used by the System Administrator to change each setting to LabSolutions Insight.

Click on the Application Configuration icon to launch the application.

A Login page will appear: Enter the password (Default: admin) to enter.



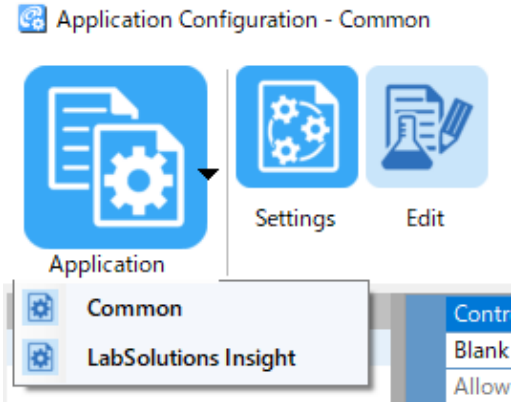
International Option: Click 'English' to change between different languages.

1.1 General Information about Configuration

The configuration settings can be changed by the administrator here.

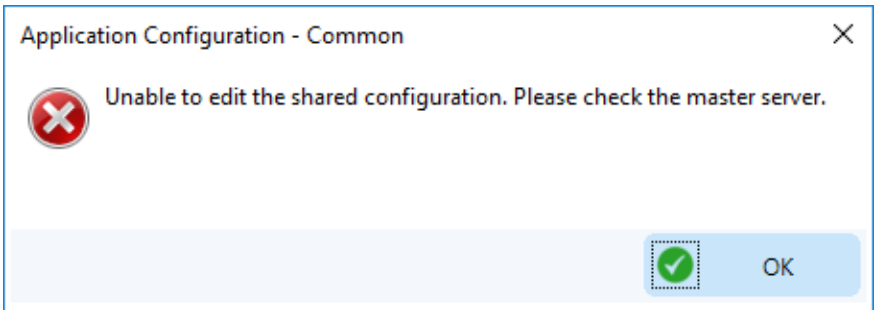
The items that can be configured are organized into sets.

Click on the configuration button to reveal a selection.

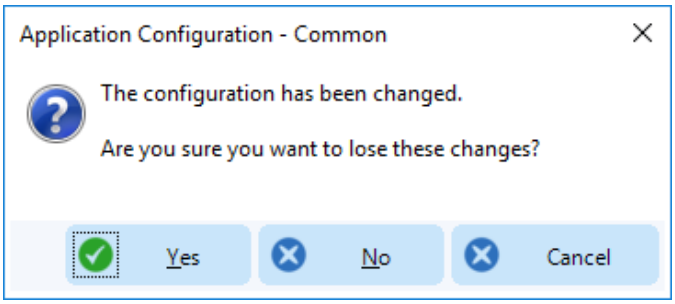


Common	General settings common to all Insight software. In order to edit any of the items, click on the Edit button. If you access any of the configuration items without clicking on the Edit button, the items will be shown as read-only.
LabSolutions Insight	 Settings particular to LabSolutions Insight.

Insight configuration parameters are shared across all master servers on the local network. A server is a PC on which LabSolutions Insight is installed. A master server is the reference server from which all servers get their configuration information from. If clicking the Edit button shows the error message below, restart the PC to re-establish network connection.

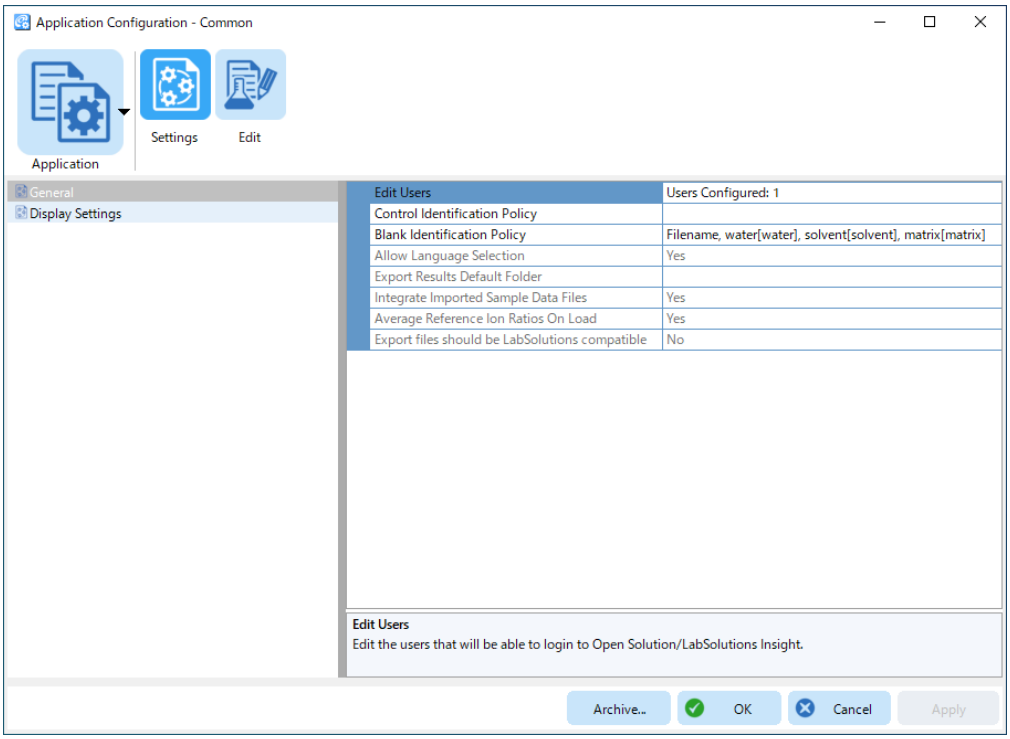


Note that closing the application with unsaved changes will show a warning message box:



Select [Yes] to close Application Configuration without applying the changes. Select [No] or [Cancel] to return to Application Configuration main window.

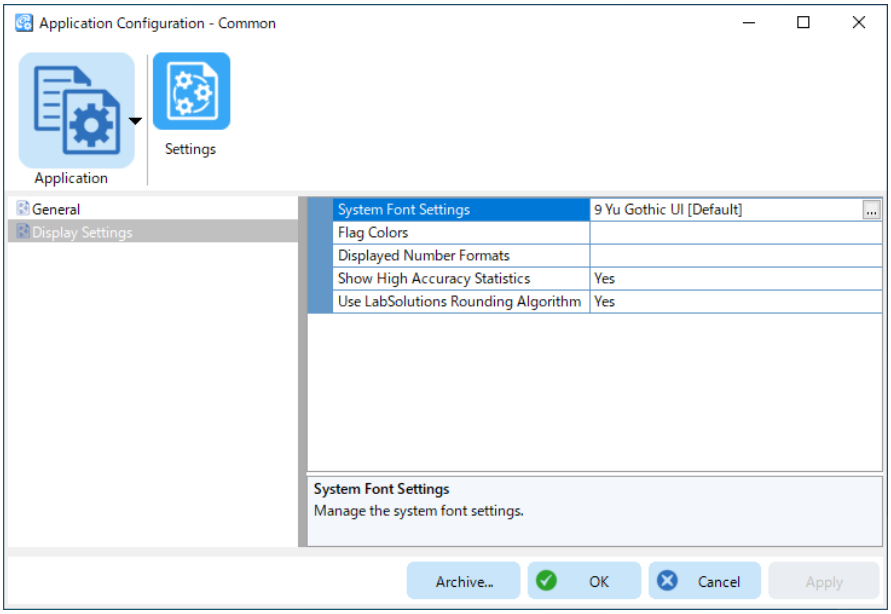
1.2 Common - General



Below is a list of settings that can be changed.

Edit Users	View and edit information about Insight users. The administrator is the only default user. The administrator account is used for logging into Application Configuration.
Control Identification Policy	Edit the method to identify the special control sample types (flag group) used for flag setting. Click on the […] button at the right end of the cell or double click in the field to open the Control Identification Configuration dialog box.
Blank Identification Policy	View and edit information on how the special blank sample types (i.e. flag groups) are identified for flagging. Click on the […] button or double click in the field to launch the Blank Identification Configuration dialog.
Allow Language Selection	Shows or hides the language selection tool in the Display Settings form of Insight. Click in the field to drop down the options.
Export Results Default Folder	Set the default folder where the export result file is saved. The folder is selected as the default folder of the export result file.
Integrate Imported Sample Data Files	Select whether the peak integration and quantitation is performed or not when the data is imported.
Average Reference Ion Ratios on Load	Averages measured reference ion ratios across all samples and updates the set reference ion ratio with the calculated average before performing peak processing and quantitation.
Export files should be LabSolutions compatible	LabSolutions Compatibility displays "——" or N.I.(low) / N.I.(high) in conc. column.

1.3 Common – Display Settings

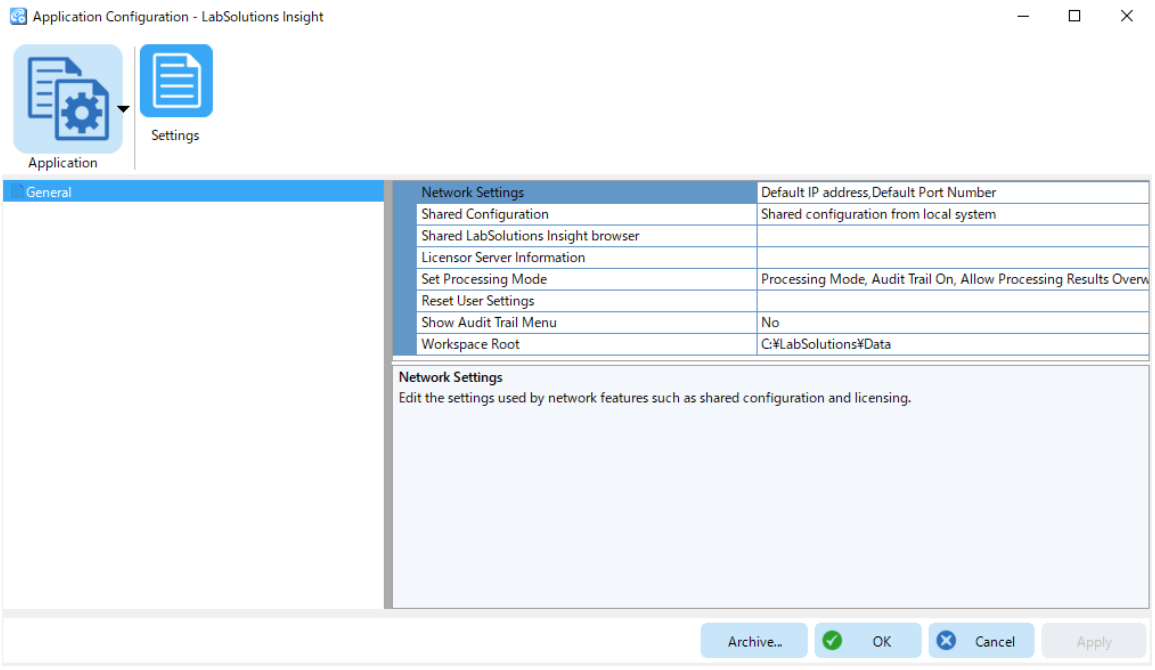


System Font Settings	Manage the system font settings. Click on the […] button or double click in the field to launch to Font Settings dialog.
Flag Colors	Manage the flag color settings.

	Click on the […] button or double-click in the field to open the Select Colors dialog box.
Displayed Number Formats	Manage the format settings to display values. Click on the […] button or double-click in the field to open the Displayed Number Formats dialog box.
Show High Accuracy Statistics	Select the level of accuracy of the statistics calculation. Select [Yes] to calculate %RSD and Standard Deviation to at least 6 decimal places. Select [No] to calculate %RSD and Standard Deviation to the same accuracy as the data for which the statistics are calculated.
Use LabSolutions Rounding Algorithm	Use either the LabSolutions rounding algorithm or Insight's own rounding algorithm. Selecting the LabSolutions rounding algorithm will ensure all calculations perfectly match between Insight and LabSolutions. Using Insight's own rounding algorithm may result in occasional (but rare) discrepancy between Insight and LabSolutions calculation results. The differences, if any, appear in the least significant figures of calculation results. Using the Insight algorithm will ensure complete consistency with previous versions of Insight.

1.4 LabSolutions Insight – General

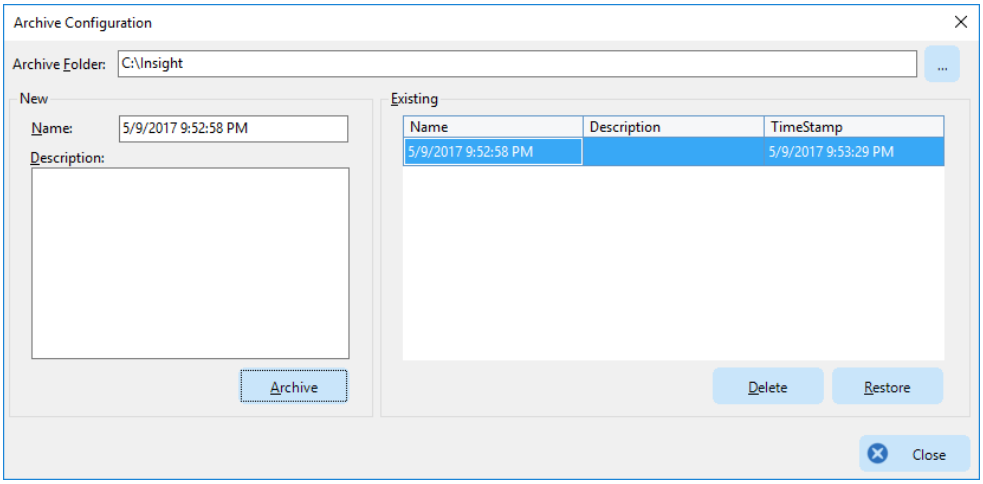
This section is for configuring items unique to LabSolutions Insight.

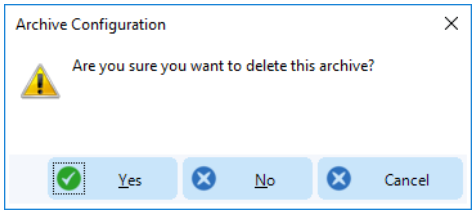


Network Settings	View and edit network information. This is required if the system is to work across a local network. If the local computer has multiple IP addresses assigned, use this setting to specify the IP address that will be used by Insight. There is no need to do this configuration if there is only one IP address. Click on the […] button or double click in the field to launch the Network Settings dialog.
Shared Configuration	Configure where the shared configuration will be shared from. The shared configuration can be shared by the local system or some remote system specified by an IP address. Click on the […] button or double click in the field to launch the Shared Configurations dialog.
Shared LabSolutions Insight browser	Set up a shared folder for sharing Insight across a network. When Insight in the folder is invoked, the Insight can be used in a computer where Insight is not installed. Click on the […] button or double click in the field to launch the Shared Browser dialog.
Licensor Server Information	View information about licenses installed on this PC. Click on the […] button or double click in the field to launch the Licensor Server Information dialog.
Set Processing Mode	Set whether to work in Processing mode or Data mode. Also set whether to enable audit trail when in Processing Mode. Click on the […] button or double click in the field to launch the [Set Processing Mode] dialog.
Reset User Settings	Initialize the window position and table columns displayed to factory default.
Show Audit Trail Menu	Select [Yes] to show the Audit Trail menu item in the [View] menu band in Insight. This option is set to [No] by default.

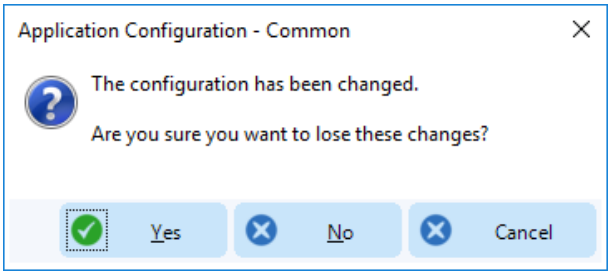
1.5 Archive Configuration

All the settings in the [Application Configuration] can be archived (i.e. backed-up) so that if necessary these can be restored at a later date. The archive dialog is opened by clicking on the Archive button on the main window.



Archive Folder	Type in the full path to the archive folder or press the […] button to choose from the standard folder selector.
New	
Name	Use the default archive name or type in a new one.
Description	Type in a brief description of the archive for easier identification when looking for archives to restore from. This can be left empty.
[Archive]	Press the [Archive] button to archive the current settings to the selected folder with the selected name.
Existing	
[Delete]	Select an archive in the [Existing] list and press the [Delete] button to delete the archive. A confirmation dialog is shown:  Select [Yes] to delete the archive and [No] or [Cancel] to keep the archive.
[Restore]	Select an archive in the [Existing] list and press the [Restore] button to restore the configuration to the selected archive. This will first create an autosave backup of the current configuration before restoring the selected existing archive.

Note that if the current configuration has been modified but not applied the following dialog will be shown when you press the Archive button:



Select [Yes] to discard any changes made to the Application configuration and proceed to open the [Archive Configuration] window. Select [No] or [Cancel] to stay in the main [Application Configuration] Window. Select [Apply] before attempting to configure the archiving options to avoid this message.

1.6 Edit Users

LabSolutions Insight utilizes three different ways in which to handle user information.

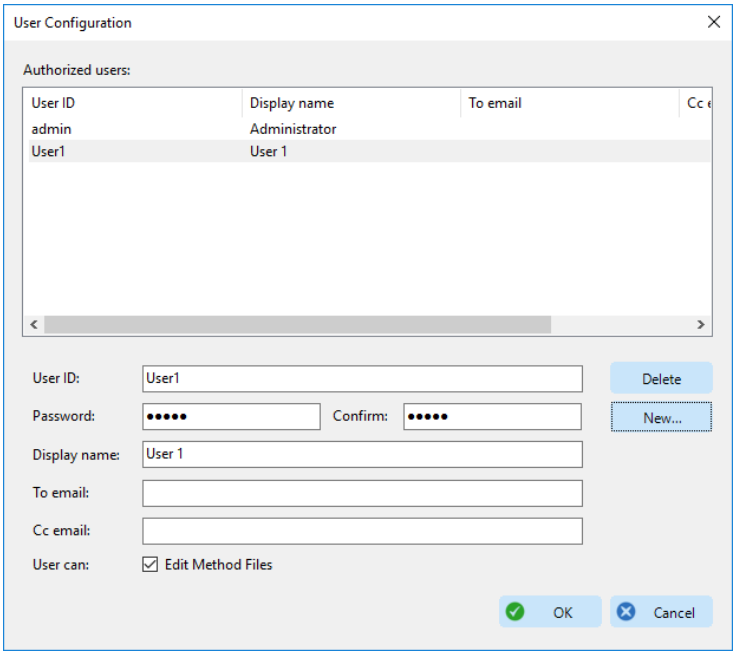
When handling GCMS data, either Insight user management database or GCMSsolution user management database will be used

For LCMS data, user management can be done by either Insight or LabSolutions (via Insight).

1.6.1 When LabSolutions LCMS and GCMSsolution Are Not Installed

Insight user management database is used when handling LCMS data without installing LabSolutions LCMS or GCMSsolution.

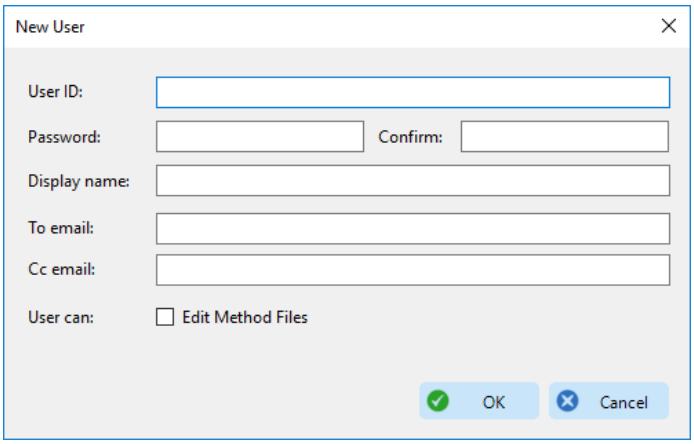
See section 1.2 “Common - General” on how to launch the User Configuration window.



The Administrator is a default user added by Insight on installation. This user cannot be deleted. （Only password change is possible.）

Use LabSolutions User DB	Select whether to use LabSolutions’ user management database.
User name	Name used to log into Insight.
Password	Password used to log into Insight. Only for the default Administrator, the same can be used to log into Application Configuration.
Confirm	Enter the password again to confirm.
Display name	The name displayed on Insight’s title bar as the currently logged in user.
To email	If the software being configured has the ability to send email notifications, the notification will be sent to this address.
CC email	If the software being configured has the ability to send email notifications, the notification will be CCed to this address.
Edit Method Files	Select whether to allow the user to edit methods.

To add users, click on the [New…] button.



Fill in the details of the new user then click [OK].

To delete a user, select the user in the list then click on the [Delete] button. Admin cannot be deleted.

1.6.2 When LabSolutions LCMS and GCMSsolution Are Installed

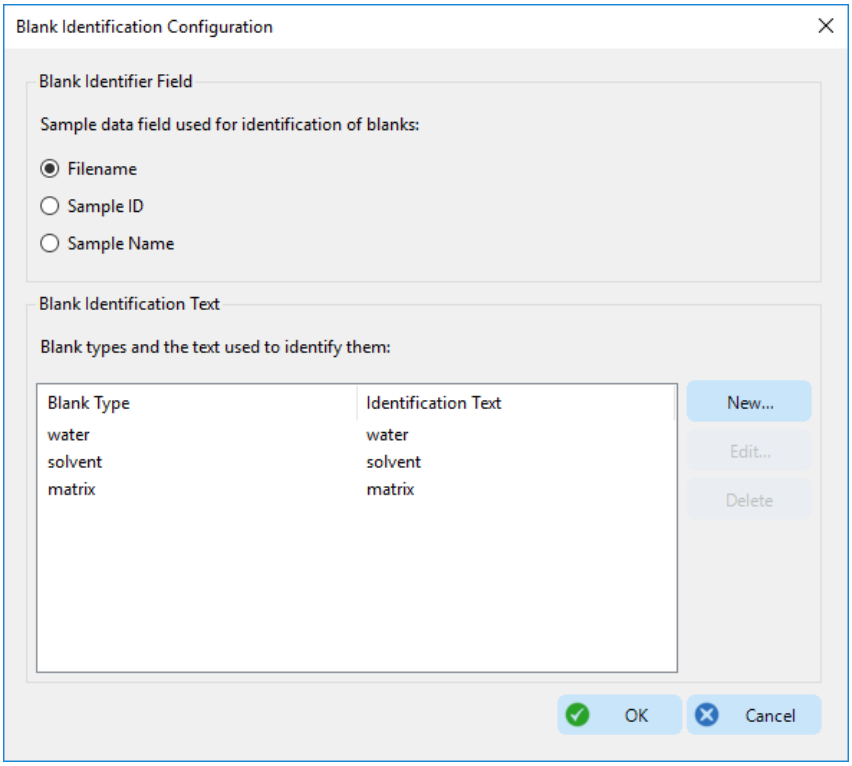
When LabSolutions LCMS or GCMSsolution is installed, the user management database will be used and Insight user management database will not be used. Please manage users using the LabSolutions LCMS or GCMSsolution user management functionality.

1.7 Control/Blank Identification Policy

Blank samples and control samples can be used as a special type of blank and control when a specific string is included in the filename, sample ID, or sample name. Because the procedure to specify them is common, this section only describes the [Blank Identification Policy] settings.

Certain blank samples can be defined as special types of blank samples. This is achieved by looking for identification keywords in the GCMSsolution or LabSolutions data fields. The blank sample type can be used as a flag group for flagging criteria.

See section 1.2 “Common - General” for how to launch the [Blank Identification Configuration] window.



Blank Identifier Field

Filename	Look for the Blank Identification Text in the sample’s data file name. For example, if the Blank Identification Text is “water”, the sample in the data file Pesticides_water.qgd(lcd) will be recognised as a Water blank whereas Pesticides_unknown.qgd(lcd) will not be.
Sample ID	Look for the Blank Identification Text in the sample’s Sample ID field in the GCMSsolution or LabSolutions data file. For example, if the Blank Identification Text is “water”, the sample with the Sample ID PEST_water will be recognised as a Water blank whereas PEST_UNK1 will not be.
Sample Name	Look for the Blank Identification Text in the sample’s Sample Name field in the GCMSsolution or LabSolutions data file. For example, if the Blank Identification Text is “water”, the sample with the Sample Name Pesticides_water will be recognised as a Water blank whereas Pesticides_unknown will not be.

Select the appropriate buttons to perform the desired operations:

Blank Identification Text

[New…] Add a new blank identification policy.

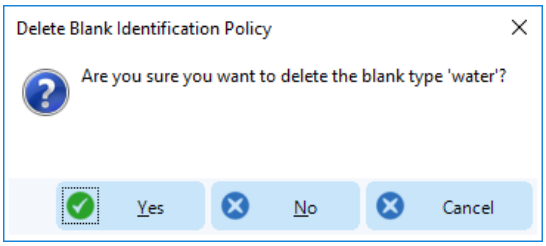
[Edit…] Edit the selected identification policy.

This button is only enabled when an existing blank identification policy is selected.

[Delete] Delete the selected identification policy.

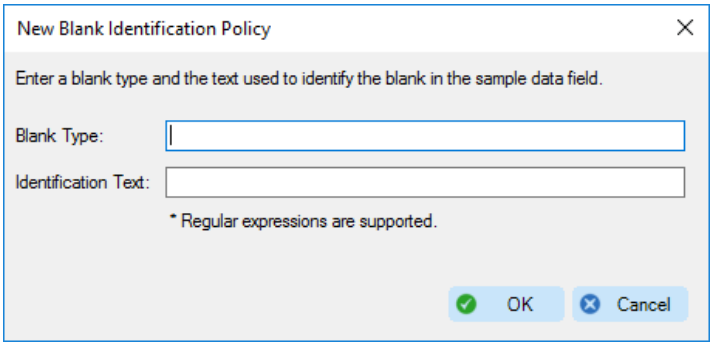
This button is only enabled when an existing blank identification policy is selected.

A confirmation message is shown. Select [Yes] to delete the selected identification policy. Select [No] or [Cancel] to keep the selected identification policy.



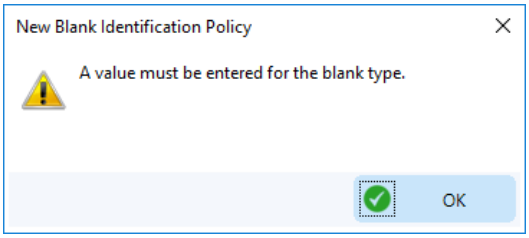
1.7.1 New Identification Policy

Click on the [New…] button on the Blank Identification Policy Configuration dialog to show the New Blank Identification Policy dialog.



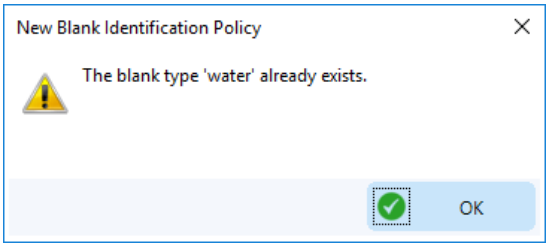
Blank Type The name of the new blank type to be configured here.

The Blank Type cannot be left blank.

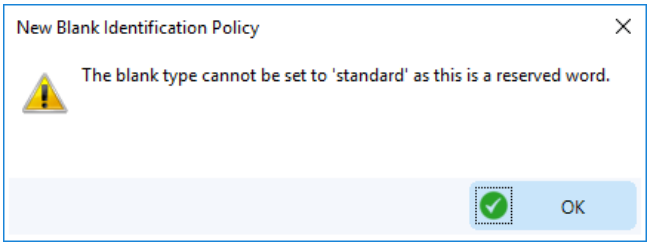


Press [OK] to go back and enter a valid Blank Type.

Blank Types must be unique so if the specified Blank Type already exists, an error message will be shown.



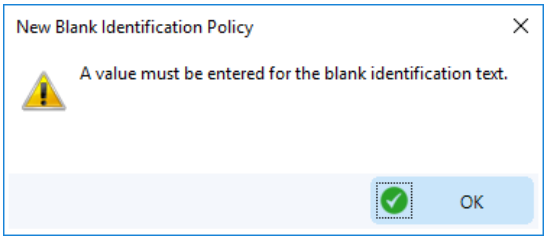
A similar message is shown if the specified Blank Type is one of the GCMSsolution sample types.



In both cases, select [OK] to go back and enter a valid Blank Type.

Identification Text — The text to search in the specified data field to identify a blank sample as the new blank type.

The Identification Text cannot be left empty:



Select [OK] to enter a valid Identification Text.

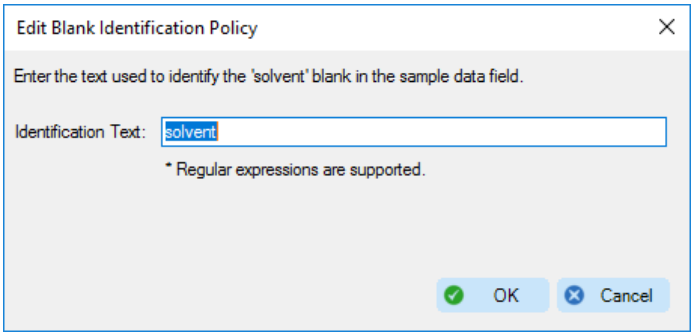
Once the Blank Type and Identification Text are entered successfully, select either [OK] or [Cancel].

[OK] — Save the new Blank Identification Policy and return to the Blank Identification Configuration dialog.

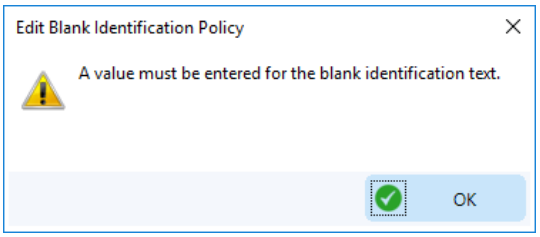
[Cancel] — Discard the new Blank Identification Policy and return to the Blank Identification Configuration dialog.

1.7.2 Edit Identification Policy

Select an existing Blank Identification Policy and click on the [Edit…] button to show the [Edit Blank Identification Policy] window.



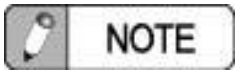
Identification Text	The text to search in the specified data field to identify a blank sample as the new blank type. The Identification Text cannot be left empty:



Select [OK] to enter a valid Identification Text.

Once the Identification Text is successfully changed, select either [OK] or [Cancel].

[OK]	Save the new Blank Identification Policy and return to the Blank Identification Configuration dialog.
[Cancel]	Discard the new Blank Identification Policy and return to the Blank Identification Configuration dialog.



Common names cannot be used in Control Identification Policy and Blank Identification Policy.

1.8 Allow Language Selection

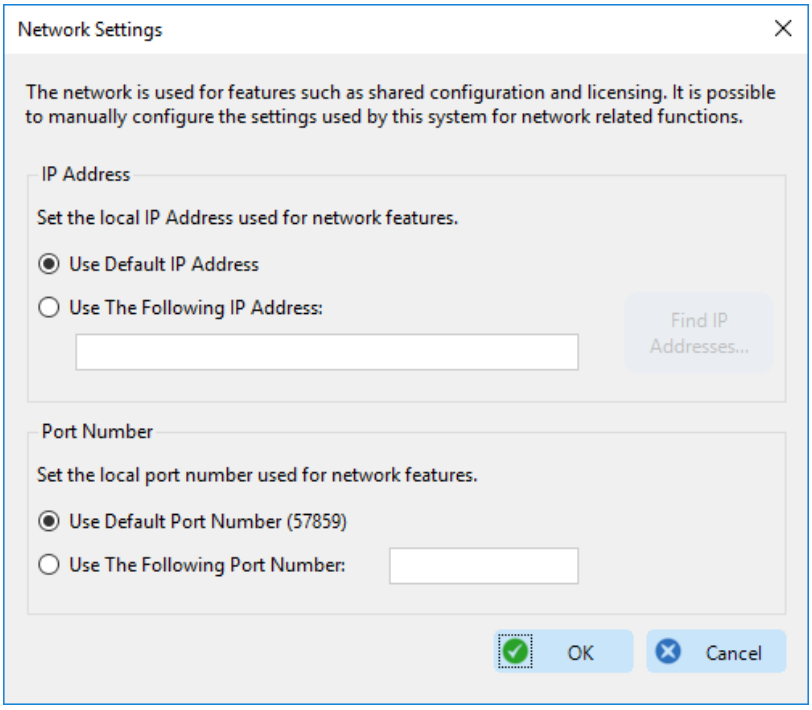
Set whether to show the language selection tool in the Insight [Display Settings] window.

Click in the field to show a drop down menu. Select [Yes] to show the language selection tool and [No] otherwise.

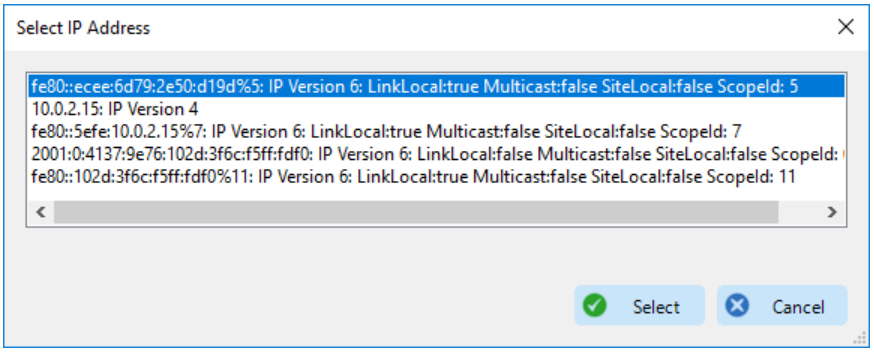
1.9 Network Settings

See section 1.4 “LabSolutions Insight – General” for how to launch the Network Settings window.

If the local computer has multiple IP addresses assigned, use this setting to specify the IP address that will be used by Insight. There is no need to use this setting if there is only one IP address on the local PC.



Select [Use The Following IP Address] to enable the option to customize the network settings. Either type an IP address directly into the text box or press [Find IP Addresses…].



Choose the appropriate IP address and press [Select].

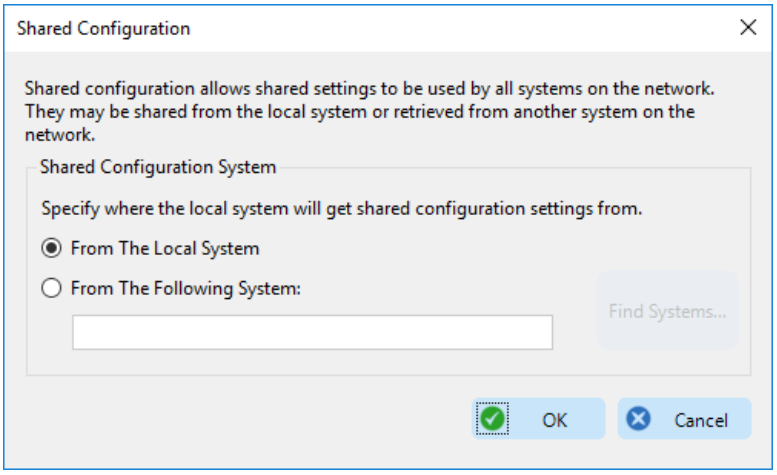
Similarly, select [Use The Following Port Number] in order to customize the port to use.

Press [OK] to apply the changes.

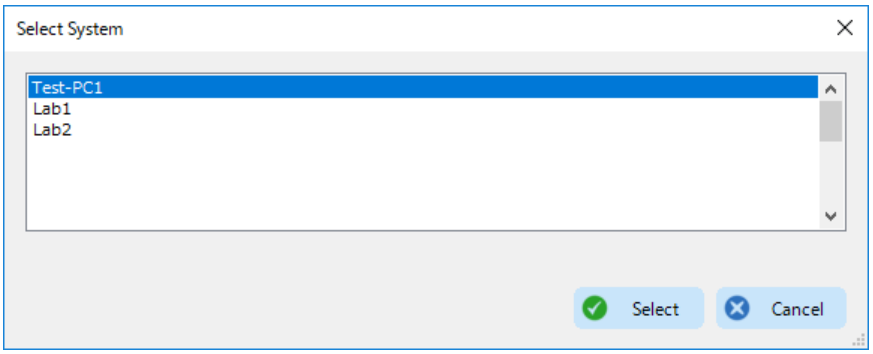
1.10 Shared Configuration

The Common settings can be shared across the local network.

See section 1.4 “LabSolutions Insight – General” on how to launch the Shared Configuration dialog.



From The Local System	Select this option to make the current PC the Master server.
From The Following System	Select a different server as the Master server. Either type in the IP address or the PC name of the Master server or click on the Find Systems… button.
Find Systems…	Click on this button to search for local systems that can be a Master server. A list of candidates is shown in a popup window. The search may take a few moments.



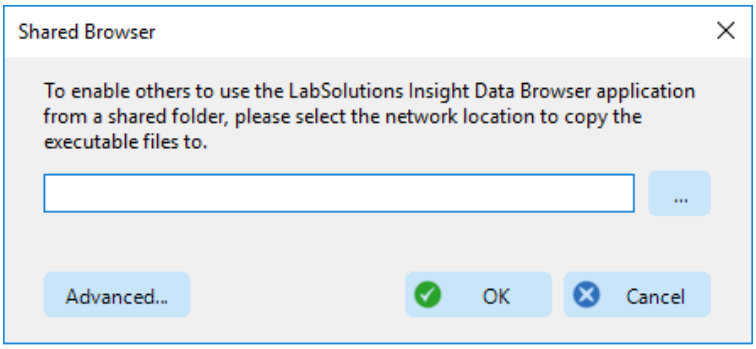
Select a system and click on [Select] or double click on the selected system to designate a system in the list as the Master server. The selected system name will be entered in the edit box.

Alternatively, click on [Cancel] to cancel the selection process.

Click on [OK] to confirm the settings or click on [Cancel] to discard the changes.

1.11 Shared LabSolutions Insight browser

See section 1.4 “LabSolutions Insight – General” for how to launch the Shared Browser window. When Insight in the folder is invoked, the Insight can be used in a computer where the Insight is not installed.

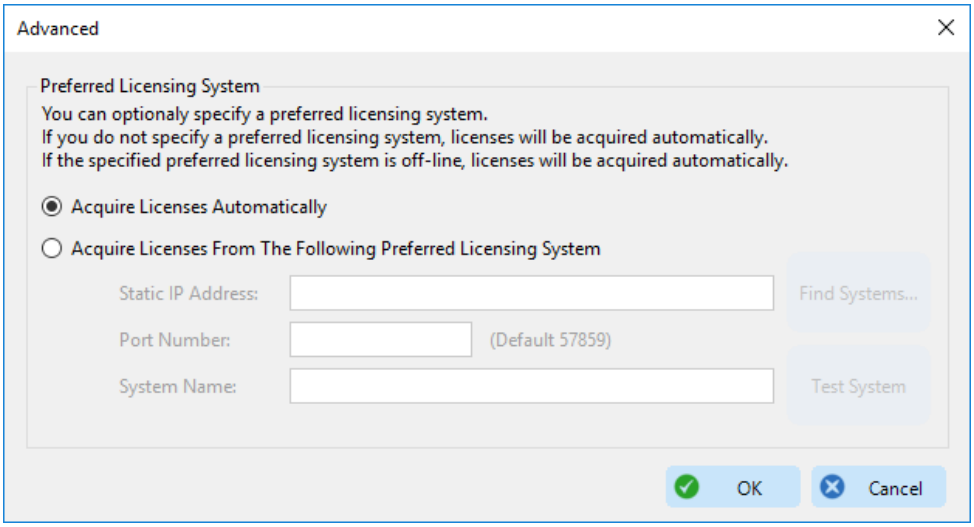


Click on the […] button to launch a folder selector window or type in the edit box directly.

It is preferable to choose a location that is not user-dependent, such as the Desktop, but a generally accessible location such as C:\LabSolutionsInsight\Shared.

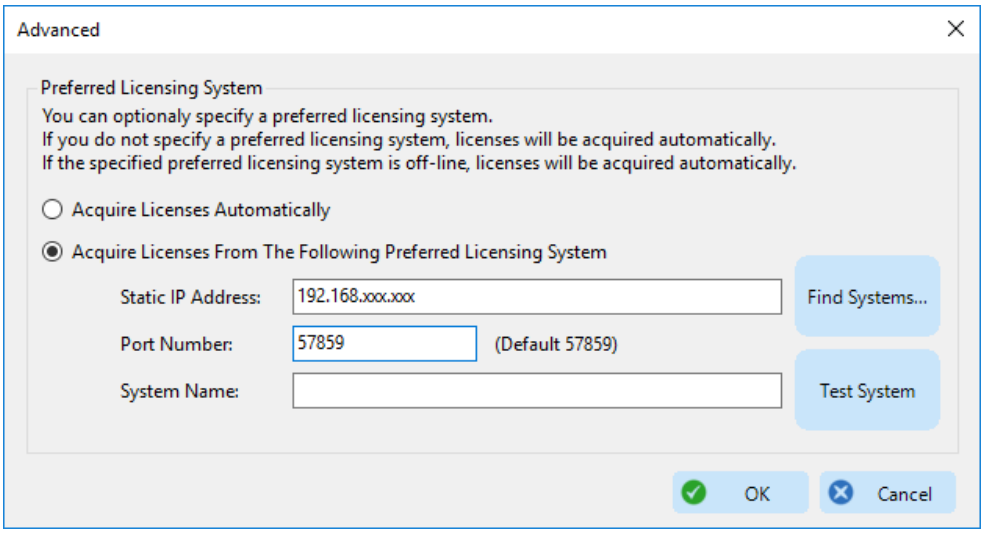
If Insight is to be shared across subnets, set up the licensing system information.

Click on the [Advanced…] button to launch the Advanced window.

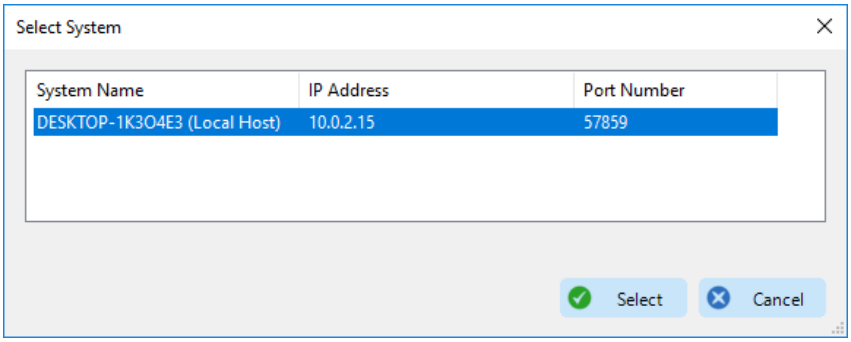


By default, Insight will search for licenses automatically. In order to cross subnets, set up the Preferred Licensing System.

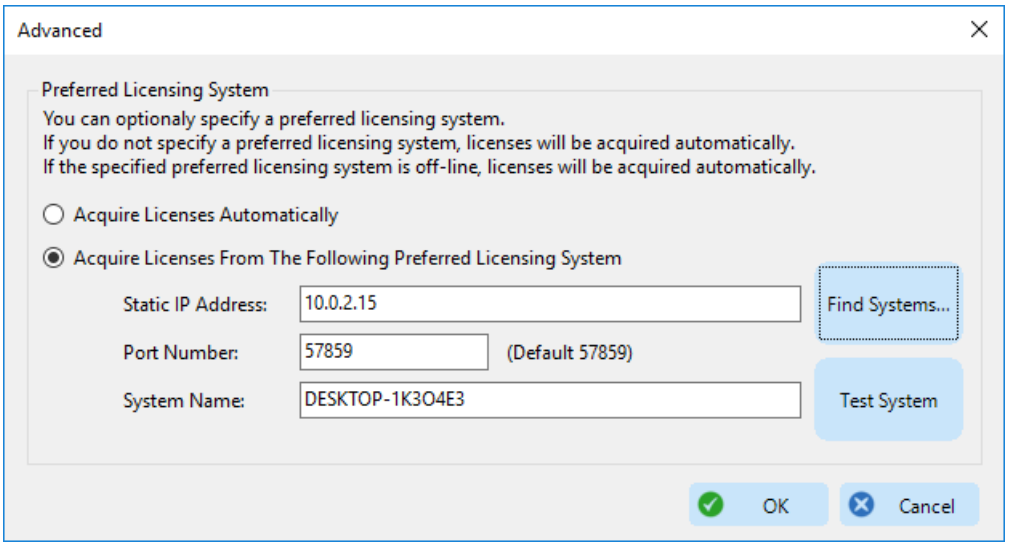
Fill in the Static IP Address of the Server PC and the port number as appropriate.



Fill in the System Name or alternatively, click on the Find Systems… button to search for available systems.



Click on the system which has the Insight license(s) installed and click on Select.

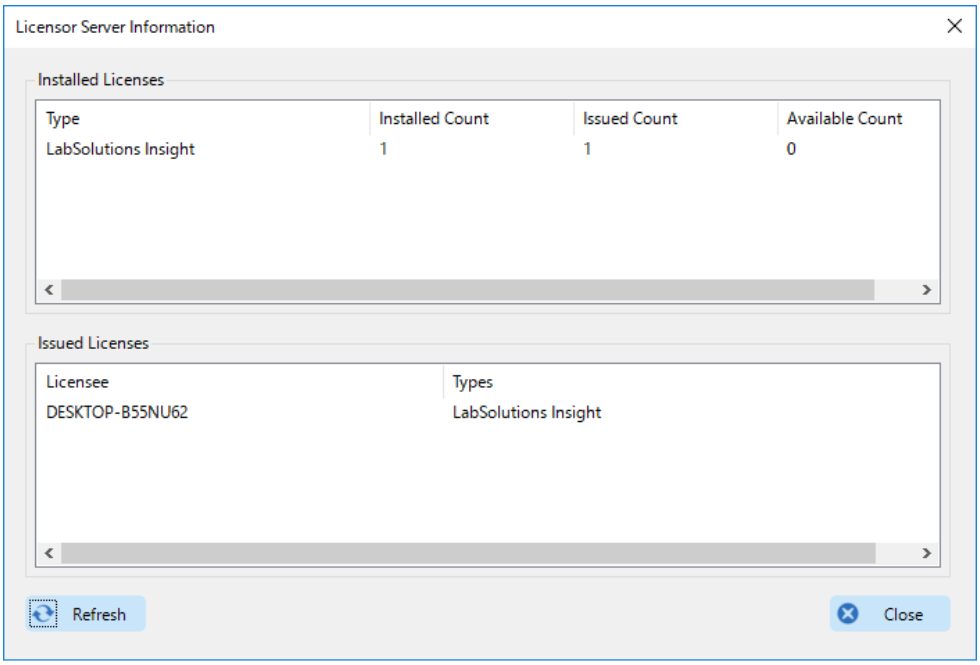


Click on Test System to test that the current settings are correct.

1.12 Licensor Server Information

See section 1.4 “LabSolutions Insight – General” for how to launch the Licensor Information window.

The Licensor Server Information window shows licenses available on the system and who the licenses are assigned to.



[Refresh]	Refresh the license list. This may take a few moments.
[Advanced…]	This button is displayed only when Insight cannot find a license. See section 1.11 "Shared LabSolutions Insight browser” on how to use this function.
[Close]	Close this dialog.

1.12.1 Installed Licenses

The Installed Licenses table displays the types and number of licenses installed on this network system. The table contains the following columns:

Type	The type of license issued.
Installed Count	The number of licenses currently installed on this pc.
Issued Count	The number of licenses that are currently issued on this network system.
Available Count	The number of licenses available on this network system.

1.12.2 Issued Licenses

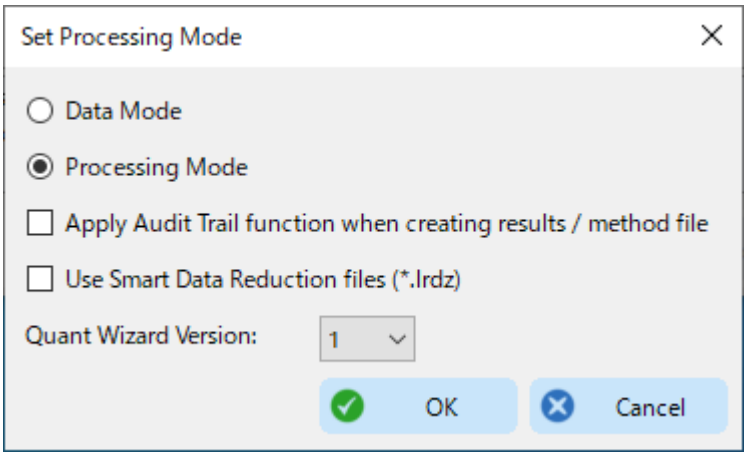
The Issued Licenses table displays details of licenses issued by this computer to the local system and other systems on the network. The table contains the following columns:

Licensee	The host name of the system that has been issued the licenses.
Types	The types of licenses installed on the system.

1.13 Setting Processing Mode

LabSolutions LCMS or GCMSsolution keeps analysis results in each data (*.lcd or *.qgd file). Insight can also keep analysis results in each data (called the Data mode) or alternatively, it can collectively manage a set of data analysis results and their analysis parameters in one file (called the Processing mode).

See section 1.4 “LabSolutions Insight – General” on how to launch the window to set this option. A detailed explanation of the Processing mode is given in section 2.1 “Operation modes”.

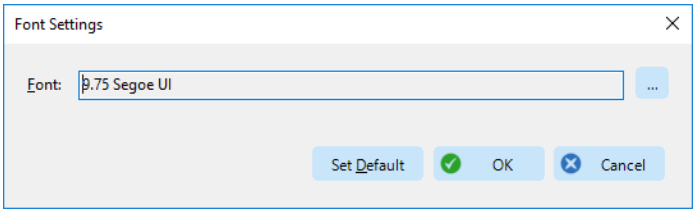


Data Mode	Data Mode : Insight opens LabSolutions files only.
Processing Mode	Processing Mode : Insight opens the processing file in addition to LabSolutions files.
[Apply audit trail function when creating processing/ method file]	Select whether to keep track of changes made to processing files and method files (audit trail). Processing files and method files created after this option is checked will be audit trailed. Check this option in order to comply with regulations such as FDA Part11.
Use Smart Data Reduction files (*.lrdz)	Enable this option when Smart Data Reduction is used at the time of acquiring data using LabSolutions. When this option is enabled, only Smart Data Reduction data files and processing files created from Smart Data Reduction data files can be read.
Quant Wizard Version	Select which version the Quant Wizard should run in. For details, please see section 3.2 [File] Wizard (Processing Mode).
[OK]	Save the settings and return to the [Application Configuration] main window.
[Cancel]	Discard the changes and return to the [Application Configuration] main window.

1.14 Font Settings

The font setting can be changed from the window shown below.

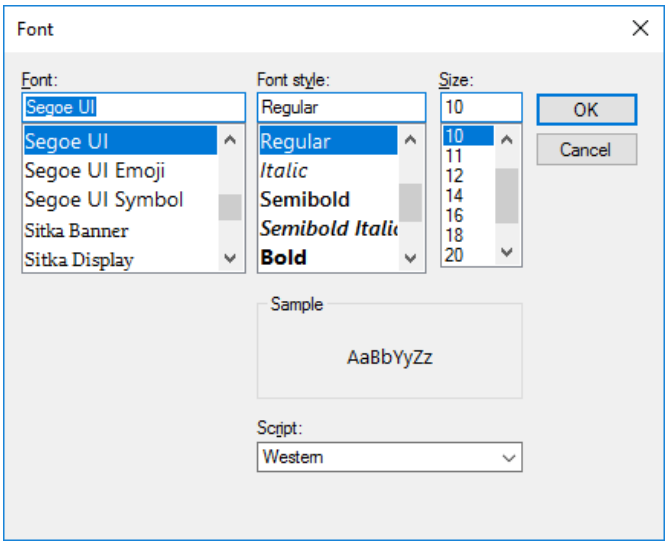
See section 1.3 "Common – Display Settings" on how to launch this window.



[Set Default]	This button is enabled only if the currently selected font is not the system default. Select this button to apply the system default font.
[OK]	Select this button to keep the new font and return to the main [Application Configuration] window.
[Cancel]	Select this button to discard any changes made to the font settings and to return to the main [Application Configuration] window.

Clicking on […] will open the font dialog.

Any changes made to the font settings will only be applied to Insight after selecting [Apply] button or the [OK] button on the main Application Configuration window.

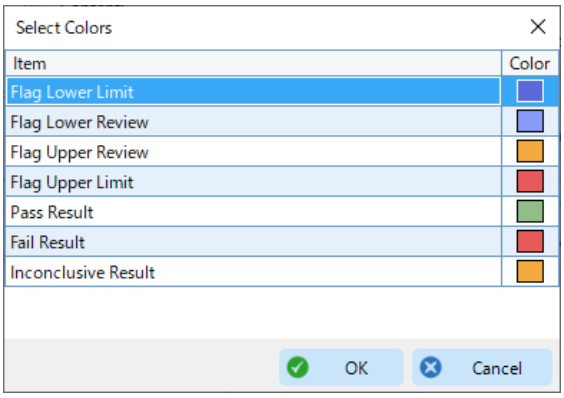


Select a font, font style, size and script and click [OK] to keep the changes. Select [Cancel] to return to the Font Settings window without applying any changes.

1.15 Flag Colors

The settings for the flag color to be used in the flag function can be changed in the window shown below.

See section 1.3 “Common – Display Settings” on how to open this window.



[OK]	Select this button to keep the new flag color and return to the main [Application Configuration] window.
[Cancel]	Select this button to discard any changes to the flag color settings and to return to the main [Application Configuration] window.

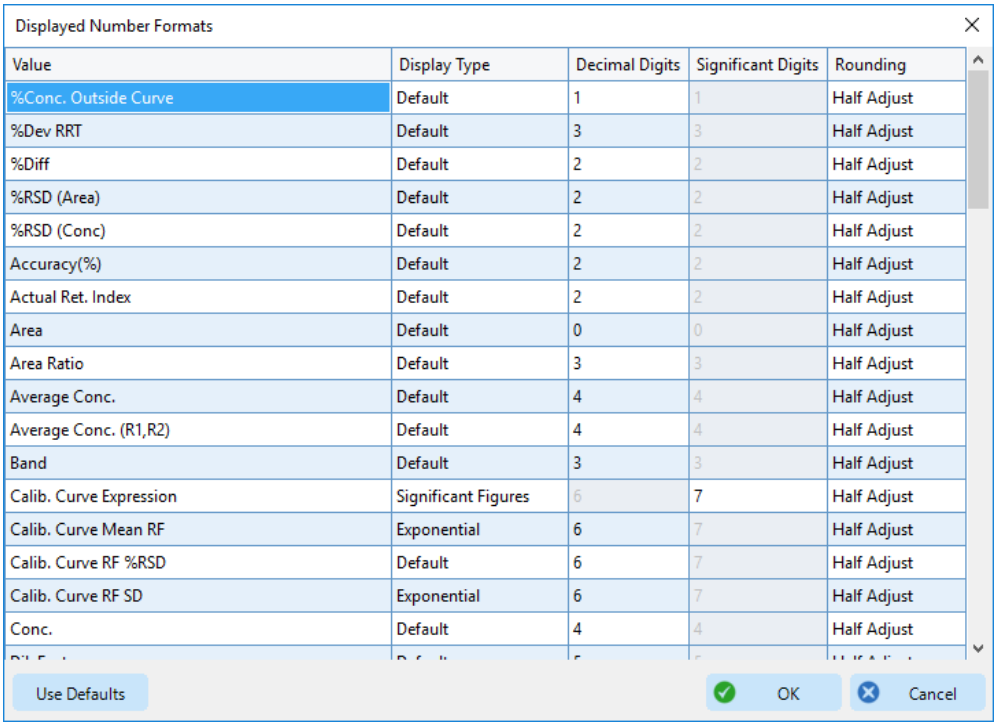
Clicking on the [Color] column for flag color setting opens the dialog box to specify the color.

Any changes made to the flag color setting is applied after clicking [Apply] or [OK] in the main [Application Configuration] window.

1.16 Displayed Number Formats

The settings for the format to display values used on the application can be changed in the window shown below.

See section 1.3 “LICENSE.Common – Display Settings” on how to open this window.



[Use Defaults]	Select this button to reset the format to display values to the default.
[OK]	Select this button to keep the new format setting and return to the main [Application Configuration] window.
[Cancel]	Select this button to discard any changes to the format settings and to return to the main [Application Configuration] window.

[Display Type], [Decimal Digits], [Significant Digits], and [Rounding] can be specified for each value. [Significant Digits] can be specified when [Display Type] is set to "Default" or "Exponential," and [Significant Digits] can be specified when [Display Type] is set to "Significant Figures". [Rounding] can be specified for all values.

[Display Type]	Specify the format to display values. Select from among "Default," "Exponential," and "Significant Figures."
[Decimal Digits]	The number of digits to be displayed after the decimal point can be specified when [Display Type] is set to " Default " or " Exponential." Enter an integer 0 to 8 in " Decimal Digits."
[Significant Digits]	" Significant Digits " can be specified when [Display Type] is set to " Significant Figures." Enter an integer 0 to 8 in " Significant Digits."
[Rounding]	"Rounding" can be specified for the digit number specified in " Decimal Digits " or " Significant Digits." Select "Half Adjust" "Round Up," or "Round Down."

Any changes made to the format setting for values to be displayed is applied after clicking [Apply] or [OK] in the main [Application Configuration] window.

1.17 Report template management

The report template used in LabSolutions Insight is managed in Report Configuration application. Please refer to the Report Configuration manual.

2 LabSolutions Insight General Information

This section gives some general information useful in operating LabSolutions Insight. The layout and general usage of the main window, the idea of flags and the proprietary data format are described.

Both Insight LCMS and Insight GCMS are ready in LabSolutions Insight.

- Insight LCMS handles LabSolutions LCMS files(lcb, lcd, lcmfle).
- Insight GCMS handles GCMSsolution files(qgb, qgd, qgm file).

2.1 Operation modes

LabSolutions LCMS and GCMSsolution stores analysis results in each data file (*.lcd files and *.qgd files).

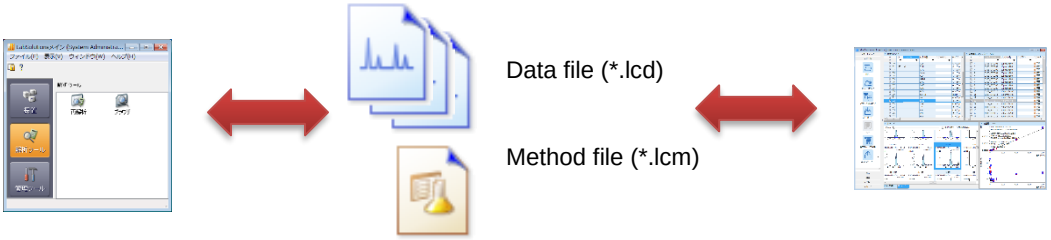
It is possible to choose whether to store the results in the data files (Data mode) or to store the set of data processing results, processing parameters and calibration curve information in a single file (Processing mode).

To switch the data processing mode, refer to "Enable Processing Mode”

2.1.1 Data Mode

LabSolutions LCMS or GCMSsolution stores integration results and quantitation results in the data (*.lcd / *.qgd) files and calibration information obtained from analysing standard samples in method (*.lcm / *.qgm) files. In Data mode, Insight stores necessary information in data files and method files. The following explanation will use LCMS as an example, but the same applies to GCMS as well.

Therefore, results processed by Insight can be read and reprocessed by LabSolutions LCMS and vice versa. If some functionality available in LabSolutions but not available in Insight must be used, it is necessary to use the Data Mode, but otherwise, it is recommended that the Processing Mode explained later is used.



Data file: Stores chromatograms, spectra and analysis results
Method file: stores instrument parameters, analysis parameters and calibration information

Benefits	● Insight processing results can be viewed in LabSolutions.
Points to consider	● Only one analysis results can be stored in a data file. ● When storing the results of analysing using a set of varying parameters, all associated data files need to be copied. ● When analysis results are saved, the original data file date and time gets updated.

2.1.2 Processing Mode

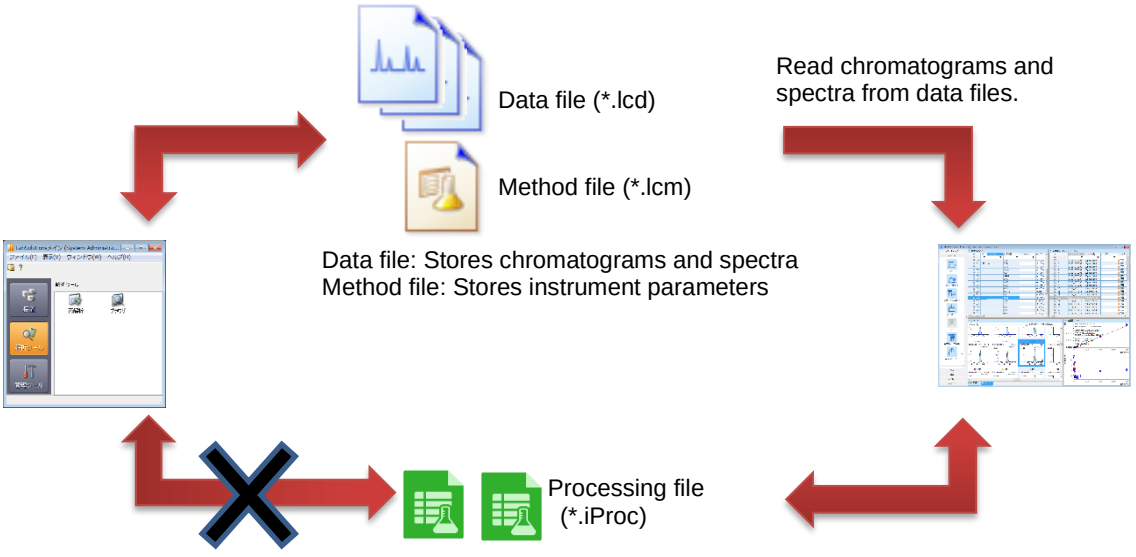
In Processing mode, all analysis results produced by Insight are stored in the LabSolutions Insight Processing file (*.iproc) (processing file for short). This file type is common to LCMS and GCMS.

Processing files store the following information:

- Analysis parameters (integration parameters, quantitation parameters, compound table etc.)
- Flag parameters
- Calibration curve information when performing quantitative processing
- Peak integration results (peak table) for the set of data files
- Quantitation results for the set of data files.
- Flagging results
- Audit trail information

However, LabSolutions LCMS cannot handle processing files so Insight's analysis results cannot be processed using the Quant Browser in LabSolutions LCMS, for example.

In this mode, Insight stores analysis results in the processing file and then reads the results again from the processing file. As an exception, Insight uses the analysis results in the data files and the calibration information in the method file when building the processing file for the first time for a particular set of data. In other words, just after switching to Processing mode using Application Configuration, Insight uses the analysis results stored in the data files and method files to create the processing files.



Benefits	● Multiple processing files can be created for a set of data files. ● Analysis results from a collection of data files are stored in a single file for easier presentation and interpretation. ● Original data and method files are unaffected when analysis results are saved.
Points to consider	● Insight is required to view Insight processing results.

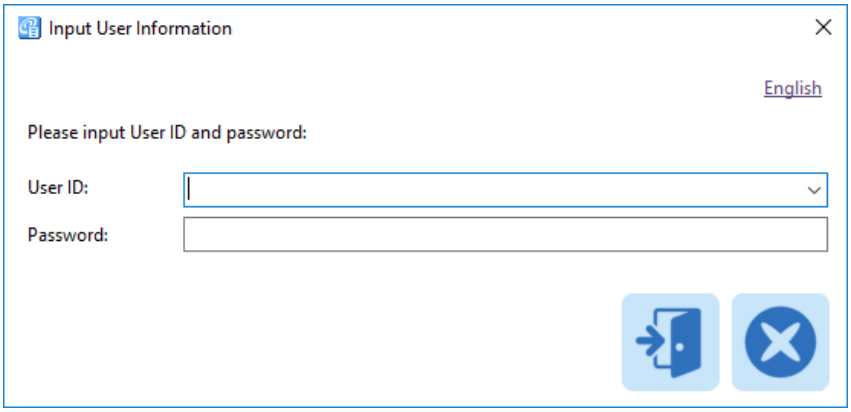
2.2 Log-in

Launch LabSolutions Insight by double clicking on the Insight icon on the desktop. Alternatively launch Insight from Windows Start menu.

Type in or select in the drop down list the appropriate user name and type in the password. The user names and passwords must be the same as those for logging into GCMSsolution, LabSolutions or Insight.

Below are the default users available at the time of installation:

Pre-installed system	User ID	Password
GCMSsolution	Admin	(blank)
LabSolutions	Admin	(blank)
none	admin	admin



If Insight is configured to allow users to change the language, there will be a hyperlink on the top right corner indicating the current language. Click on the hyperlink to show a list of languages to choose from. Currently, Insight supports English and Japanese.

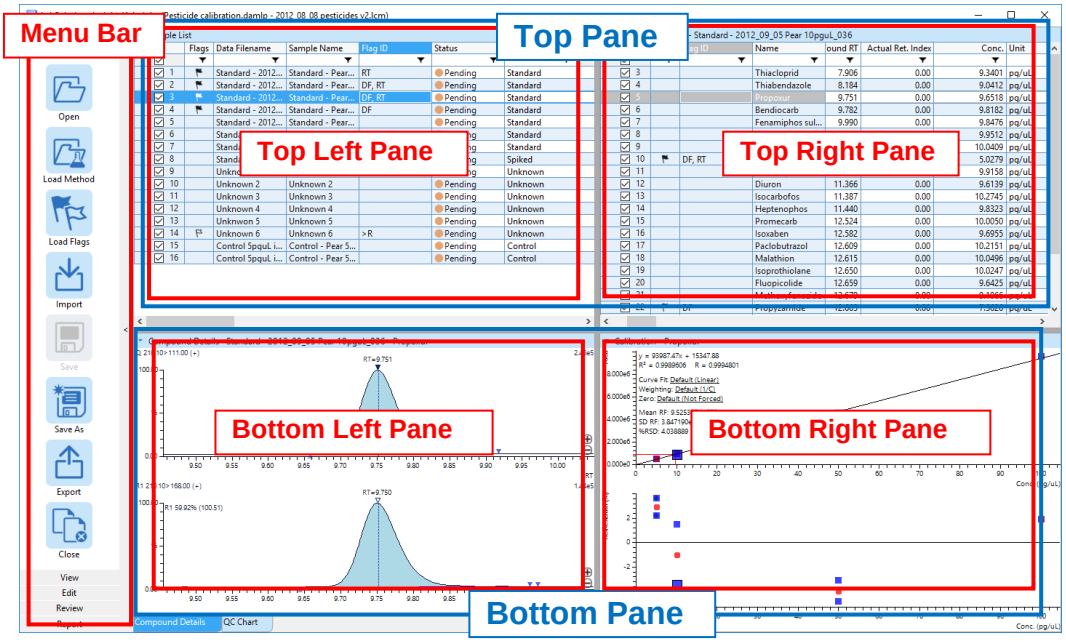
See section 1.2 “Common - General” on how to enable/disable language selection.

2.3 Main Window

There are, in large, two parts to the main window; the menu bar on the left and the rest of the window which is used for displaying data. The menu bar and data panes are described briefly below.

2.3.1 Display

The display consists of the menu bar on the left, the top data pane for showing quantitative results and the bottom pane for showing additional information.



Pane layout can be customized by floating and or docking each pane. Here, brief description of each pane is given assuming the default layout. See sections 2.3.3 “Data panes” and 3 “LabSolutions Insight Functions” for details.

The top pane is divided into the left and right panes. The type of information shown in each pane depends on the selected view.

Compound View	Top Left pane	[Sample List] pane
	Top Right pane	[Compound Results] pane
Sample View	Top Left pane	[Compound List] pane
	Top Right pane	[Sample Results] pane
Summary View	Top pane	[Summary] table pane occupies the entire top pane

The bottom pane shows chromatograms. The following two views are available and they can be switched by selecting the appropriate tab.

Compound Details	Show chromatograms and calibration curve for one compound.
Survey	Show all compound chromatograms for all samples.

QC chart or calibration curve can be displayed in the bottom pane.

Calibration Curve	Show the calibration curve for one compound and residual plot.

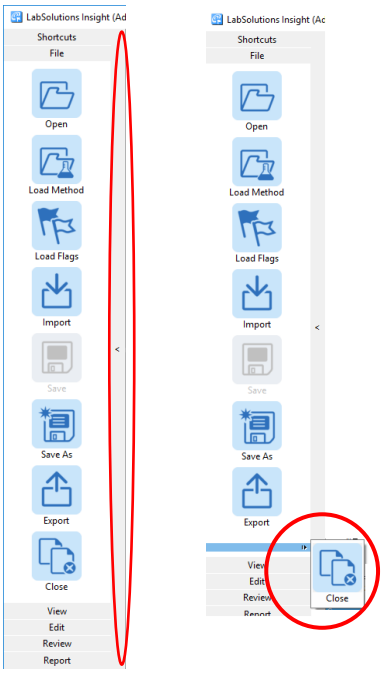
QC Chart	Show a graph in which the quantitative values are plotted or error bar.

2.3.2 Menu bar

The menu bar is on the left of the main window which comprises a set of menu “bands” holding buttons for performing related operations. One menu band is reserved for user-definable “Shortcuts”, into which the most commonly-used tool buttons may be grouped.

The menu bar can be collapsed by clicking on the divider.

Depending on the window size, all the menu buttons cannot be shown. Click on the bottom right button to show all the buttons.



Shortcuts Shortcuts menu band with favourite items

File File menu band with file-related operations.

Open

Open a batch file and a DAMLP file.

Load Method

Load a method file.

Load Flags

Load flag setting and setting to hide compounds from the DAMLP file.

Import

Import Unknown type data files.

Save

Save current work.

Not available in Read Only mode.

Save as

Save the current method file and DAMLP file under a new name.

Save Flags

Save the current flag settings as a DAMLP file. (Processing Mode only)

Export

Export results and method to file or text.

[Results to File] Export quantitative results as text.

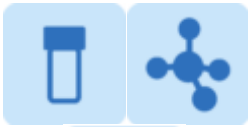
[As New Method] (Processing mode only) Save quantitation parameters and compound table information to a new LabSolutions method (*.lcm) file. This can be used to run acquisition based on analysis done in Insight.

Close

Close current batch, data and method files.

View

View menu band with view-related operations.

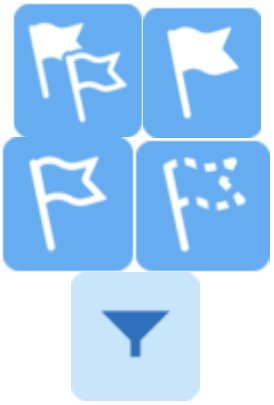


Compound

Sample

Summary

Switch between three different views.



Flags Filter

Outliers or Review

Outliers only

Review only

No Outliers or Review

All

Filter results according to flag status.

Compound Details

Launch Compound Details pane.

Calibration Curve

Launch Calibration Curve pane.

Survey

Launch Survey pane.

QC Chart

Launch QC Chart pane.

Select whether to show [Levey-Jennings chart] or [Error bar chart].

Settings

Configure display settings.

Audit Trail

Audit Trail setting can be changed.

Show the audit trail log saved in a file.

Edit

Edit menu band with edit-related operations.

Edit Method

Edit Integration, Identification and Quantitation parameters.

Integrate Batch

Perform automated peak integration on all compounds in all samples.

Unavailable if the data file is opened in Read Only mode or if the user does not have edit rights.

Integrate Sample

Perform automated peak integration on all compounds in the current sample.

Unavailable if the data file is opened in Read Only mode or if the user does not have edit rights.

Integrate Compound

Perform automated peak integration on the current compound in the all sample.

Unavailable if the data file is opened in Read Only mode or if the user does not have edit rights.

Integrate Result

Perform automated peak integration on the current compound in the current sample.

Unavailable if the data file is opened in Read Only mode or if the user does not have edit rights.

Edit Table

Edit settings in the sample list or quantitative results table. A mark is added to the item name in the table when the value can be edited.

Unavailable if the data file is opened in Read Only mode or if the user does not have edit rights.

Edit Flags

Edit flag criteria.

Operates in read-only when the user does not have edit rights.

Hide compounds

Select compounds not to be displayed on the table.

Review

Review menu band with review-related operations.

Accept

Change the status of the selected result to Accept.

Rerun

Change the status of the selected result to Rerun.

Pending

Change the status of the selected result to Pending.

Send

Determine the status and save the DAMLP file.
This is enabled when the HL7 option software is installed.
Unavailable if the data file is opened in Read Only mode or if the user does not have edit rights.
Unavailable when Edit Tables mode is ON.

Report

Report menu band with print-related operations.

Reports

Select the report template and print reports

Report

Print GCMSsolution or LabSolutions report. Report is printed using the report format stored in the selected data file.

This option is unavailable if neither GCMSsolution nor LabSolutions is installed.

(Data Mode only)

2.3.3 Data panes

All data panes can be pulled out to float or docked in any user-defined region. The proportions of the client area assigned to each pane can be adjusted by grabbing and dragging their borders.

Below are explanations of the panes as they appear by default.

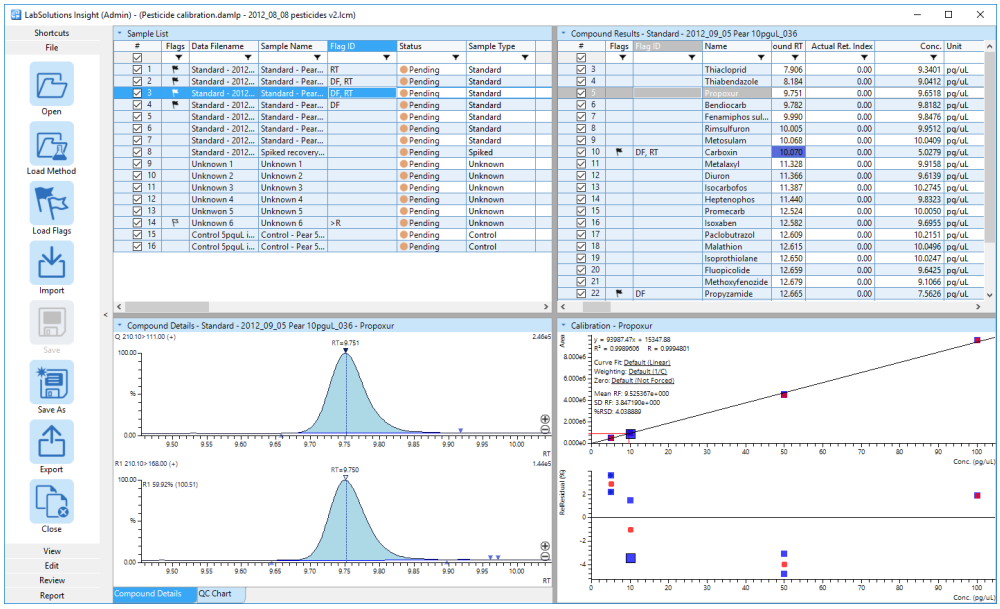
Top Left pane	This pane holds the primary list for listing items to choose the quantitation results by. In Compound View, the samples (data) are listed here. In Sample View the compounds are listed here. The pane is only available in Compound or Sample views.
Top Right pane	This pane holds the results table for listing quantitation results for the selected item in the left pane. For Compound View this lists the quantitation results for each compound. For Sample View, this lists the quantitation results for each sample. The pane is only available in Compound or Sample views.
Top pane	This is used to show a grid of results for all compounds and all samples. The pane is only available in Summary view.
Bottom Left pane	This pane is used to show the chromatograms, and QC chart. If this pane is not shown, click [Compound Details], [Survey], or [QC Chart] to show the pane.
Bottom Right pane	This pane is used to show the calibration information. If this pane is not shown, click [Calibration Curve] to show the pane.
Bottom pane	This pane is used when either all tabs in the Bottom Left pane are disabled or when the calibration curve is not showing.

2.3.3.1 Docking panes

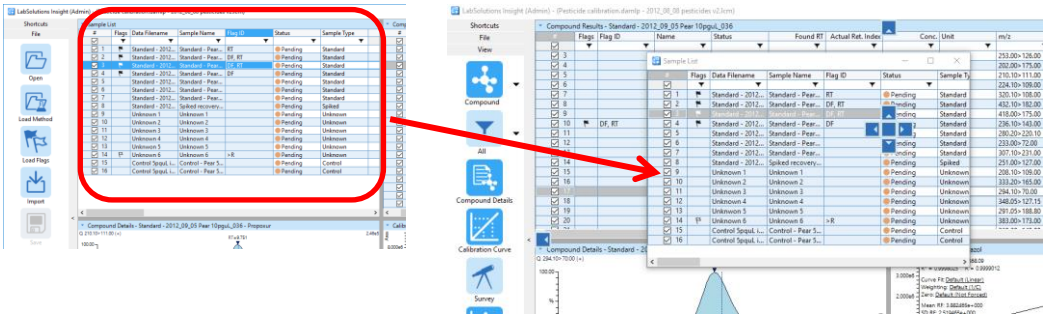
Floating forms may be docked back inside the main form client area at a number of target positions - docked to left-hand side, right-hand side, top and bottom or into the middle of the client area.

If a docked form already exists in the target position, then the new form will be added as a new tab in that position.

Default Layout



Changing Layout

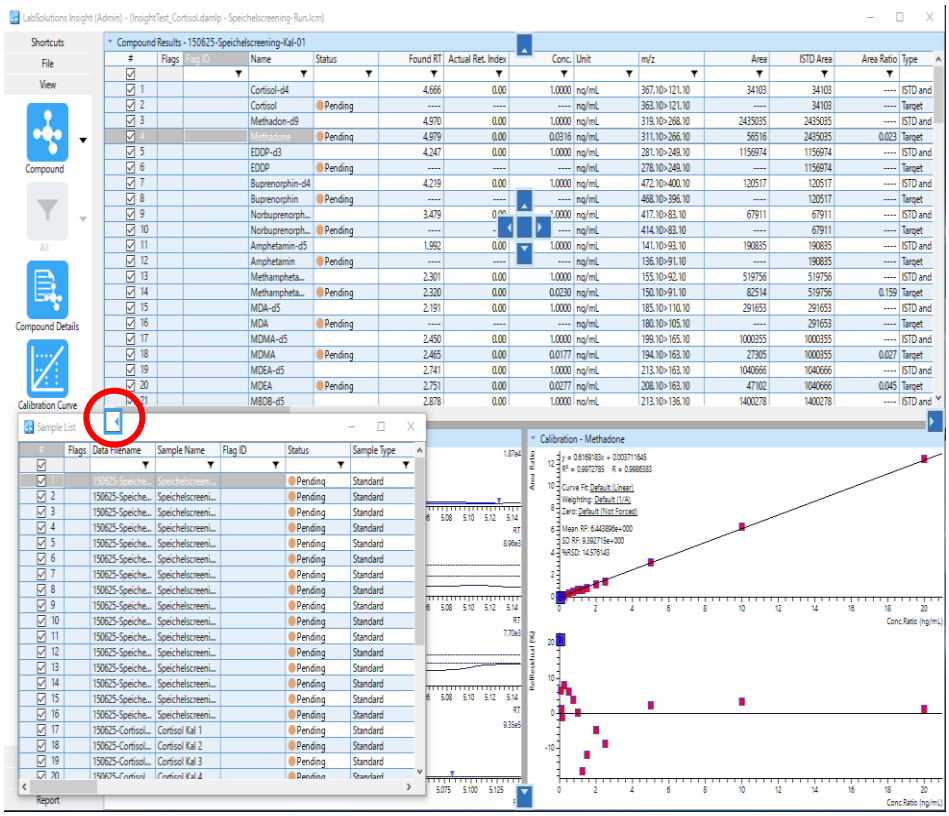


Grabbing pane header and moving the mouse floats out the pane.

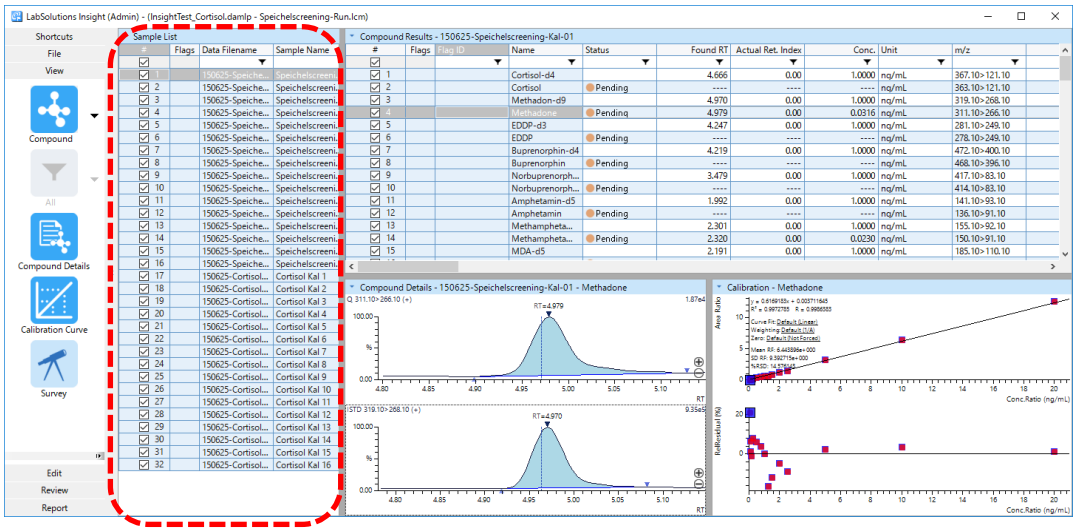
Dock indicators are shown so that the pane can be docked back into the main window.

Dock Left

Drag the pane over the left dock indicator and release it.



Floating pane is now docked left.



Similarly, floating panes can be docked in all directions and locations in accordance with the dock indicators.

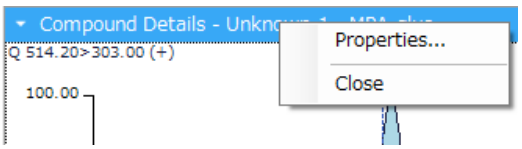
> **NOTE**
>
> Docking the Sample List to the right does not change the View to Sample View. Similarly, docking the Compound List to the right does not change the View to Compound View.

2.3.3.2 Docked Captions and Menus

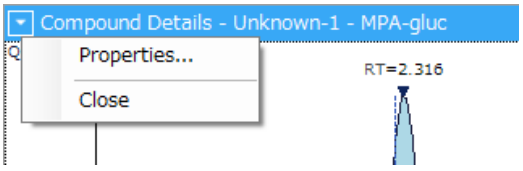
When a pane is docked, it will display a mini caption to facilitate dragging and floating out and also to access a pane menu to allow closure and access to Options for that pane (when available).

Accessing a pane's caption menu:

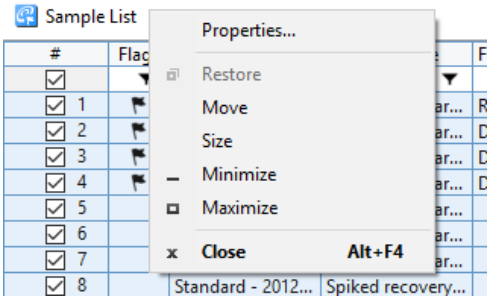
Right-click on the docked pane's caption.



Click on the docked pane's drop down control.



Right-click on the floating pane's window caption to access extended system menu.



The same menu can be accessed by clicking on the icon of the floating pane's window caption.

2.3.3.3 Persistence

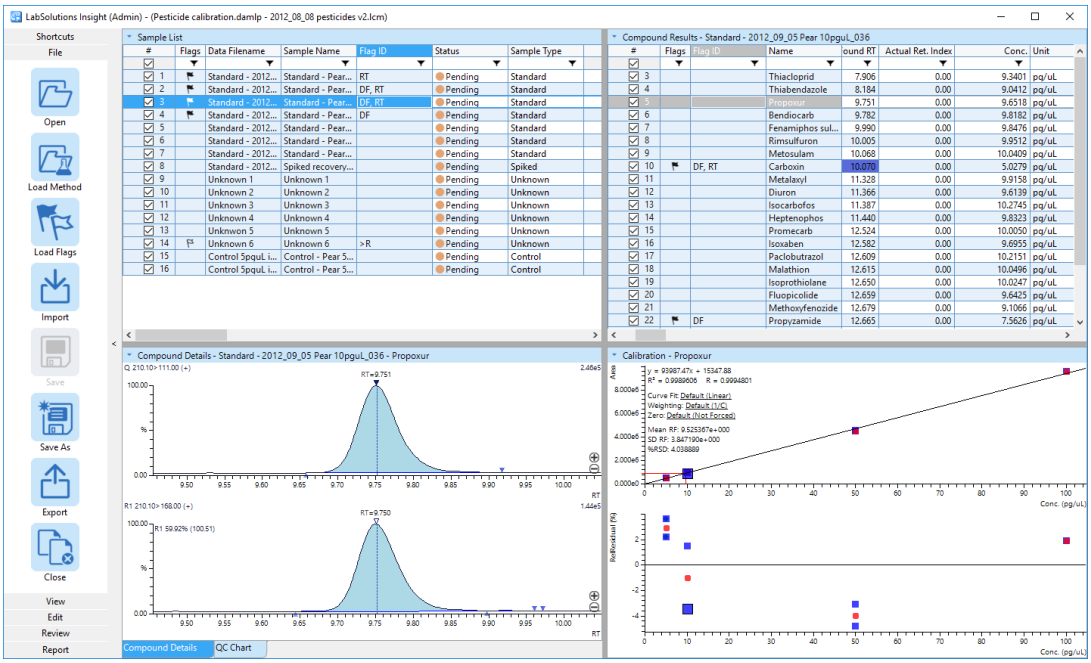
When the Insight browser is closed the position and state (minimized, normal or maximized) of the main window is persisted along with the docked and floating window positions of the internal list, details and chromatograms. Then when Insight is subsequently started all of these settings will be restored to the same state as when the program closed. If a second display is no longer available, then those windows will be brought back onto the primary or reset to default positions (as appropriate).

2.4 Views and Panes

LabSolutions Insight has three views by which it displays quantitative results; Compound, Sample and Summary. There are also two auxiliary views for showing detailed information or for viewing the data in a different way.

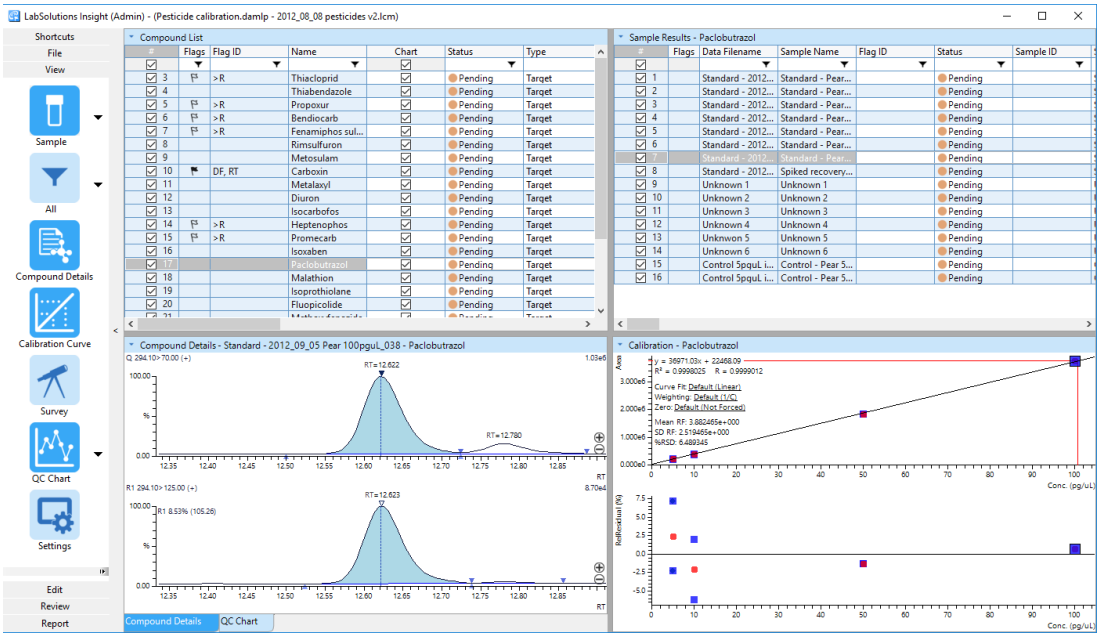
2.4.1 Compound View

This view is for viewing results for each compound by selecting a sample of interest. By default, the Sample List is in the left pane and the Compound Results are in the right pane.



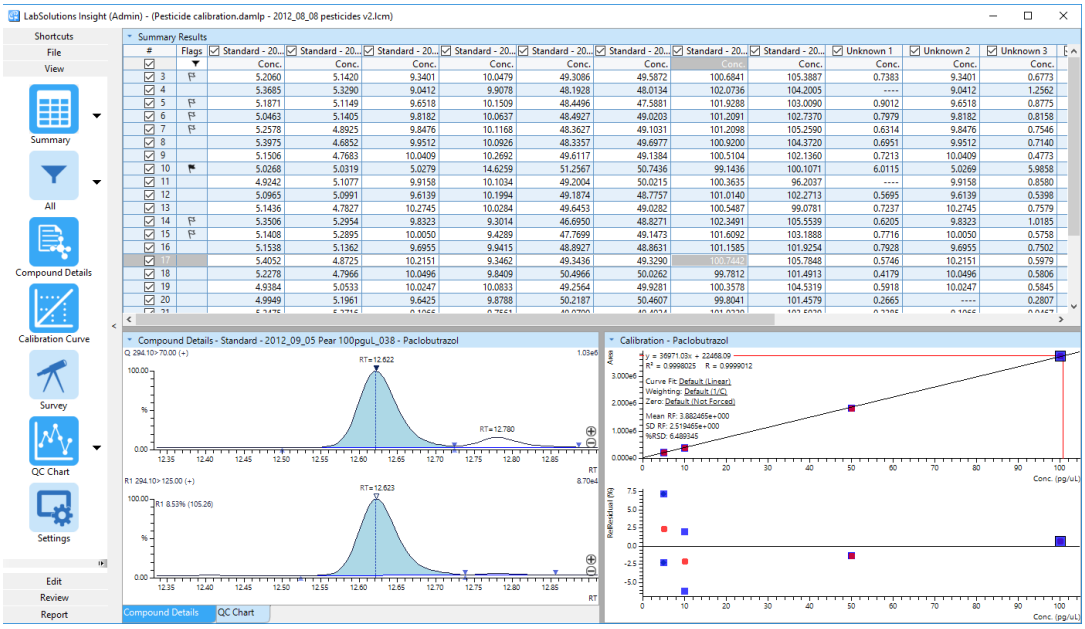
2.4.2 Sample View

This view is for viewing results for each sample by selecting a compound of interest. By default, the Compound List is in the left pane and the Sample Results are in the right pane.



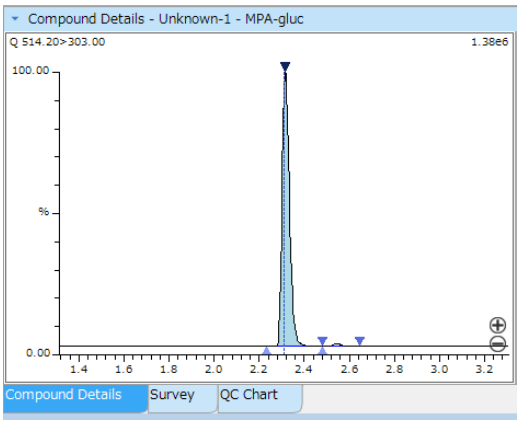
2.4.3 Summary View

This view is for viewing results as a grid. Values such as Concentration, Area, Area Ratio, Height and Retention Time are shown for all compounds and all samples. By default, the summary is shown in the top pane.



2.4.4 Compound Details Pane

This view is for showing peak chromatograms and calibration information for each compound. By default, this view is shown in the bottom pane. If Survey or QC Chart is also enabled, it will become a tab sheet in the bottom pane.

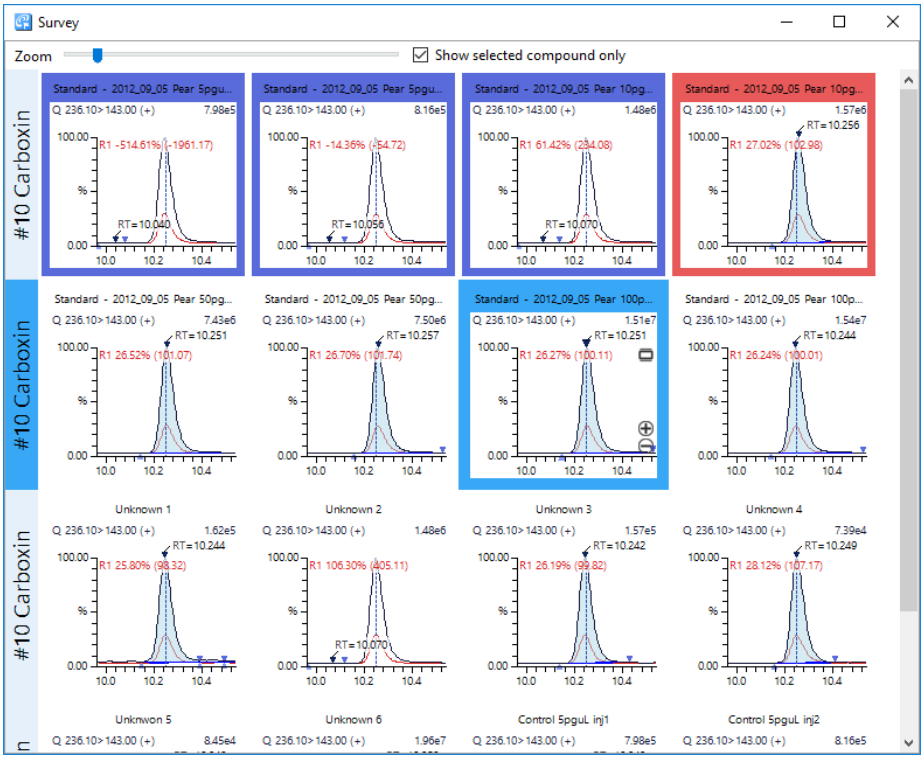


The button for showing or hiding Compound Details is a toggle button. Press it once when it is turned OFF (light blue) to enable the view and or to bring it to the front. Press it once when it is turned ON (darker blue) and showing on top to close it.

When this view is enabled, the peaks, calibration curves and residual plots are shown for the currently selected Compound from the currently selected Sample. Only a single instance of a Compound Details is shown at any time. Its contents are automatically refreshed when a different sample or compound is selected in the results.

2.4.5 Survey Pane 1.3.1

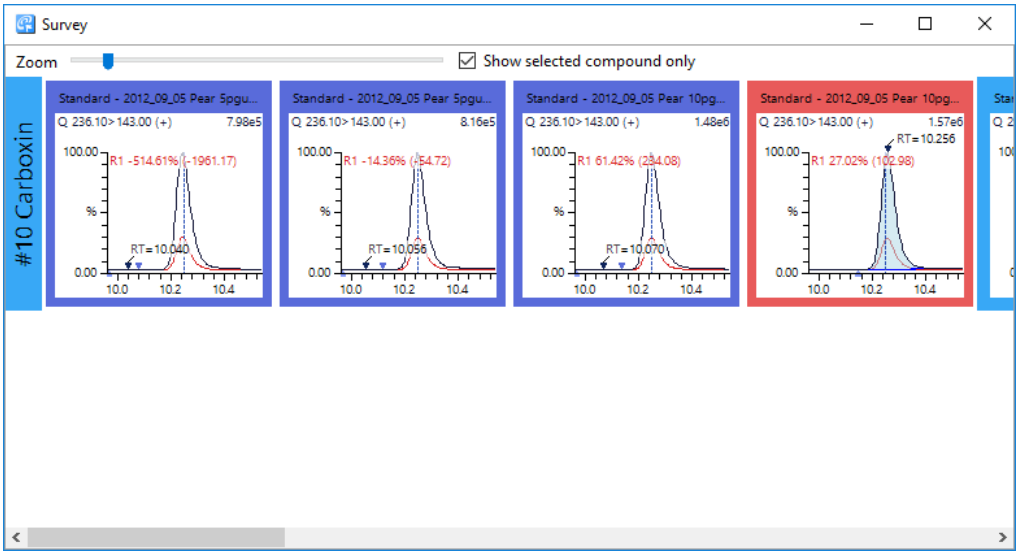
This view is for comparing chromatograms across compounds. Chromatograms are shown as tiles with compounds listed in the vertical direction and samples in the horizontal direction. It can be changed to a tile format where samples are listed in the vertical direction and compounds in the horizontal direction. By default, this view is shown in the bottom pane. If Compound Details or QC Chart is also enabled, it will become a tab sheet in the bottom pane.



The button for showing or hiding Survey is a toggle button. Press it once when it is turned OFF (light blue) to enable the view and or to bring it to the front. Press it once when it is turned ON (darker blue) and showing on top to close it.

When this view is opened, the quantified peak for each compound in the checked sample(s) is shown.

The number of peaks shown for each compound is controlled by the number of samples that are checked in the Sample List, Sample Results or Sample columns in the Summary Results and the number of compounds that are checked in the Compound List, Compound Results or the Compound rows in the Summary Results. If the Compound List or Compound Results are sorted the order of rows will be changed if Flags Filter status is toggled, then those samples that are filtered out appear faint or are not displayed. In this pane, the user can select a mode where chromatograms are displayed in a single row or a mode where they are displayed in multiple rows when they do not fit in a single row.



Mode where chromatograms are displayed in a single row

Mode where they are displayed in multiple rows

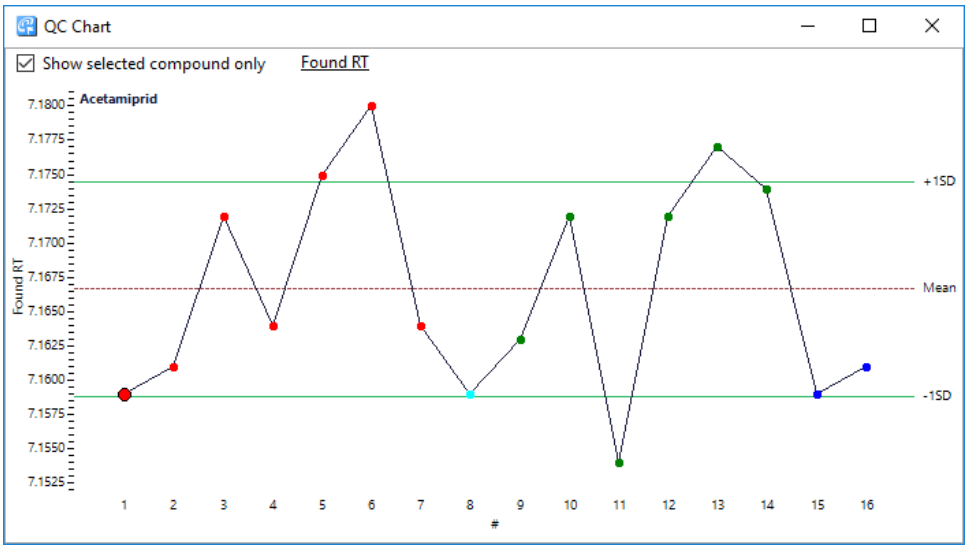
Checking the “Show selected compound only” checkbox will show a single row (a single compound) in the pane. The compound row shown is determined by the currently selected compound in the results. Similarly, selecting the "Show selected sample only" checkbox will show only the samples currently selected on the results table.

NOTE

In [Survey], specified compounds or samples are displayed in a horizontal arrangement. The user can select to display filtered chromatograms in gray or hide them after filtering is performed on a list or results table from options.

2.4.6 QC Chart Pane

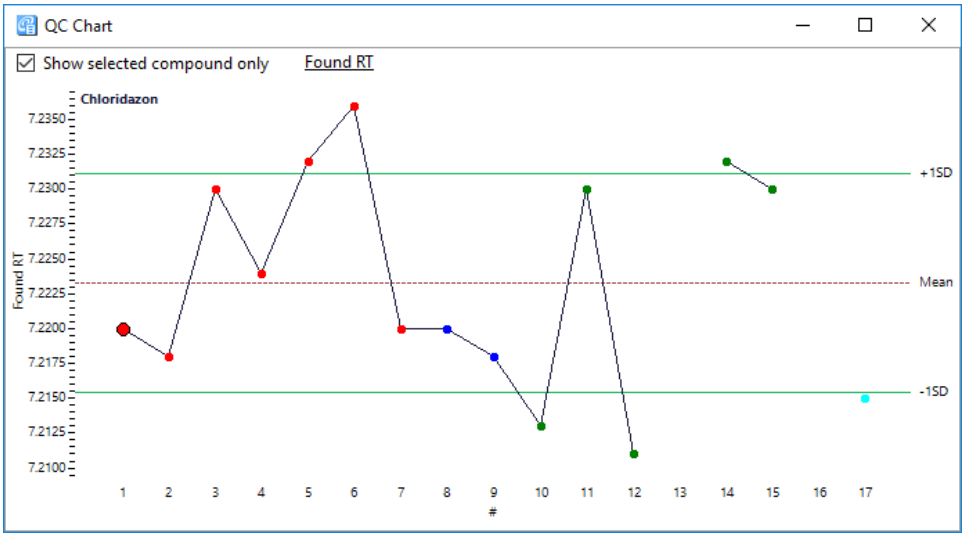
This pane displays the quantitative results of the selected compounds in a chart format. By default, this view is displayed on the lower pane. When [Compound Details] or [Survey] is activated, it is displayed on the lower pane as a tab sheet.



The user can switch to display and hide [QC Chart] using a button on the menu band. Press it once when it is turned OFF (light blue) to enable the view and display it in front. Press it once when it is turned ON (darker blue) to close the displayed view.

Select the graph to display in the [QC Chart] pane from "Levey-Jennings Chart" and "Error Bars Chart." This section uses Levey-Jennings Chart for explanation. For details, see section 3.18 "[View] QC Chart".

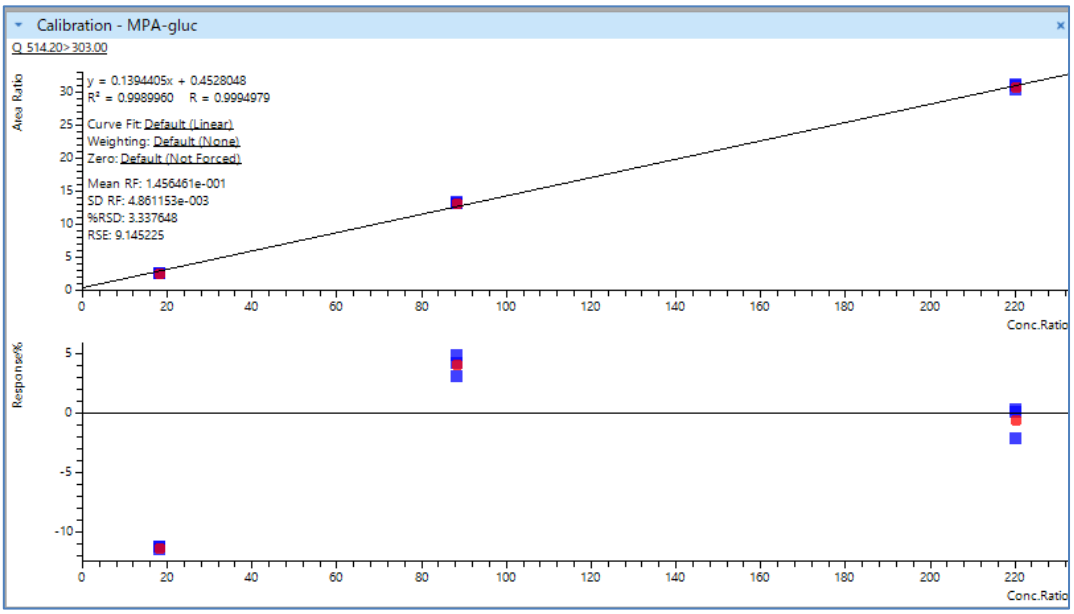
When this view opens, the quantitative results for the compound selected on the table are displayed in chart format. The target quantitative values are shown on the vertical axis and sample IDs on the horizontal axis. The name of the selected compound is displayed in the upper left area of the chart. Quantitative results to be displayed can be selected by clicking the quantitative result item name in the upper part of the chart. Select samples to display on the chart using the checkbox for the [Chart] item in [Sample List] or [Sample Results]. When there are no applicable quantitative results, data points are not displayed. However, since applicable sample IDs are displayed, the chart is displayed with unconnected points.



Data points for the currently selected sample are displayed larger than other data points. The color, shape, and size of data points can be set for each sample type. The line connecting neighboring data points can be displayed or hidden.

2.4.7 Calibration Curve Pane

This pane displays the calibration curve and residue plot of the selected compound. By default, this view is displayed on the right side of the bottom pane. When [Compound Details], [Survey], or [QC Chart] is activated, it is displayed on the right side of them.



Switch to display and hide [Calibration Curve] using a button on the menu band. Press it once when it is turned OFF (light blue) to enable the view and display it in front. Press it once when it is turned ON (darker blue) to close the displayed view.

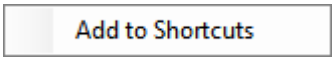
When this view opens, the quantitative results for the compound selected on the table are displayed. Calibration points on a calibration curve correspond to the samples for which [Calibration Curve] checkbox is selected in [Sample List] or [Sample Results] table. The [Calibration Curve]

checkbox is enabled when the sample type of the respective sample is "Standard" or "Control." (Only the "Standard" sample type is used for calibration points.)

2.5 Shortcuts

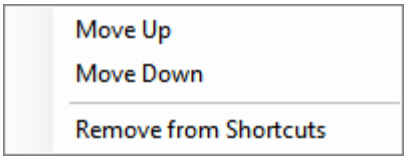
Shortcuts are located at the top of the menu bar and are user-definable. Any menu item can be added into the shortcuts band for quicker access. Items within the shortcuts band may be arranged and removed via the context menu on each item.

Right click on any menu button to show the following context menu.



Selecting this context menu adds a copy of the selected button to the Shortcut band in the Menu bar.

Right click on any shortcut button in the Shortcut band to show the following context menu.



Select Move Up or Move Down to order the shortcut buttons in the desired order.

> **NOTE**
>
> When selecting the topmost item in the band, Move Up is disabled. When selecting the bottommost item in the band, Move Down is disabled.

Select Remove from Shortcuts to delete the selected item from the Shortcut band. Since shortcut buttons are copies, the original buttons are never lost by this operation.

Shortcut menu items are persisted between sessions on a per-user basis.

The status (e.g. enabled/disabled, check state etc.) between the original buttons and their shortcut buttons, or if it is a drop down button, the status between the original drop down items and their shortcut drop down items, are always synched.

2.6 Flags

In the list, results and graph panes, where values are found that are out of some expected range, these are flagged up as such either in dedicated flag columns or beside a property in graphs.

Please also note that even if the target compound is correctly identified, if the internal standard is not identified correctly, or if the calibration curve is a quadratic curve where the maxima is smaller than the target compound area or height and therefore does not have a solution at that area or height, the concentration cannot be calculated and will be shown as “0.000”. Please be aware of this behaviour when applying flags to the concentration values.

> **NOTE**
>
> When the target compound is misidentified the flagging functionality may report outcomes erroneously. In order to interpret the results correctly, please view the chromatograms carefully and make sure target compounds are correctly identified.

2.6.1 Flag colors

Two types of colors are used to indicate flagged values:

1. Cool colors such as blue are where the value is below the flag’s lower threshold, or where it is implied that an outlier must be below the set threshold.
2. Warm colors such as red are where the value is above the flag’s higher threshold, or where it is implied that an outlier must be above the set threshold.

Details of the value found and the range it exceeds are captured at the point of discovery and stored as flag details. The flag color can be changed in Application Configuration

2.6.2 Flag types

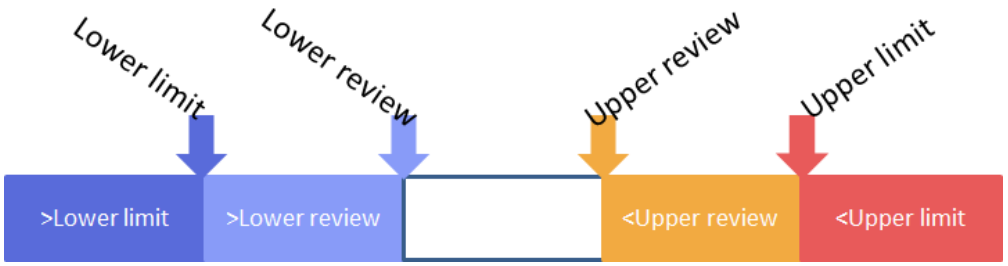
There are two discrete types of flags, “Review” and “Outlier”, for concentration.

In general, the idea is that Outlier type flags indicate that there is a problem with the data integrity, possibly because the sample analysis had an issue or the sample preparation wasn’t carried out correctly, etc.

The Review type flag indicates that the sample was analysed correctly by the instrument but the results indicate that the sample has failed to meet a required criterion.

The different types of flags will be highlighted with different colors on the Browser UI and filtering is available for the results based on flag type.

The only flags that are “Review” type are “Lower Conc. Review” and “Upper Conc. Review”.

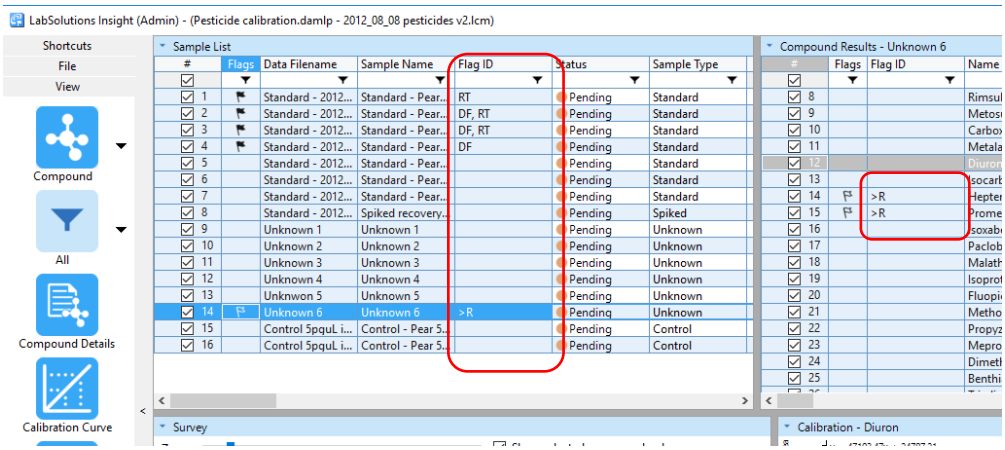


2.6.3 Flag ID

When a flag is applied to a value in the results, the ID of the flag is also displayed to aid the understanding of the reason for the flags being raised.

The Flag IDs are shown in the Flag ID columns in Sample List, Compound Results, Compound List and Sample Results.

If multiple flags are applied, they are listed separated by a comma.



The Flag IDs are defined as shown below:

		Flag Groups					
Flag ID	**Corresponding Flag**	**Unknown**	**Standard**	**Control**	**Spiked**	**Unspiked**	**Blank**
<L	Lower Conc. Limit	✓					
<R	Lower Conc. Review	✓					
>R	Upper Conc. Review	✓					
>L	Upper Conc. Limit	✓					
RT	Retention time	✓	✓	✓	✓	✓	✓
RT%	Retention time (%)	✓	✓	✓	✓	✓	✓
IRr	Ion ratio (relative)	✓	✓	✓	✓	✓	
IR	Ion ratio (absolute)	✓	✓	✓	✓	✓	
R2	R^2		✓				
CR	Calibration Range	✓					
BC	Blank concentration						✓
DF	%Difference		✓	✓	✓		
AC	Accuracy(%) (*)		✓	✓	✓		
CVc	%RSD conc.		✓	✓			
CVa	%RSD area		✓	✓			
SN	S/N	✓	✓	✓	✓	✓	✓
RC	Recovery(*)	✓	✓	✓	✓	✓	✓

ISs	ISTD peak area deviation (Standards)(*)	✓		✓	✓	✓	✓
ISc	ISTD peak area deviation (QC)(*)	✓	✓		✓	✓	✓
TF	Tailing factor (Symmetry factor)	✓	✓	✓	✓	✓	✓
S	Saturation	✓	✓	✓	✓	✓	✓
LSI	Min. Library Similarity Index (Screening/Explore)	✓	✓	✓	✓	✓	✓
RTi	Retention time (absolute ISTD)	✓	✓	✓	✓	✓	✓
RTs	Retention time (absolute Standards)	✓	✓	✓	✓	✓	✓
eRT	Lib. errRT (Screening/Explore)	✓	✓	✓	✓	✓	✓
RRT %	Relative Retention Time (%)	✓	✓	✓	✓	✓	✓
RRT	RRT (absolute)	✓	✓	✓	✓	✓	✓
<RFD	RF Deviation		✓				
SI	Minimum Similarity Index (GCMS)	✓					
Conf	Confidence	✓	✓	✓	✓	✓	✓
ASM	Asymmetry	✓	✓	✓	✓	✓	✓
mDa	Mass Error（mDa） (LCMS)	✓	✓	✓	✓	✓	✓
ppm	Mass Error（ppm） (LCMS)	✓	✓	✓	✓	✓	✓
NAME	Lib. Compound Name (Screening/Explore)	✓	✓	✓	✓	✓	✓
ISO	Iso Score (Explore)	✓	✓	✓	✓	✓	✓
QR	Quantitation Result	✓	✓	✓	✓	✓	✓
R	R		✓				
SCR	Score	✓	✓	✓	✓	✓	✓
H	Height	✓	✓	✓	✓	✓	✓

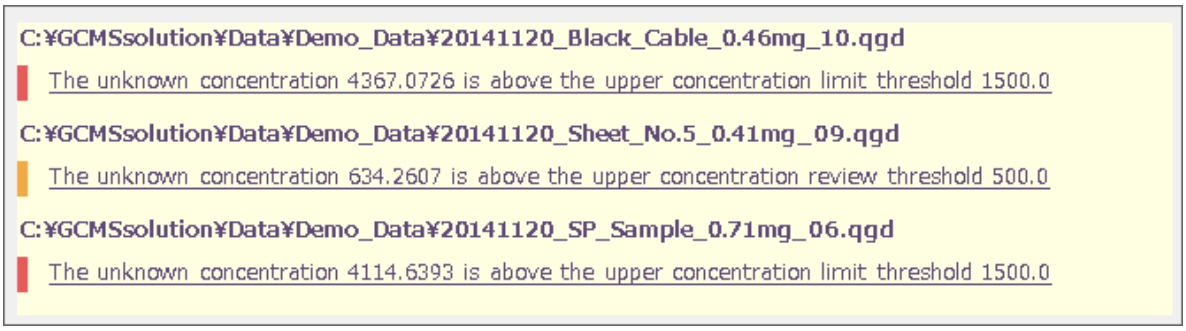
<Isa	ISTD Peak Area (min)	✓	✓	✓	✓	✓	✓
>Isa	ISTD Peak Area (max)	✓	✓	✓	✓	✓	✓
Q	Q-value (min) (GCMS)	✓	✓	✓	✓	✓	✓
<A	Peak Area (min)	✓	✓	✓	✓	✓	✓
>A	Peak Area (max)	✓	✓	✓	✓	✓	✓
PW	Peak Width (50%)	✓	✓	✓	✓	✓	✓
RSE	RF RSE (Curve)		✓				

(*) These flags check the measured value is within a range rather than above or below a fixed limit.

See section 3.27.2 "Setting flags" for detailed description of the flags.

2.6.4 Confirming flags

The following caption-less pop-up is displayed whenever a flag is clicked.



Two levels of text are displayed, a header text identifying the sample or the compound depending on the current view, and the flag details.

The colored bar on the left gives an indication of which way the value exceeded threshold.

To display the flag pop-up left-click on a flag icon within a cell in the list, results or summary pane. The caption-less flag pop-up is displayed next to the flag (like a tooltip).

To navigate between flagged items within the flag pop-up move the mouse over a hyperlink item. The item is bolded to indicate the hyperlink can be activated and followed to inspect the problem item.

Left-clicking follows the hyperlink. Alternatively use the [SPACE] or [ENTER] key.

[UP] and [DOWN] cursor keys can be used to move up and down through the list of flagged items. A highlight rectangle is placed around the current item, the item is bolded to indicate the hyperlink can be activated and followed inspect the problem item.

To 'peek' and view information that is behind the flag pop-up hold down the [CTRL] key. The flags pop-up is made less opaque so that it is possible to see what is behind it.

To dismiss the flag pop-up instantly left-click outside of the pop-up. Alternatively, move the mouse cursor outside of the pop-up and perform no action. The flags pop-up will be closed after a few seconds (like a tooltip).

2.7 LabSolutions Insight file structures

Files used by Insight differs between Data mode and Processing mode. Their roles are explained in turn in the following sections. See 2.1 Operation modes for details on the different operation modes.

2.7.1 Data Mode

In Data mode, Insight operations mainly involve the LabSolutions Insight Project file (DAMLP, pronounced as DAML-P, where DAML is pronounced like “camel” and P like “pea”, file for short).

DAMLP file

The names and paths of each data file in a set of experimental data and their method file(s) are stored as well as any applied flags (thresholds) and their results.

Insight workspace can be saved to DAMLP file, and reloading can restore the previous workspace.

LabSolutions data file (*.lcd, *.qgd)

Data files created by LabSolutions.

Data file holds chromatograms, spectra, integration results, quantitation results etc. Integration and quantitation results obtained using Insight will be stored in data files in the same way as in LabSolutions.

LabSolutions method file (*.lcm, *.qgm)

Method file edited by LabSolutions.

Method file holds instrument parameters, analysis parameters and calibration curve information. Analysis parameters edited in Insight and calibration information create d by Insight will be stored in the method file in the same way as in LabSolutions.

LabSolutions batch file (*.lcb, *.qgb)

Batch file created by LabSolutions.

Names of the data files obtained from a batch run and the name of the method file used to process the data files are stored in the batch file.
Insight cannot edit and save batch files. If data files are deleted or added to a batch, this information is not reflected in the batch file.

2.7.2 Processing Mode

In Processing mode, Insight operations mainly involve the LabSolutions Insight Processing file (processing file for short).

Processing file

Analysis parameters, calibration curve information and results obtained uses these parameters as well as the data and method file names for a set of data are stored. In addition, flag settings (thresholds) and their results are stored.

Loading a saved processing file can restore all information required by Insight to display the results. Multiple processing files can be created for the same batch data set.

LabSolutions data file

Data files created by LabSolutions.

Insight uses the chromatograms and spectra stored in the data files. Insight does not use integration and quantitation results produced by LabSolutions DB/CS. (Integration and quantitation results are used only when creating new processing files.)

Integration and quantitation results produced by Insight are all stored in the processing file. The original LabSolutions data files are not altered.

LabSolutions method file

Method file edited by LabSolutions.

Method file holds instrument parameters, analysis parameters and calibration curve information.

Analysis parameters and calibration curve information edited by Insight are all stored in the processing file. The original LabSolutions method file is not altered.

LabSolutions batch file

Batch file created by LabSolutions.

Names of the data files obtained from a batch run and the name of the method file used to process the data files are stored in the batch file.
Insight cannot edit and save batch files. If data files are deleted or added to a batch, this information is not reflected in the batch file.

Processing Method file

File holding analysis parameter information.

Processing Method file is used for loading analysis parameter information only.

DAMLP file

File holding flag (threshold) information.

DAMLP file is used for loading flag information only.

2.8 LabSolutions Insight Project File (DAMLP file)

Part of the work done using Insight is stored in the DAMLP file and can be reused. The role of this file depends on whether Insight is operating in Data or Processing mode. DAMLP files have the extension “damlp”.

2.8.1 Data Mode

Any work done in LabSolutions Insight can be saved as a DAMLP file. It holds information such as the data file references and method file references in a batch and the flagging criteria applied to the batch.

DAMLP files can be loaded like batch files from the Open button or like methods from the Load Method button.

2.8.2 Processing Mode

In Processing mode, DAMLP files are used to store and load flagging thresholds. Flag information shipped with methods from Shimadzu corporation can be utilized in this way.

DAMLP files are used when [Load Flags] or [Save Flags] in the [File] menu band are used.

In Processing mode, analysis parameters, quantitative results and flag information are all stored in the processing file. DAMLP is not used in a normal flow of operations.

3 LabSolutions Insight Functions

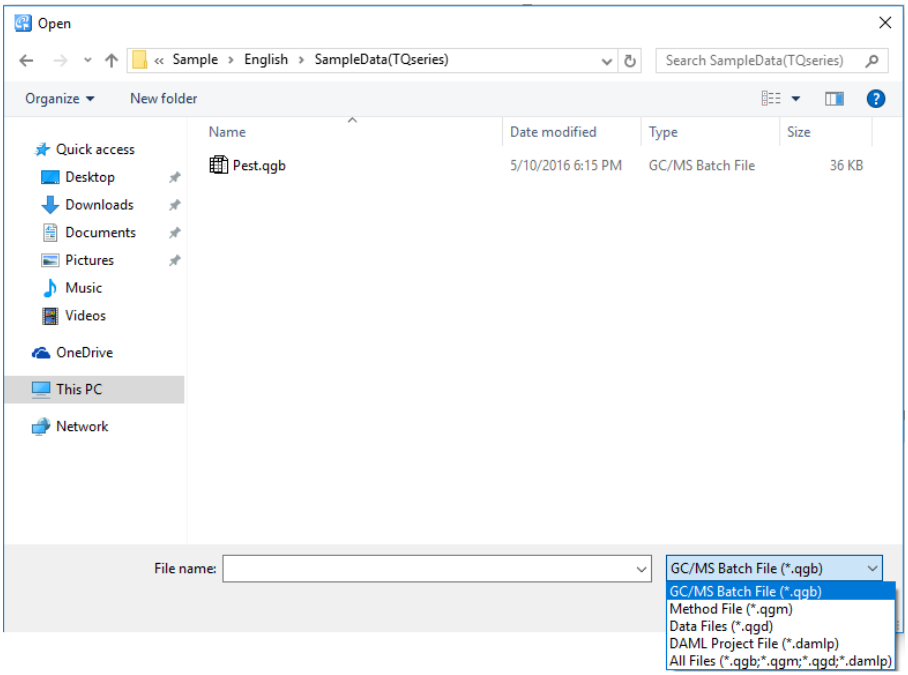
This section describes every operation that can be accessed via the menu items in the menu bar.

3.1 [File] Open

This is the primary method for loading data into Insight. Click on the [Open] button and the standard Windows file selector window is shown. The file selection window differs slightly depending on the version and mode of Insight so they are explained in turn in the following subsections.

3.1.1 GCMS Data Mode

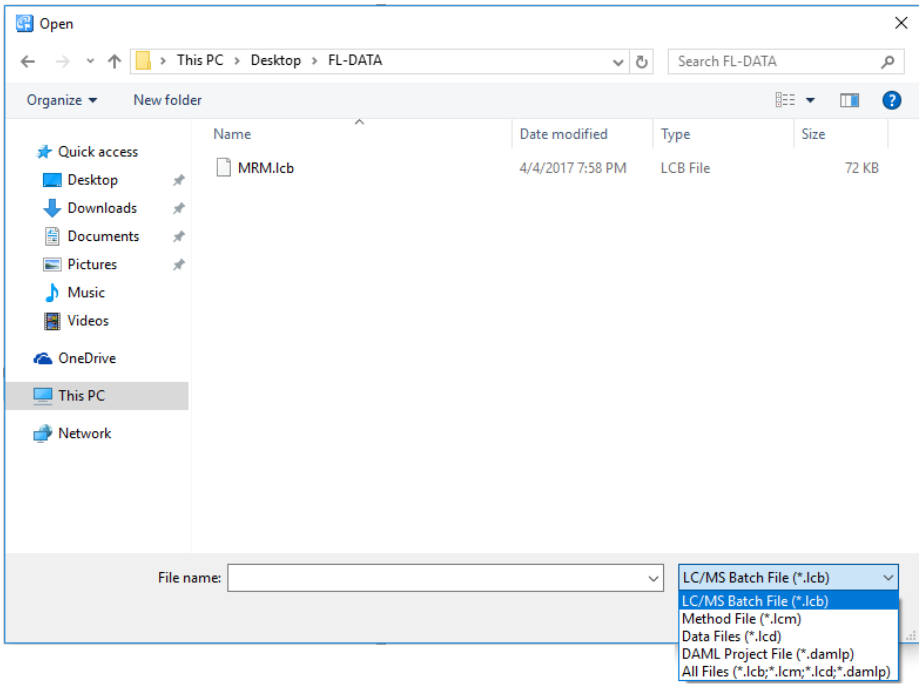
GCMSsolution batch file, method file, data file or a DAMLP file can be loaded. By default, Insight expects to open a qgb file.



3.1.2 LCMS Data Mode

LabSolutions batch file, method file, data file or a DAMLP file can be loaded. By default, Insight expects to open an lcb file.

Use the drop down list to change the file type to filter on. It is not possible to open a processing file.



NOTE

When a standard data files that are referenced directly by the selected file is missing, the name of the missing standard data file will be shown in Insight followed by “Not Available”. The data is not loaded.

When the standard data files referred to by the method file referred to by the selected file is missing, a similar action is taken.

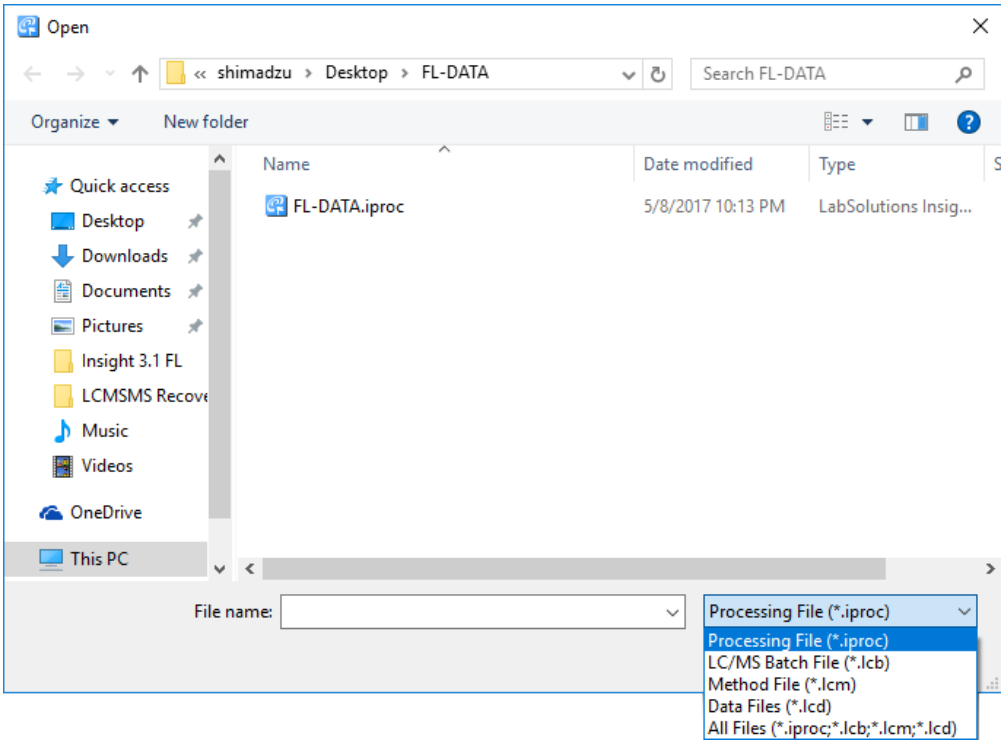
NOTE

When a data file other than a standard data file is missing, or if a standard data file that is not referred to by the method is missing, that data file is simply not loaded and its file name is not shown in Insight.

3.1.3 Processing Mode

LabSolutions batch file, method file, data file or a processing file can be loaded. By default, Insight expects to open a processing file.

Use the drop down list to change the file type to filter on. It is not possible to open a DAMLP file.



NOTE

When the DAMLP file is loaded as a batch file, the Save operation will always automatically overwrite the current DAMLP file.

NOTE

When data files referred directly by or by the method referred to by the processing file, LabSolutions batch or method file is missing, the name of the missing data file will be shown in Insight followed by “Not Available”. The data is not loaded.

NOTE

When a standard data file not referred to by a method or a data file other than standards referred to by the LabSolutions batch file are missing that data file is simply not loaded and its file name is not shown in Insight.

NOTE

When a method file is not available in the location specified in the batch file, the batch will open without showing any samples or compounds.

3.2 [File] Wizard (Processing Mode)

The quantitation Wizard is available only in Processing Mode.
The wizard helps create a processing method and processing results files using LabSolutions batch, method and data files in just 3 steps.

Step 1	Select a batch file used during acquisition and select data files from the batch that will be used for analysis.
Step 2	A processing method to be used for analysis can be selected from an existing set or created anew. If a new processing method is to be created, proceed to Step 3.
Step 3	A list of compounds registered in the acquisition method is shown. (Only LCMS) Using a reference data (a good and representative data from a group of data to be used for further analysis) and its chromatograms for each compound, adjust integration parameters and retention times.

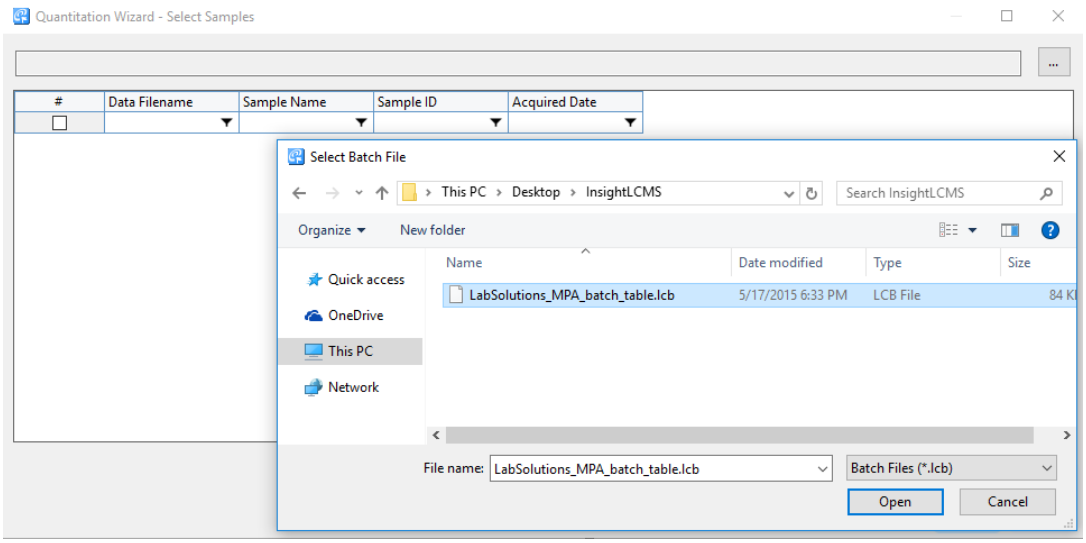
A processing method file (*iprom) is created once the Wizard is finished. The browser shows a list of data selected in Step 1 and the quantitation results calculated based on the processing method parameters defined in Steps 2 and 3.

3.2.1 Step1: Sample Selection

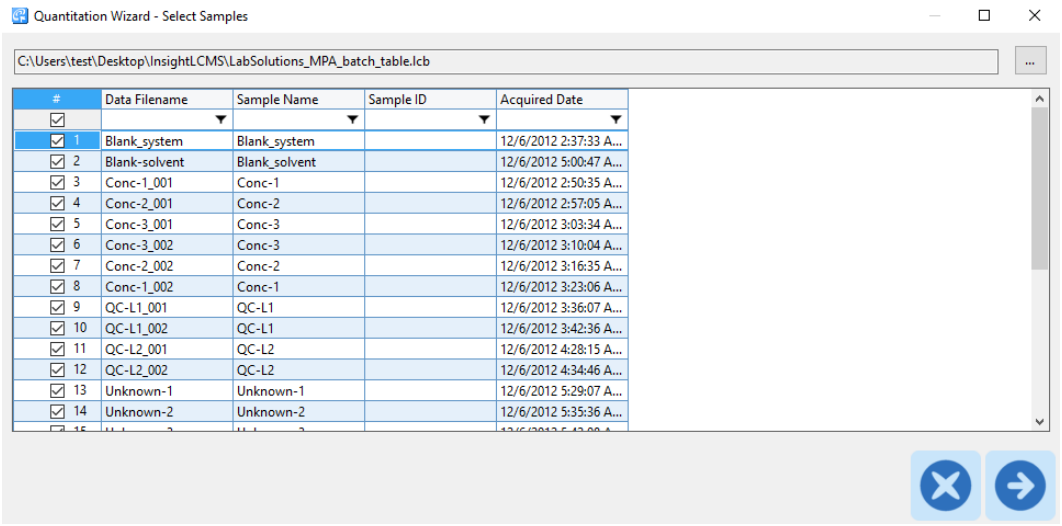
Select the [File] menu band and click on the [Wizard] button to open the quantitation Wizard.

In Step 1 of the quantitation Wizard, select a batch file or a Smart Data Reduction data file (lrdz file), then select the data in the batch or lrdz file to use in the following data analysis.
Click on the [Wizard] button to select a batch file or an lrdz file.

In Step 1 of the quantitation Wizard, select a batch file or an lrdz file, then select the data in the batch or lrdz file to use in the following data analysis.
Click on the [Wizard] button to select a batch file.



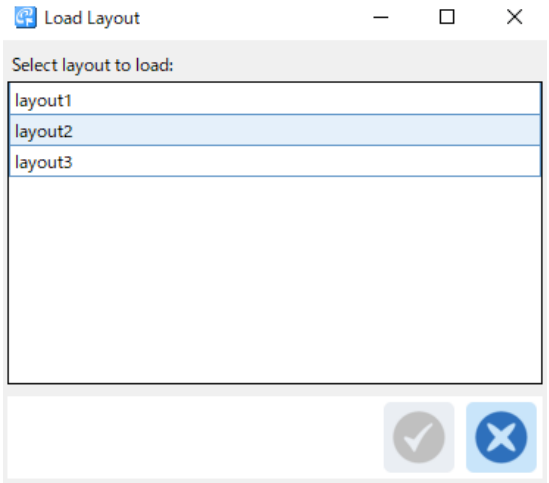
When a batch file is selected, a list of available data files is shown.



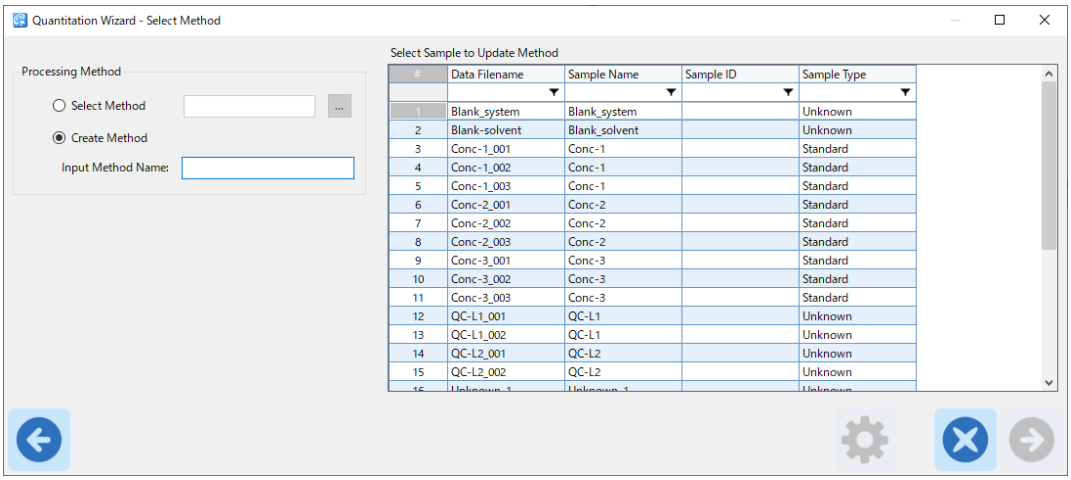
Data files with the left hand side check box ticked will be used for analysis. If a data file is not to be used in analysis (e.g. Blank), untick the check box.

Click on the right arrow button at the bottom right of the window to confirm the current selection ad to proceed to the next step. Click on the Cancel button to abort the Wizard.

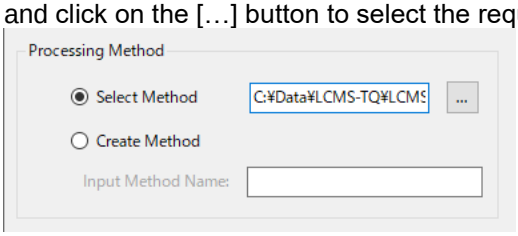
Click on the cogwheel button to select a saved layout.



3.2.2 Step2: Method Selection



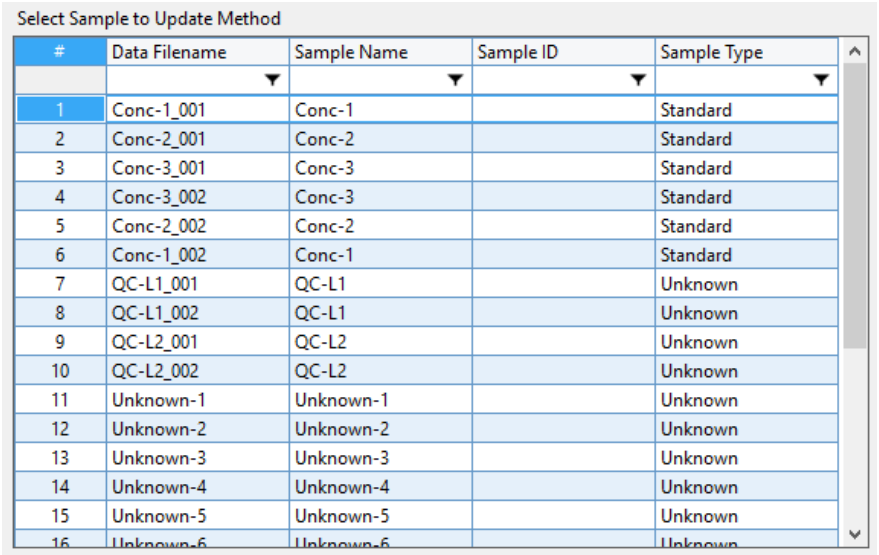
In Step 2, select a processing method to be used in the analysis.
To use an existing processing method to analyze this data, select the [Select method] radio button and click on the […] button to select the required processing method.



Once a method file is selected, the button at the bottom right of the window becomes enabled.

Click on the Check button to finish the Wizard and proceed to producing the analysis results. Click on the Cancel button to abort the Wizard.

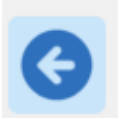
To create a new processing method, select the [Create method] radio button and enter the name of the new processing method file to be created. Next, select a sample to use for creating the method in Step 3. The highlighted row will be used in Step 3.



When a valid processing method file name is entered and a sample for creating the method is selected, the button at the bottom right of the window becomes enabled.

Click on the right arrow button to confirm the current settings and to proceed to the next step. Click on the Cancel button to abort the Wizard.

Click on the left arrow button at the bottom left of the window in order to go back a step and to modify the settings.



3.2.3 Step3: Update Parameters (LCMS Only)

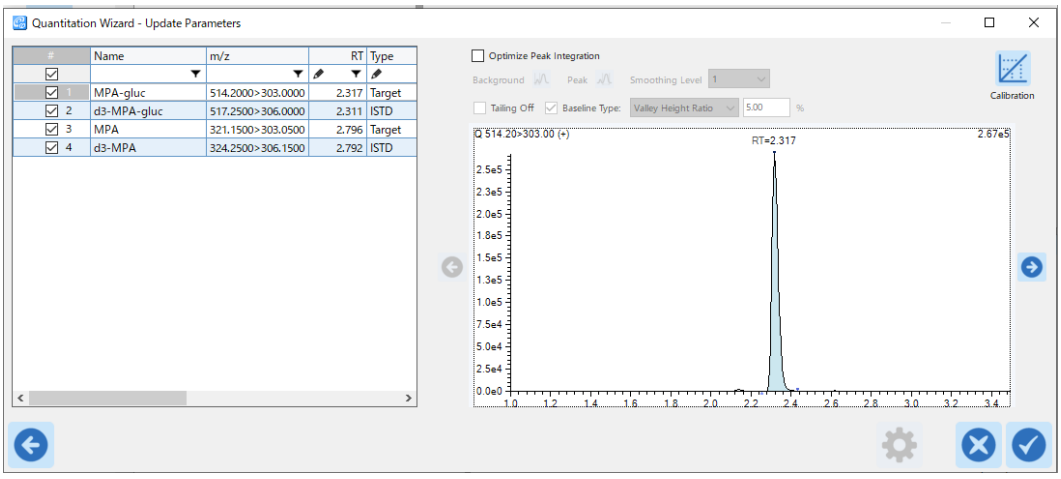
Only LCMS parameters can be update. For GCMS, it is only possible to view and confirm the compound list.

In Step 3, the chromatograms and peaks for each compound registered at the time of acquisition can be reviewed. There are multiple versions of the Update Parameters page and which version to use can be selected in the Application Configuration. When the version is changed in the Application Configuration, please restart Insight to apply the selection.

If a compound is not going to be required for data analysis, untick the check box at the left hand side to remove that compound from further processing.

#	Name	m/z	RT
1	MPA-gluc	514.20>303.00	2.317
2	d3-MPA-gluc	517.25>306.00	2.311
3	MPA	321.15>303.05	2.796
4	d3-MPA	324.25>306.15	2.792

3.2.3.1 Version 1

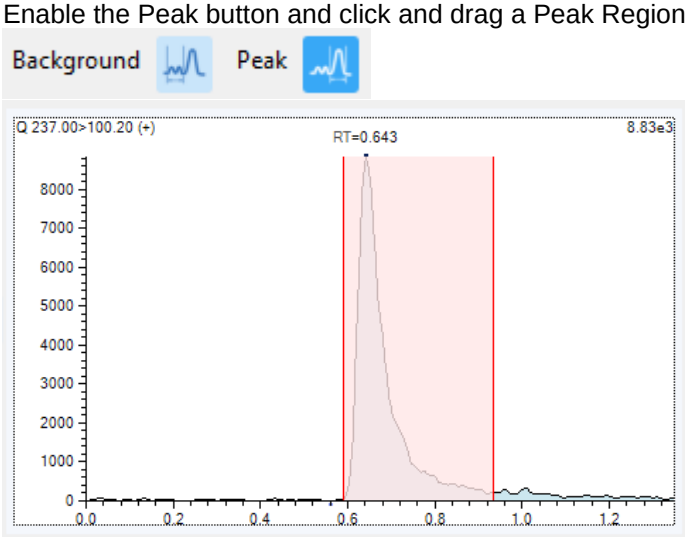


Peak integration parameters can be updated easily by selecting peak and background regions and setting the smoothing level appropriately.

When peak integration parameters are not set appropriately, a combination of the following operations can help improve peak integration.

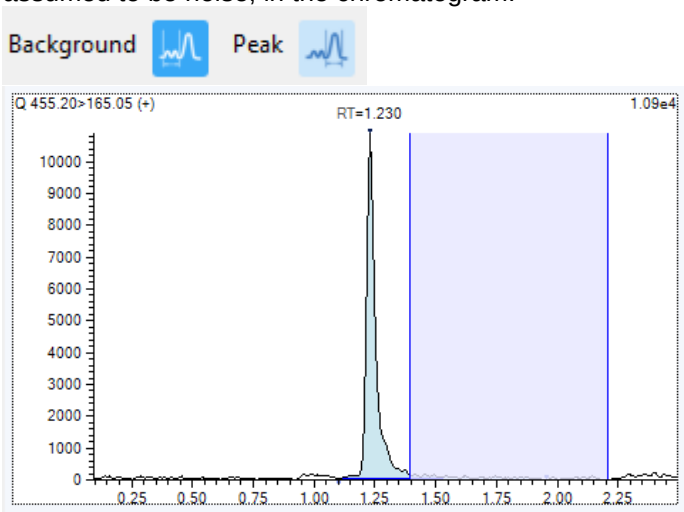
1. Select Peak

Enable the Peak button and click and drag a Peak Region in the chromatogram.



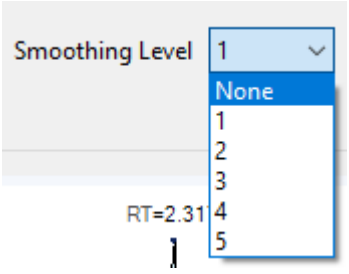
2. Select Background

Enable the Background button and click and drag a Background Region, where the signal is assumed to be noise, in the chromatogram.



3. Select Smoothing Level

Select a smoothing level if the chromatogram needs smoothing. The larger the level number, the more smoothed the chromatogram will become.

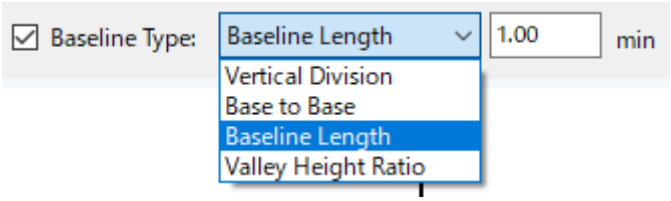


4. Tailing Off

Tailing processing detects smaller peaks located on top of the tail of a previous bigger peak. This processing option is turned ON by default but by ticking the Tailing Off check box, it is possible to turn it off.

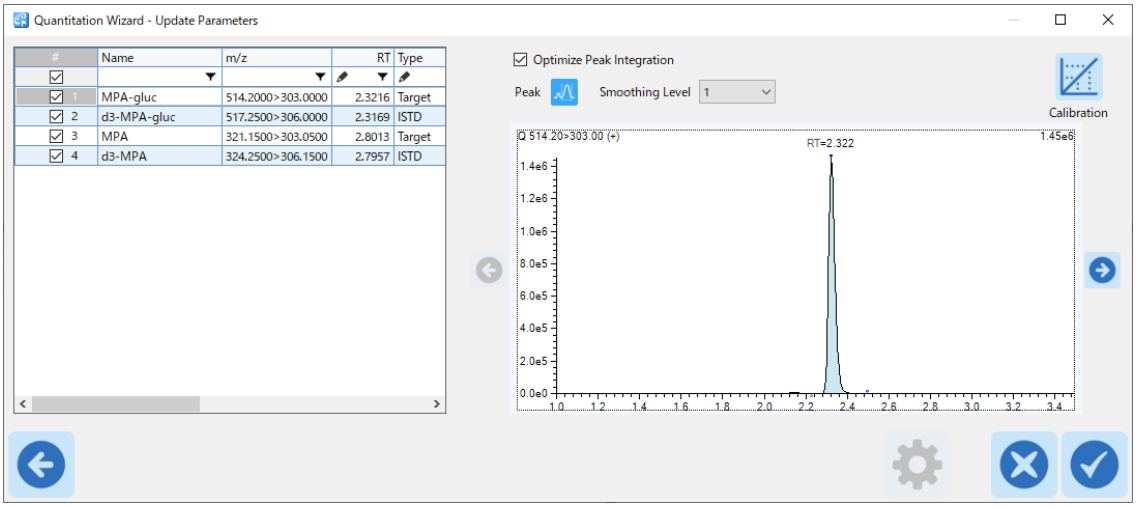
5. Baseline Type

Tick the [Baseline Type] check box in order to apply baseline processing and select the method by which to process the basline from the drop down list.



For [Baseline Length] and [Valley Height Ratio], enter the appropriate parameters in the adjacent box. For details on baseline processing please refer to LabSolutions DB or LabSolutions CS users manual or online help.

3.2.3.2 Version 2

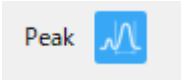


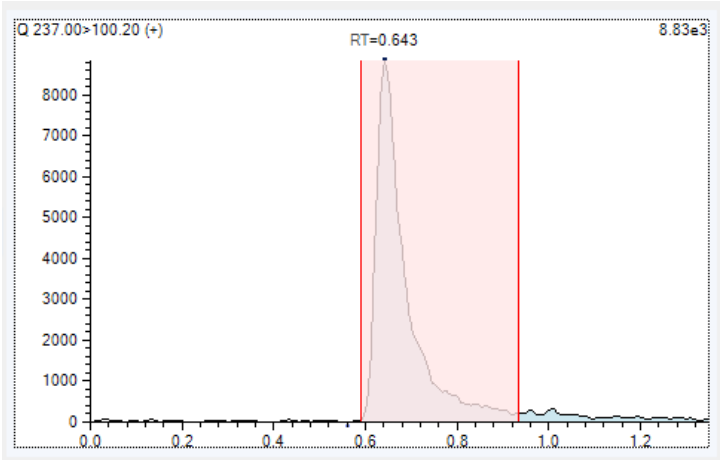
Peak integration parameters can be updated easily by selecting the peak and setting the smoothing level appropriately.

When peak integration parameters are not set appropriately, tick the [Optimize Peak Integration] option then a combination of the following operations can help improve peak integration.

1. Select Peak

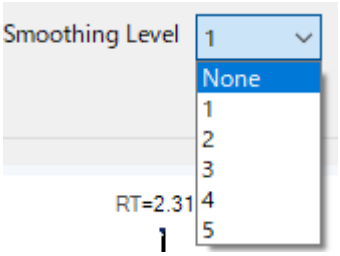
Enable the Peak button and click and drag a Peak Region in the chromatogram.





2. Select Smoothing Level

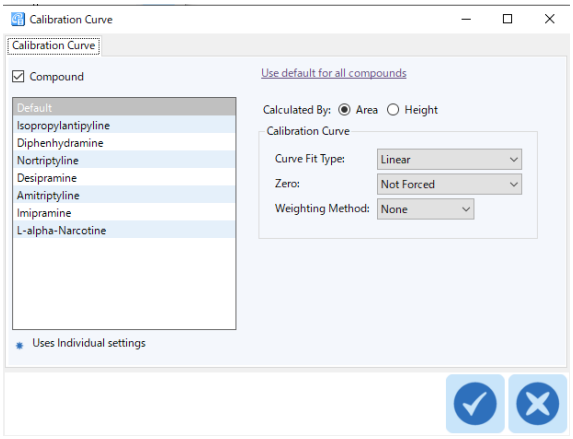
Select a smoothing level if the chromatogram needs smoothing. The larger the level number, the more smoothed the chromatogram will become.



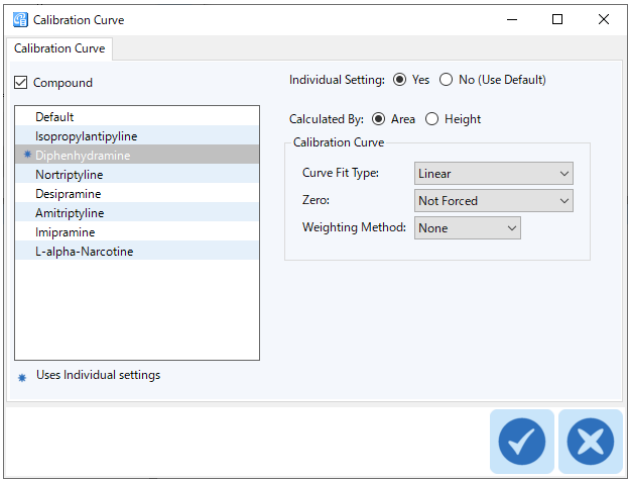
Tailing processing is unaltered, and the baseline type is set to “Base to Base”.

3.2.3.3 Calibration curve

It is possible to configure the calibration curve by clicking on the Calibration button  .



Here, you can configure whether to use area or height, calibration curve type, zero through behaviour and weighting. Please refer to the LabSolutions DB or LabSolutions CS user guide or online help for details on each of the options.



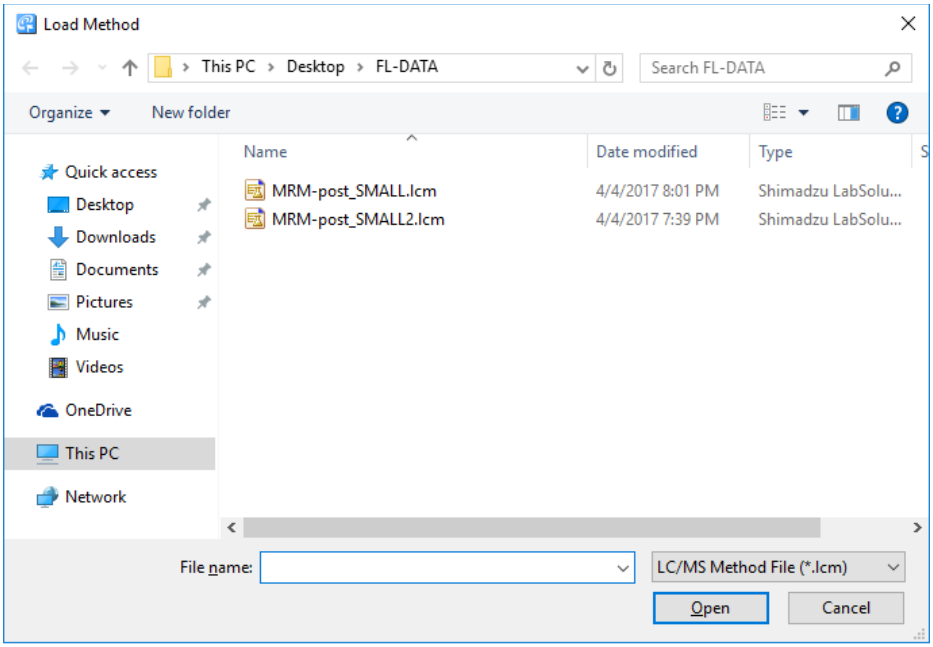
It is also possible to select whether to use the default calibration curve settings for all compounds or to configure a compound separately. A compound for which calibration configuration is set separate to the default is marked with *.

3.3 [File] Load Method

Use this function to apply a new quantitation method.

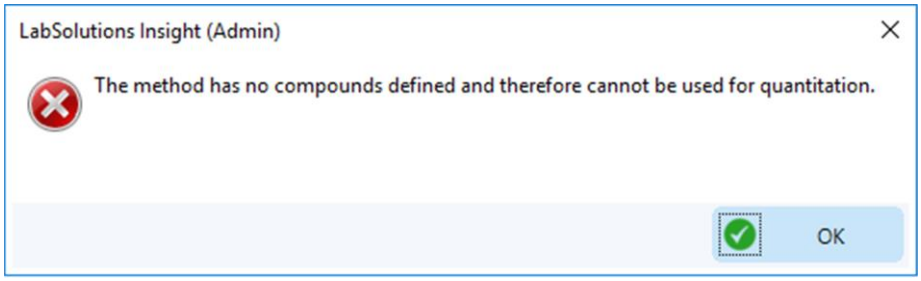
Click on the [Load Method] button and the standard Windows file selector window is shown. Select a method to load. A method can be a qgm file (GCMSsolution method file) or an lcm file (LabSolutions LCMS method file).

In Processing mode, Insight expects to open a processing file by default. Use the drop down list to change the filtering on the file type as appropriate.



NOTE

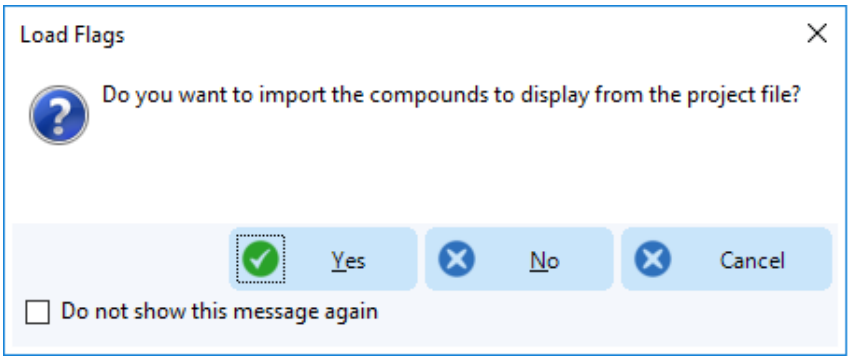
When a method file with no compounds registered in its compound table is loaded, an error message is shown and that method cannot be used in Insight.



3.4 [File] Load Flags

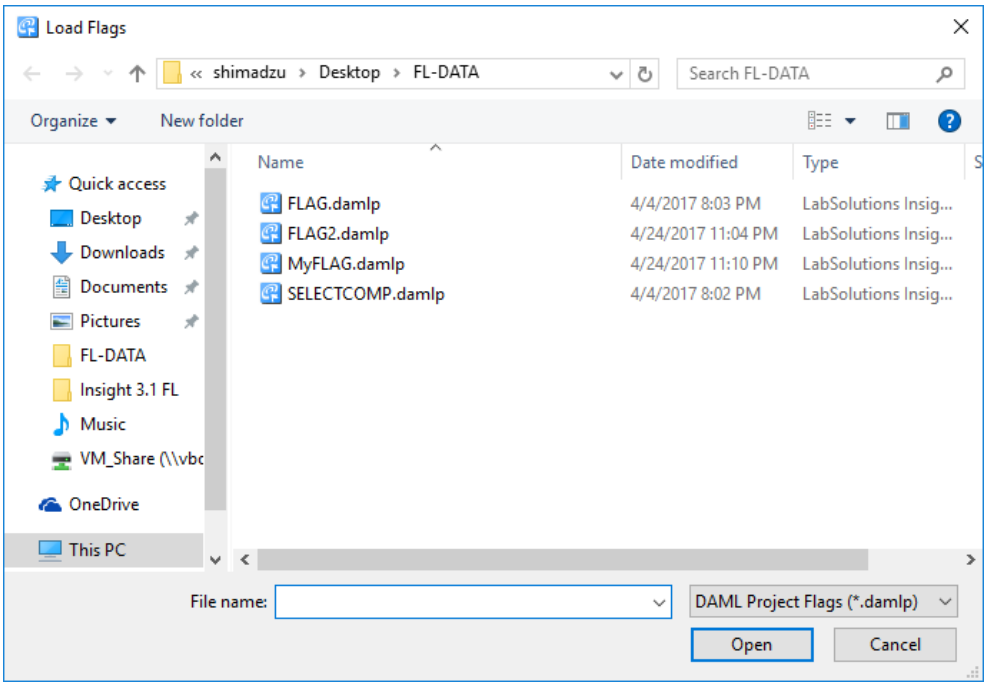
Click on the [Load Flags] button to apply a new set of flag criteria.

When the setting to select compounds has been saved in the selected file, this setting can also be loaded.



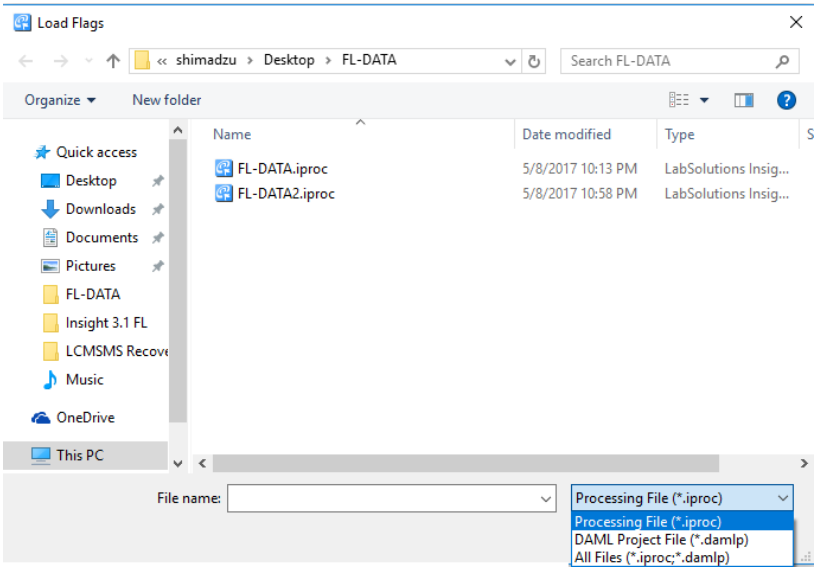
3.4.1 Data Mode

Select a DAMLP file to load.



3.4.2 Processing Mode

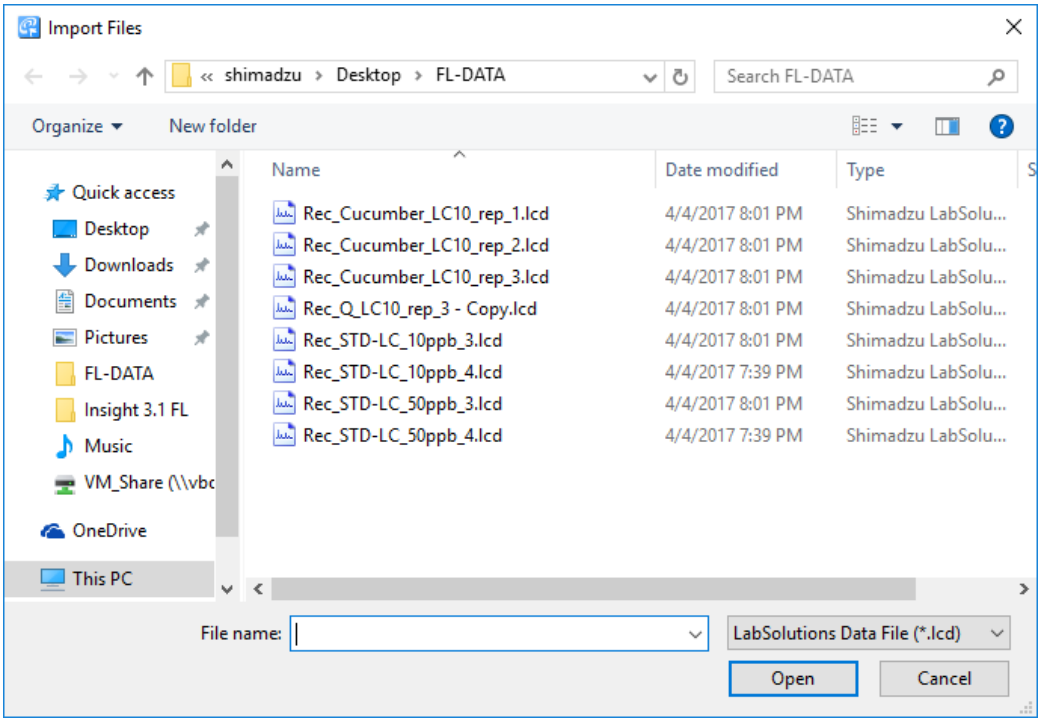
Select a processing file or DAMLP file to load.



3.5 [File] Import

One or more data files can be appended to an existing batch or processing file.

Click on the [Import] button and the standard Windows file selector window is shown. Select one or more data files to load.



NOTE

A method file, a batch file or a processing file must be opened prior to importing data files.

NOTE

Data files appended to an existing batch can only be saved to a DAMLP file in Data mode or processing file in Processing mode, not to a GCMSsolution or LabSolutions batch file.

3.6 [File] Save

Work done in Insight can be saved by clicking on the [Save] button.

3.6.1 Data Mode

Data files, method files and DAMLP files can be saved.

When a set of data is loaded into Insight without using a DAMLP file, an option to save it as a DAMLP file is presented.

When data is loaded from a DAMLP file, the current file is always overwritten.

When the data had been loaded without using a DAMLP file and a DAMLP file has been opened subsequently to apply flags, the Save operation will always offer to save the current data as a new DAMLP file.

NOTE

If any one of the following are read-only, this menu item is made disabled: user rights, data file, method file.

3.6.2 Processing Mode

Processing files can be saved.

If data had been loaded without using a processing file, the Save operation will always offer to save the current data as a new processing file.

If data had been opened using a processing file, the Save operation will always overwrite the current processing file.

When the data had been loaded without using a processing file and a processing file has been opened subsequently to apply flags, the Save operation will always offer to save the current data as a new processing file.

If audit trail is enabled and the current data was opened without using a processing file, an audit trail log stating the file path of the method currently in use will be created on saving the data as a new processing file.

NOTE

If any one of the following are read-only, this menu item is made disabled: user rights, processing file.

NOTE

If audit trail is enabled and set up to ask for reasons for any changes made, Insight will display a window for entering the reason for change.

See section 3.20.2 “Entering the Reason for Change” for details on being prompted for reason for change.

See sections 1.13 "Enable Processing Mode (LCMS only)” and 3.19 "[View]—Audit Trail” for more information on setting up Insight to perform audit trail and to view audit trail logs.

3.7 [File] Save as

Click on the [Save as] button to save the current work done in Insight under a new name.

This menu item is enabled even when the method file or processing file is read-only.

3.7.1 Data Mode

Method files and DAMLP files can be saved under a new name. If a data file has been altered for example by performing manual peak integration, the current data file is overwritten and saved.

3.7.2 Processing Mode

The current work done in Insight can be saved to a new processing file. Any changes made to methods and data files are saved to the processing file and not to each LabSolutions method and data files.

NOTE

If audit trail is enabled and set up to ask for reasons for any changes made, Insight will display a window for entering the reason for change.

See section 3.20.2 “Entering the Reason for Change” for details on being prompted for reason for change.

See sections 1.13 "Enable Processing Mode (LCMS only)” and 3.19 "[View]—Audit Trail” for more information on setting up Insight to perform audit trail and to view audit trail logs.

3.8 [File] Save Flags

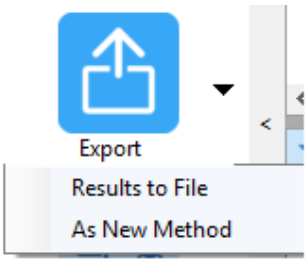
This operation is only available in Processing mode.

Click on the [Save Flags] button to save the current flags to a DAMLP file. The [Save Flags] button becomes enabled when a new flag file is applied or when flag settings are changed or when selected compounds are changed. Save Flags will always prompt to save as a new DAMLP file.

3.9 [File] Export

Click on the [Export] button to export results as text.

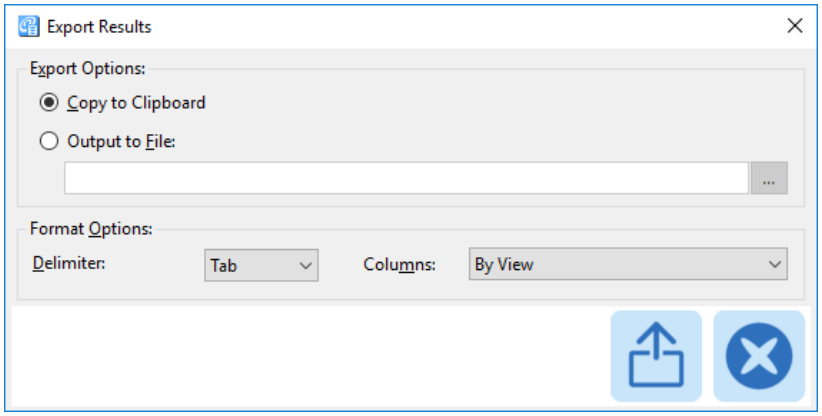
In Processing mode, clicking on the [Export] button shows a drop down menu. An additional option to export a method file is shown.



3.9.1 Results to File

This function provides the ability to export quantitative result information to the clipboard or Comma Separated Variables (csv) / Tab Separated Text (txt) /Tab Separated Variables (tsv) file. The output format depends on the current results view.

Click on the Export button to show the window below:



Export Options	
Copy to Clipboard	Copy the results to Clipboard. The content can subsequently be pasted to third-party software such as word processing software.
Output to File	Write the results out to the file specified below. Click on the […] to select a file or type the full output file path in the box. The file name extension depends on the delimiter options: Tab: txt / tsv Comma: csv
Delimiter Options	
Tab Comma	Select the required delimiter from the drop down list.
Columns	

By View Fixed Format (Compound vs Sample) Fixed Format (Sample vs Compound	Select the format of the applicable export result from the drop down list.
	Export the results using the options set above.
	Cancel the export operation.

> **NOTE**
>
> Due to the specification of this software, information irrelevant to the current configuration of the software may be exported.

3.9.1.1 Format: By View (Compound View)

This format is used when [By View] is selected for the format option and [Compound View] is selected for the current display setting.

Layout is changed according to the table style of the view.

Below is an example. The details of the format are available in “Appendix A”.

```
ID#     1
Name    Dichlorvos
        Data Filename   Name    Type    ISTD Group      m/z     Found Ret. Time Std. Conc.      ISTD A
1       pest_std_003    Dichlorvos      Target  0       185.00  6.211   100.0                   0.0
2       pest_std_002    Dichlorvos      Target  0       185.00  6.208   500.0                   0.0
3       pest_std_001    Dichlorvos      Target  0       185.00  6.207   1000.0                  0.0
4       pest_unknown_001        Dichlorvos      Target  0       185.00  6.209

ID#     2
Name    Fenobucarb
        Data Filename   Name    Type    ISTD Group      m/z     Found Ret. Time Std. Conc.      ISTD A
1       pest_std_003    Fenobucarb      Target  0       150.00  9.607   100.0                   0.0
2       pest_std_002    Fenobucarb      Target  0       150.00  9.607   500.0                   0.0
3       pest_std_001    Fenobucarb      Target  0       150.00  9.607   1000.0                  0.0
4       pest_unknown_001        Fenobucarb      Target  0       150.00  9.607

ID#     3
Name    Simazine
        Data Filename   Name    Type    ISTD Group      m/z     Found Ret. Time Std. Conc.      ISTD A
1       pest_std_003    Simazine        Target  0       201.00  10.927  100.0                   0.0
```

3.9.1.2 Format: By View (Summary View)

This format is used when [By View] is selected for the format option and [Summary View] is selected for the current display setting.

Below is an example. The details of the format are available in “Appendix A”.

Data Filename	Sample Name	Sample ID	Dichlorvos	Fenobucarb	Simazine		Propyz
pest_std_003	Pest13Compounds 1ug/mL	STD-0003	6.211	9.607	10.927	11.371	11.532	11.828
pest_std_002	Pest13Compounds 1ug/mL	STD-0002	6.208	9.607	10.927	11.371	11.532	11.829
pest_std_001	Pest13Compounds 1ug/mL	STD-0001	6.207	9.607	10.930	11.373	11.533	11.829
pest_unknown_001	Pest13Compounds 1ug/mL	UNK-0004	6.209	9.607	10.927	11.372	11.532	

3.9.1.3 Format: Fixed Format (Compound vs Sample)

This format is used when [Fixed Format (Compound vs Sample)] is selected for the format option.

The details of the format are available in "Appendix A."

3.9.1.4 Format: Fixed Format (Sample vs Compound)

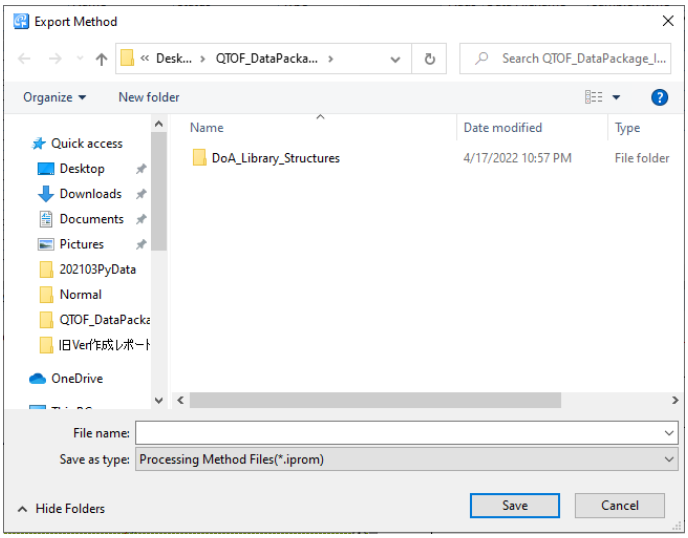
This format is used when [Fixed Format (Sample vs Compound)] is selected for the format option.

The details of the format are available in "Appendix A."

3.9.2 As New Method

This menu is enabled only in Processing mode.

Export the current method as a new method file. The new method file can only be exported to the current project.



Enter a name for the new method file and click on  .

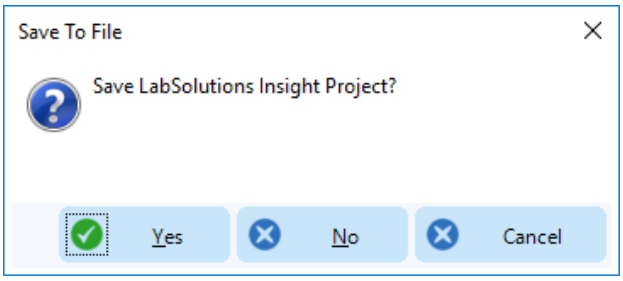
3.10 [File] Close

Use this function to close all current files.

3.10.1 Data Mode

If any changes have been made, an option to save them will be presented.

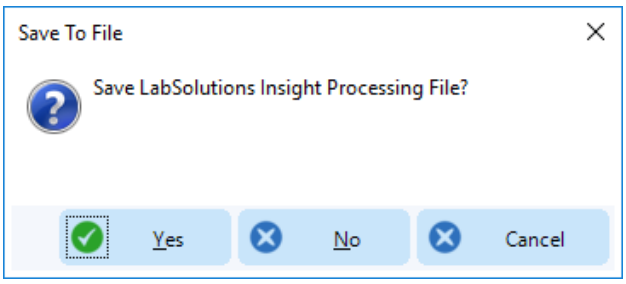
If the set of data files were opened without using a DAMLP file, an option to save the data, method and flag files (if applicable) as a DAMLP file will be presented.



3.10.2 Processing Mode

If any changes have been made, Insight will offer to save the changes to the current processing file.

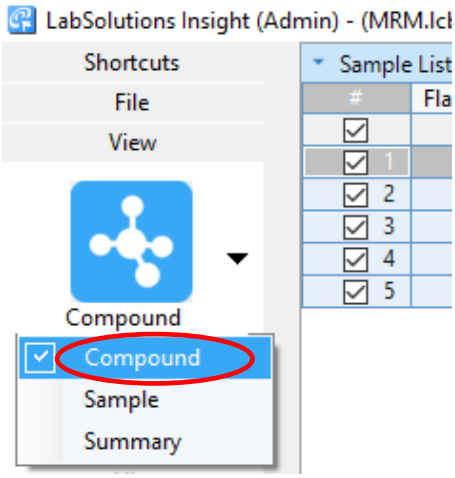
If the current data was opened without using a processing file, Insight will offer to save the current data as a new processing file.



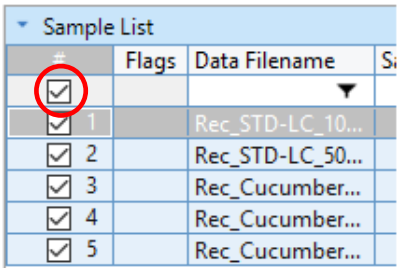
3.11 [View] Compound

In Compound view, the Sample List shows the list of samples in the loaded batch and the Compound Results table shows the results for all of the compounds in the current selected sample.

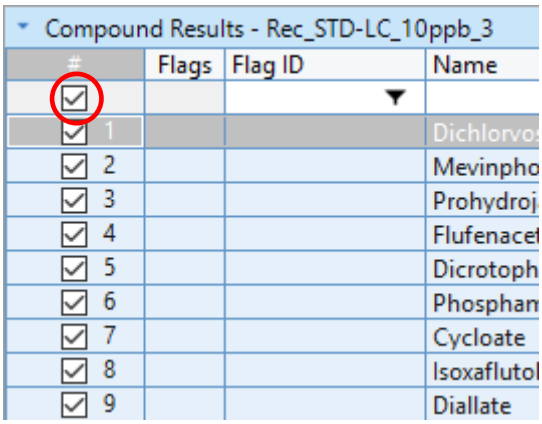
Click on the first button in the View menu band and select Compound from the drop down list that appears under the button.



Check the checkboxes in the Sample List to include that sample in the Survey view. The checkbox in the header can be used to check/uncheck all the samples at once.



Similarly, check the checkboxes in the Compound Results table to include that compound in the Survey view. The checkbox in the header can be used to check/uncheck all the compounds at once.

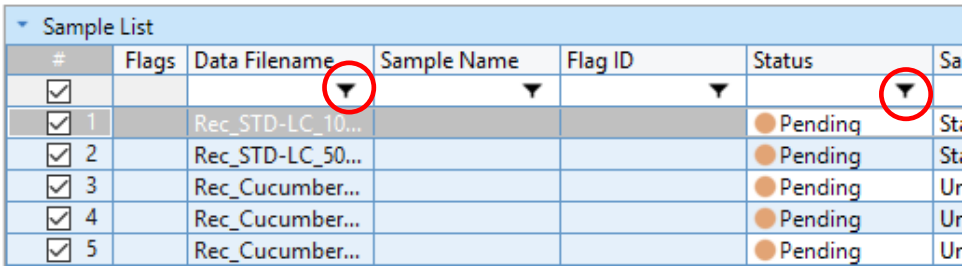


The order of the items shown in the Sample List and Compound Results tables can be changed by clicking on a column header to sort the list by the values under that column (for example, clicking on the “Sample Name” column header in the Sample List table will sort the results displayed in that list alphabetically by sample name). Clicking on the column header again will toggle between ascending and descending sort order (as is standard Windows behaviour).

If either the Sample List or Compound Results tables are closed, they can be restored by selecting Compound again from the View menu band.

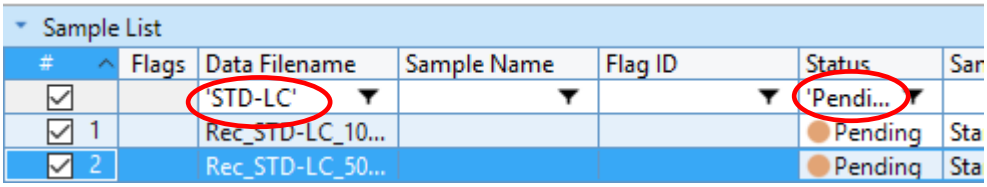
3.11.1 Filtering

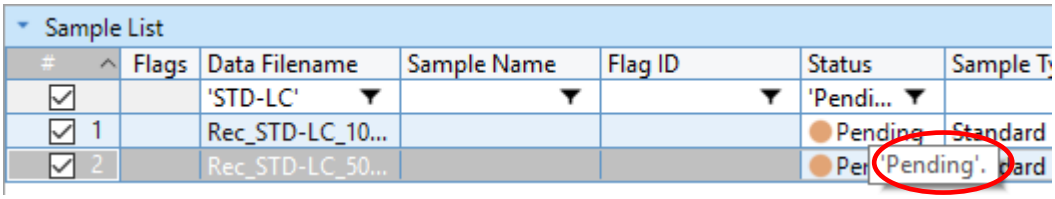
Lists and Results can be filtered using the filter buttons located under each column header. Filtering only affects the visibility of the samples/compounds in the lists; it does not affect the actual data in the batch in any way.



Filter criteria can be set by clicking on a filter icon. Filtering can be applied for multiple columns and the effects of each filter are combined to restrict the range of values shown within the corresponding list. When the filter criteria pop-up window is dismissed (by clicking anywhere outside of the popup window or hitting the [Return] key) the filter is immediately applied to the list contents so that the effects of applying that filter can be seen on the fly.

Once a filter has been applied for a list column, the header for that column shows details of the filter as shown below. If the filter description text is too long for the current column width (as the description for Level is in this example), then it is truncated with ellipses and a tooltip can be used to reveal the complete description.





Click on the filter icon again to remove the current filter.

The criteria that need to be specified in order to filter the list contents by the values under a specific column are dependent on the type of the column. There are six different criteria types: String, Numeric, Options List, Date, Status and Level.

> **NOTE**
>
> When filtering is activated, it affects the chromatograms shown in Survey. However, the filtering is intended to be controlled based on the Lists and Results and not the chromatograms. It is advised to simply view chromatograms when filtering is activated.

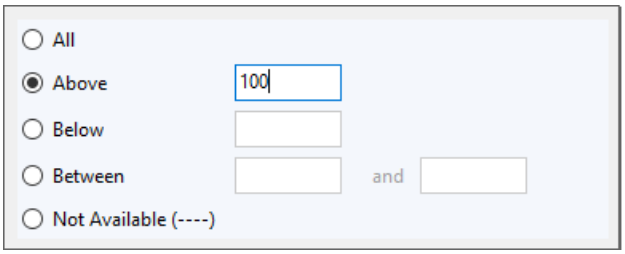
3.11.1.1 String Filtering

For a string filter type (for example, for the “Data Filename” column), the filter criteria is set in a pop-up window shown below.

Enter a string of characters to search in the corresponding column. Only those items containing exactly the specified string will be shown and the rest will be hidden. The matching portion in the items listed can be anywhere in each item as long as the specified string is found as a contiguous and complete piece. String filtering is case insensitive (therefore filtering on “STD” and “std” performs the same operation). Deleting the string in this pop-up window will remove any filtering applied to the corresponding column.

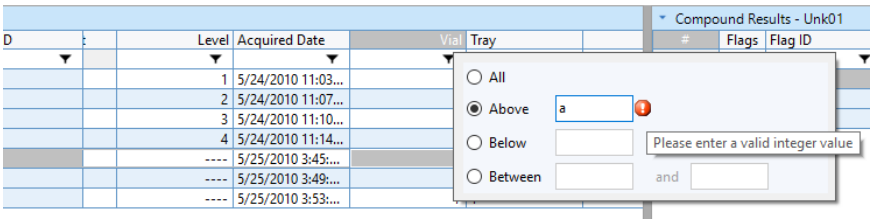
3.11.1.2 Numerical Filtering

For a numerical filter type (for example, the “Area” column), the following filter criteria pop-up window is shown.



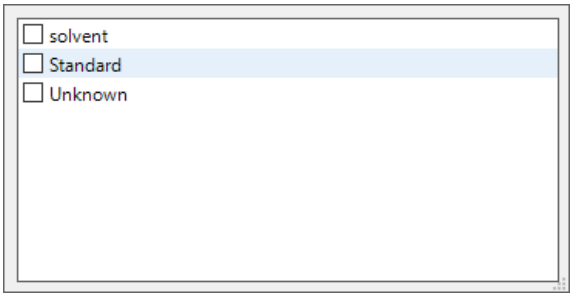
All	Show all items. This is equivalent to switching off filtering.
Above	Show values greater than the specified value (not including the entered value).
Below	Show values less than the specified value (not including the entered value).
Between	Show values between the specified values (including the entered values).
Not Available (----)	Show the items which have no value. Not Available is not shown if there are no (---) in the selected column.

An error icon is shown if an invalid value is entered. Hovering the mouse pointer over the error icon will show a tooltip explaining the reason for the error.



3.11.1.3 Options List Filtering

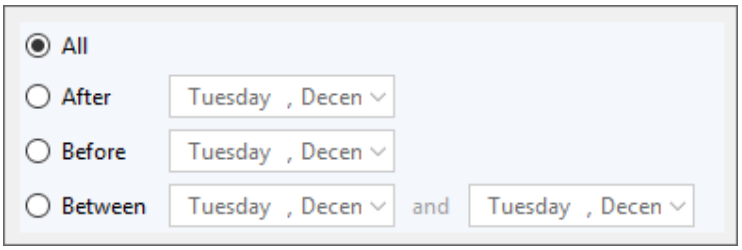
When a filter is to be applied to a column that contains values that are from a list of several available options (such as the “Sample Type” column in the Sample List table), the following dialog box is shown. Only the options that are present in the table’s column data are shown in the list.



Check the boxes for the items to show. Unchecking all options listed in the filter pop-up window removes all filtering previously applied to the corresponding column.

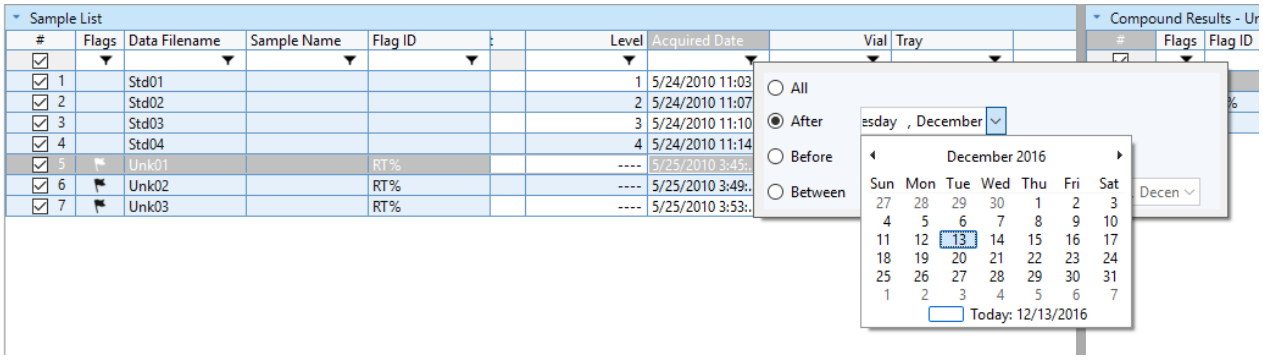
3.11.1.4 Date Filtering

Date and time values can be filtered using the following pop-up window.



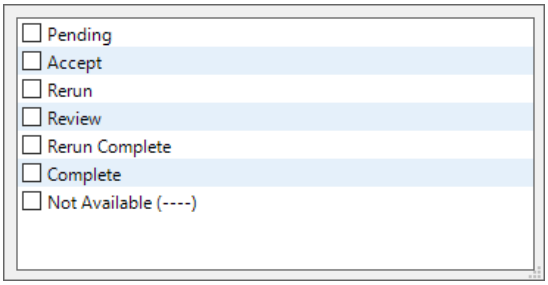
All	Show all items. This is equivalent to switching off filtering.
After	Show values after than the specified date (not including the entered date).
Before	Show values before than the specified date (not including the entered date).
Between	Show values between the specified dates (including the entered dates).

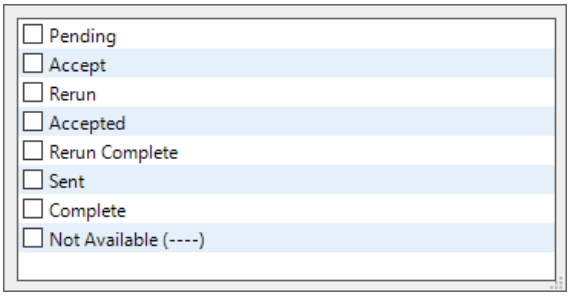
Dates can be entered directly into the fields using the keyboard or by clicking on the down arrow button which will show the standard date selector pop-up as shown below:



3.11.1.5 Status Filtering

The Status values can be filtered using the following pop-up window.





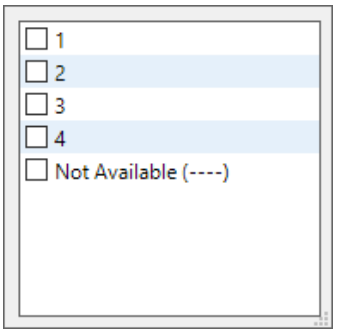
Sample List Compound Results

Pending	Show the compound or sample for which the status is “Pending”.
Accept	Show the compound or sample for which the status is “Accept”.
Rerun	Show the compound or sample for which the status is “Rerun”.

Accepted	Show the compound or sample for which the status is “Accepted”.
Rerun Complete	Show the compound or sample for which the status is “Rerun Complete”.
Sent	Show the compound or sample for which the status is “Sent”.
Complete	Show the compound or sample for which the status is “Complete”.
Not Available （----）	Show the compound or sample for which the status is “Not Available”.

3.11.1.6 Level Filtering

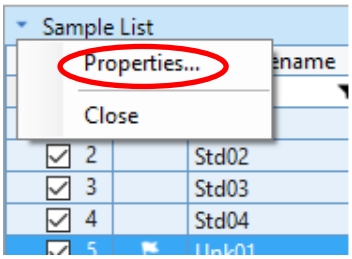
The Level values can be filtered using the following pop-up window.



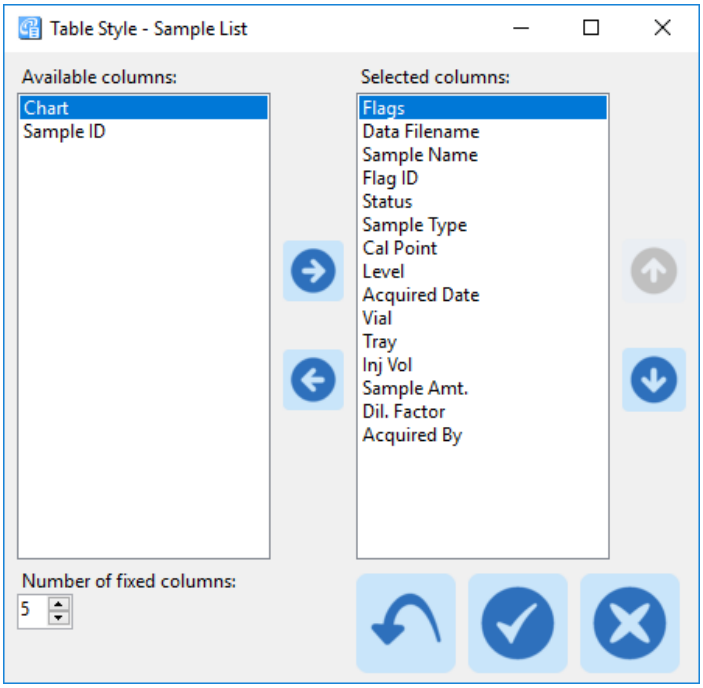
1, 2, 3 …（Numerical）	Show the sample which has the same level.
Not Available（----）	Show the sample in which the level is “---”.

3.11.2 Table style

The configuration of columns that are shown in the Sample List and Compound Results tables can be edited using each pane’s caption menu and selecting the “Properties…” menu item.



Selecting this menu item displays the Table Style dialog box:



This dialog box shows the columns that are currently selected for display in the Sample List table in the right hand list and the remaining available columns in the left hand list. Columns can be added to the “Selected columns” list by selecting one or more items in the “Available columns” list and clicking the right arrow button; the selected column(s) will then be added to the end of the “Selected columns” list.

Selected columns	List of columns currently displayed in the corresponding list or table. The columns are listed in the order they appear in the corresponding list or table where the topmost is the leftmost and the bottommost is the rightmost.
Available columns	List of columns currently hidden from the corresponding list or table.
	Select a column in the Available columns list and click this button to send the selected column to the Selected columns list. The selected column will be shown in the corresponding list or table.
	Select a column in the Selected columns list and click this button to send the selected column to the Available column list. The selected column will be hidden from the corresponding list or table.
	Select a column in the Selected columns list and click this button to send the selected column up the list. The column will be moved left along the corresponding list or table.
	Select a column in the Selected columns list and click this button to send the selected column down the list. The column will be moved right along the corresponding list or table.
Number of fixed columns	The specified number of columns from the left side can be fixed from among the columns displayed in the corresponding list or results.

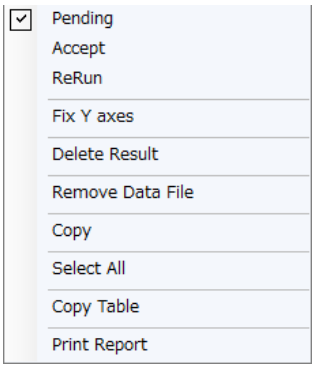
Certain types of columns are mandatory and must always be present (such as the “#” [sample number] and “Flags” columns in the Sample List table), therefore these columns are not presented for configuration in the Table Style dialog box. The mandatory columns are always included at the start of the table, followed by the columns as configured in the Table Style dialog box.

	Reset to default settings.
	Apply the changes and close the Table Style dialog.
	Discard the changes and close the Table Style dialog.

The Table Style settings for all tabular views can also be accessed through the Table Styles section of the Display Settings window.

3.11.3 Sample List operations

Right click on a row in the Sample List to show the following context menu:



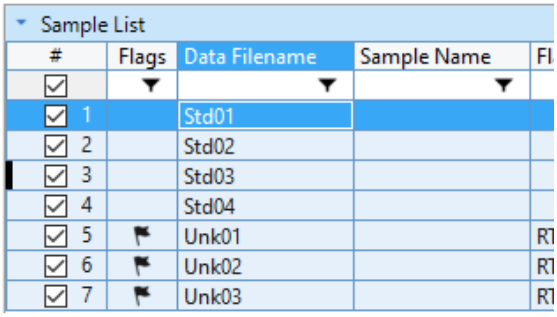
For Pending, Accept and Rerun see 3.29 Review.

3.11.3.1 Fixing the Y-axis

Select [Fix Y axes] from the Sample List context menu.

Now, the Y-axes of all the chromatograms shown in the Survey are fixed to show the selected sample optimally. Using this option allows for the comparison of all sample chromatogram intensities against the selected reference chromatogram.

The selected reference chromatogram is indicated by a black bar on the far left of the Sample List:

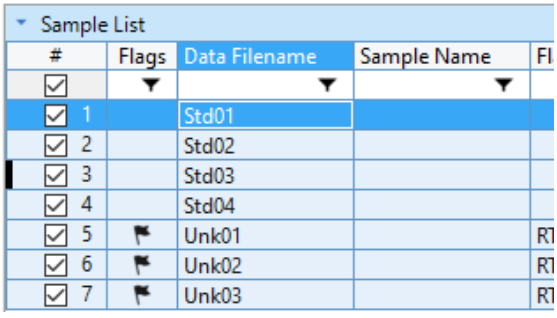


3.11.3.2 Overlay plot

Select [Overlay plot] from the Sample List context menu to specify the sample as the reference chromatogram. This menu is enabled only when the selected sample type is "Standard."

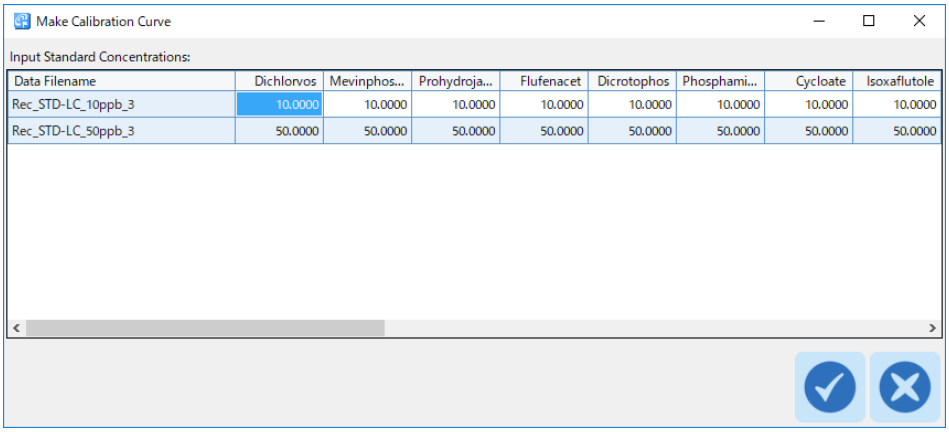
The chromatogram of the sample specified in this item is displayed overlaid with all displayed chromatograms. The y-axis is fixed to the intensity axis of the chromatogram of the sample specified in this item. Using this option, all sample chromatograms can be easily compared with the selected reference chromatogram.

A black bar is shown on the left side of the selected reference chromatogram in Sample List.



3.11.3.3 Make Calibration Curve from Selected Sample(s)

Select at least one sample and select [Make Calibration Curve from Selected Sample(s)] in order to create calibration curves for all compounds.



Enter standard concentrations for each level for every compound and click on the check box. The levels are set from 1 at the top of the list to however many samples are selected to make the calibration curve from.

Here, the right click context menu item other than the standard Windows items are explained.

Fill down	Apply the selected value to all rows below.
Sample Identifier	Select which information to identify each sample by -Data file name -Sample name -Sample ID

All samples not selected for calibration curve creation will be set to Unknown.

3.11.3.4 Delete Result

Select [Delete Result] from the Sample List context menu to delete the quantitative results of the selected compound.

3.11.3.5 Removing Data Files

Select [Remove Data File] from the Sample List context menu to remove the selected file from the list.

This option is only available for non-standard samples and is therefore disabled when the current selected row is of “Standard” sample type.

3.11.3.6 Copy

Select [Copy] from the Sample List context menu to copy the currently selected cell.

3.11.3.7 Select All

Select [Select All] from the Sample List context menu to select all items displayed in the Sample List.

> **Hint**
>
> Drag the mouse to select a desired range.

3.11.3.8 Copying the Table

Select [Copy Table] from the Sample List context menu to copy the current table as tab-delimited text to the clipboard.

The text can be used in 3rd party software as a table.

3.11.3.9 Printing Reports

This option is available for Data mode only.

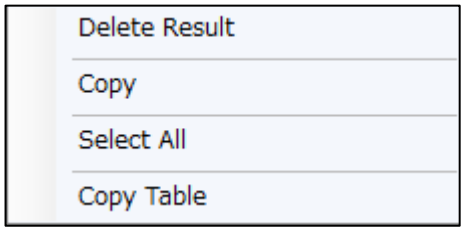
Select [Print Report] from the Sample List context menu to print a GCMSsolution Report or LabSolutions LCMS report for the selected data file. See "3.31 [Report] Report " for details.

3.11.3.10 Properties

Selecting [Properties…] in the Sample List context menu displays the sub-window to edit the table style as described in 3.11.2 Table style.

3.11.4 Compound Results operations

Right click on a row in the Compound Results table to show the following context menu:



3.11.4.1 Deleting Results

Select [Delete Result] in the Compound Results context menu to remove the compound result for the currently selected sample in the Sample List, in the same way as in GCMS Quant Browser.

3.11.4.2 Copy

Select [Copy] in the Compound Results context menu to copy the currently selected cell.

3.11.4.3 Select All

Select [Select All] in the Compound Results context menu to select all items displayed in Compound Results.

3.11.4.4 Copying the Table

Select [Copy Table] from the Compound Results context menu to copy the current table as tab-delimited text to the clipboard.

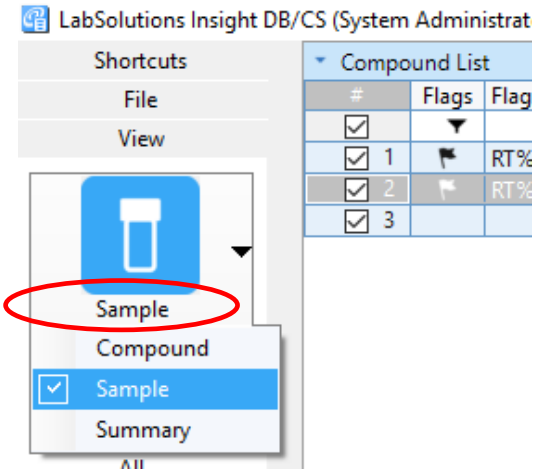
The text can be used in 3rd party software as a table.

3.12 [View] Sample

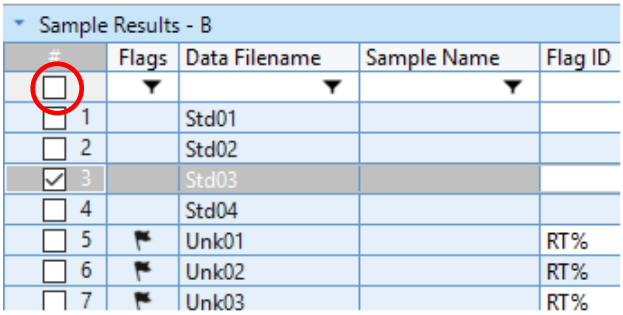
In Sample view, the Compound List shows the list of compounds contained in the samples and the Sample Results table shows the results for the samples for each of the compounds selected in the Compound List.

Click on the first button in the View menu band and select Sample from the drop down list that appears under the button.

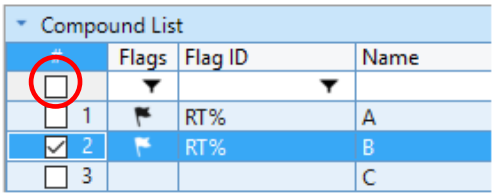
If either the Compound List or Sample Results tables are closed, they can be restored by selecting Sample again from the View menu band.



Check the checkboxes in the Sample Results to include that sample in the Survey view. The checkbox in the header can be used to check/uncheck all the samples at once.



Similarly, check the checkboxes in the Compound List to include that compound in the Survey view. The checkbox in the header can be used to check/uncheck all the compounds at once.



The order of the items shown in the Compound List and Sample Results tables can be changed in the same way as for Sample List and Compound Results in Compound View.

Filtering of items in the Compound List and Sample Results tables is also supported in exactly the same way as that specified for the Compound view above.

The configuration of columns that are shown in the Compound List and Sample Results tables can be edited using each pane's caption menu and selecting the "Options…" menu item in the same way as that specified for the Compound view above.

Sample List operations available in Sample View are now available in Sample Results.

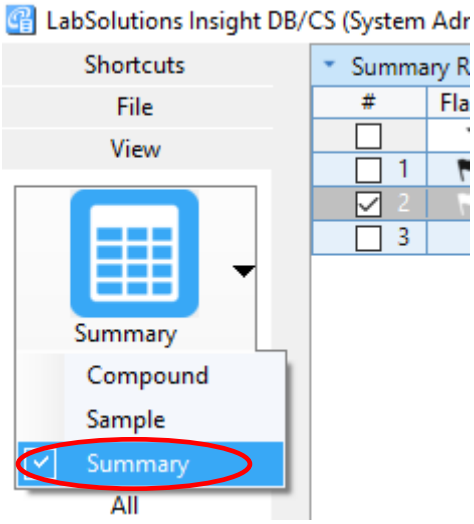
Compound Results operations available in Sample View are now available in Compound List except that it is not possible to delete compounds from the Compound List.

3.13 [View] Summary

In Summary view the results are summarized in a single table with a row for each compound and a column for each sample – this orientation matches the orientation of the Survey pane. The values shown in the table cells correspond to a single data value for the specific sample / compound combination.

Click on the first button in the [View] menu band and select [Summary] from the drop down list that appears under the button.

If the [Summary Results] table is currently closed, it can be restored by selecting [Summary] again from the [View] menu.



When showing compounds vs samples, the check boxes for selecting samples to display in [Survey] are along the top next to the sample names. Similarly, the check boxes for selecting compounds are next to the compound IDs (#). All compounds can be selected or unselected using the check box under the column header for Compound ID (#) as shown below.

Summary Results

#	Flags	Data Filename	MPA-gluc	d3-I
			Conc. (mg/L)	Co
1		Blank_system	----	
2		Blank-solvent	-3.082	
3		Conc-1_001	18.200	
4		Conc-2_001	88.300	
5		Conc-3_001	218.716	
6		Conc-3_002	218.488	
7		Conc-2_002	91.539	
8		Conc-1_002	15.888	
9		QC-L1_001	44.697	
10		QC-L1_002	43.723	
11		QC-L2_001	133.579	
12		QC-L2_002	135.381	
13		Unknown-1	87.186	
14		Unknown-2	19.168	
15		Unknown-3	63.201	

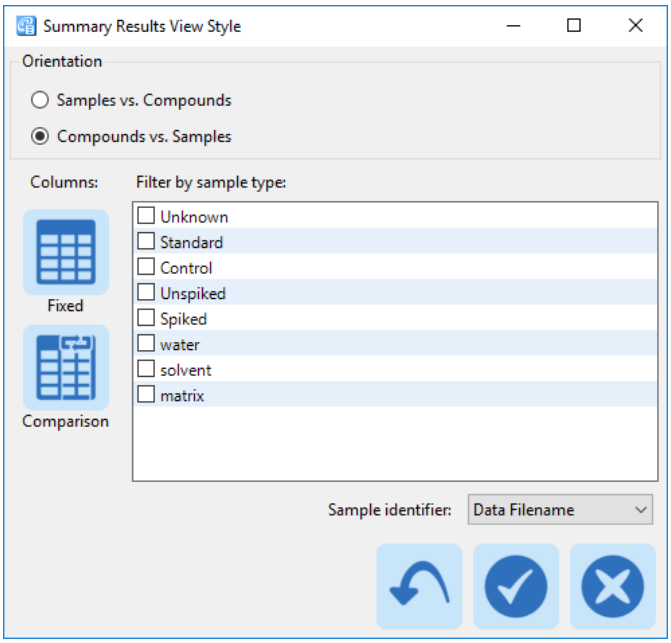
Similarly, when showing samples vs compounds, the check boxes for selecting compounds are displayed next to compound names across the top. The check boxes for selecting samples are

displayed next to the sample IDs going down. All samples can be selected or unselected using the check box under the Sample ID header.

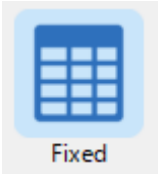
Filtering can only be applied to the “Flags” and “Name” columns in this table (the “Flags” and “Data Filename” columns when selecting “Samples vs. Compounds” orientation). The procedure for setting the flagging criteria is the same as for the Compound View.

3.13.1 Summary Results Options

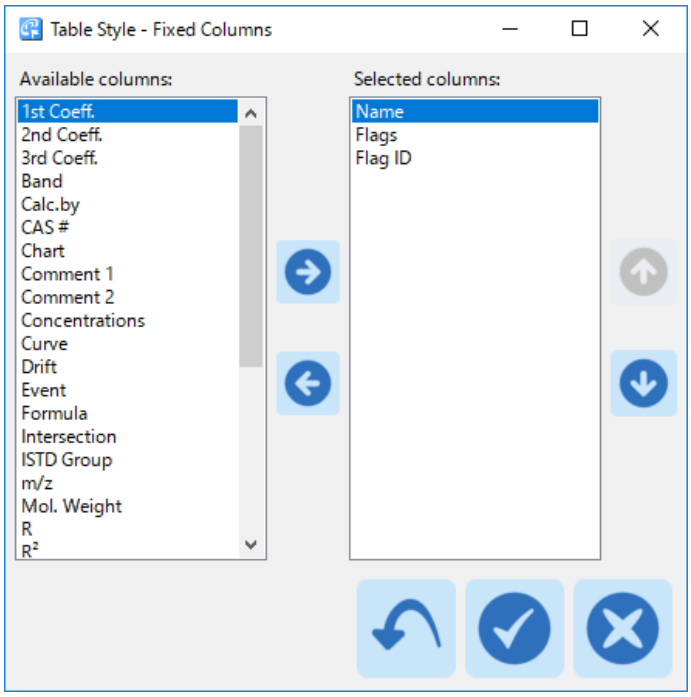
The type of data to be displayed in the Summary table can be specified by selecting the [Properties...] caption menu and using the [Summary Results View Style] popup window.



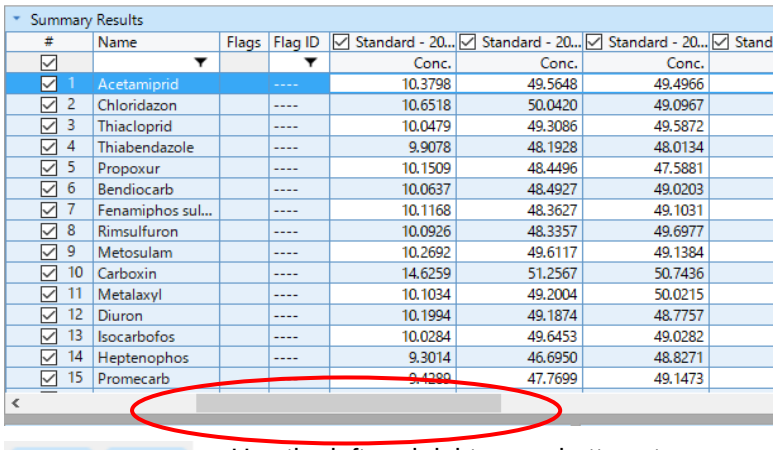
Select the items to be displayed in the Summary view here. Click [Fixed] to select the items to display on the fixed column on the left side of the summary table. Click [Comparison] to select the items to display on the comparison column on the right side of the summary table.



Configure which columns to fix at the left hand side of the summary table. These columns will stay visible even when the table is scrolled to the right.

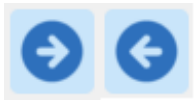


Fixed columns do not scroll:



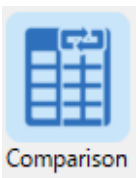
Summary Results

#	Name	Flags	Flag ID	Standard - 20... Conc.	Standard - 20... Conc.	Standard - 20... Conc.	Stand
1	Acetamiprid		----	10.3798	49.5648	49.4966	
2	Chloridazon		----	10.6518	50.0420	49.0967	
3	Thiacloprid		----	10.0479	49.3086	49.5872	
4	Thiabendazole		----	9.9078	48.1928	48.0134	
5	Propoxur		----	10.1509	48.4496	47.5881	
6	Bendiocarb		----	10.0637	48.4927	49.0203	
7	Fenamiphos sul...		----	10.1168	48.3627	49.1031	
8	Rimsulfuron		----	10.0926	48.3357	49.6977	
9	Metosulam		----	10.2692	49.6117	49.1384	
10	Carboxin		----	14.6259	51.2567	50.7436	
11	Metalaxyl		----	10.1034	49.2004	50.0215	
12	Diuron		----	10.1994	49.1874	48.7757	
13	Isocarbofos		----	10.0284	49.6453	49.0282	
14	Heptenophos		----	9.3014	46.6950	48.8271	
15	Promecarb			9.4289	47.7699	49.1473	

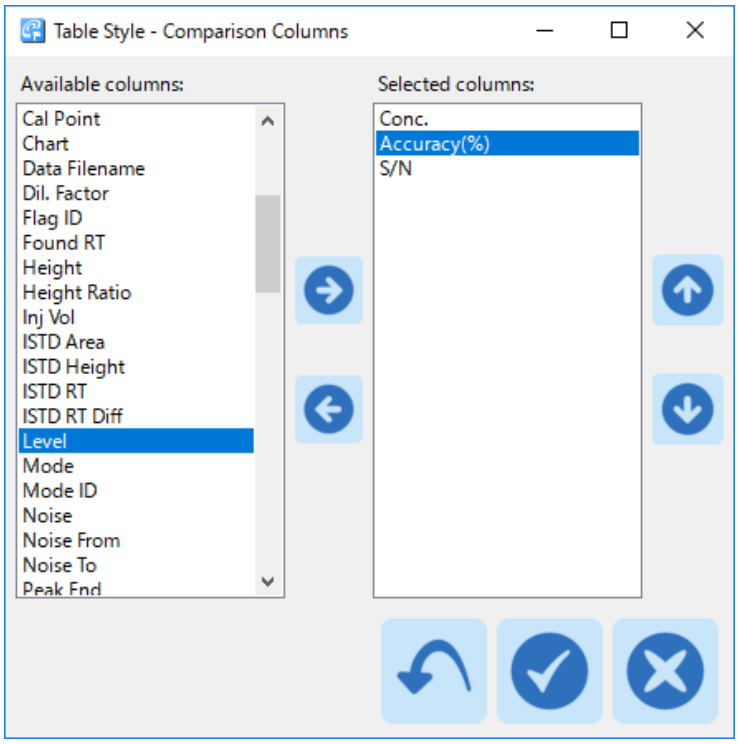


Use the left and right arrow buttons to move columns between the [Available columns] and [Selected columns] lists. Columns listed in the [Selected columns] list will appear in the Summary table as fixed columns on the left.

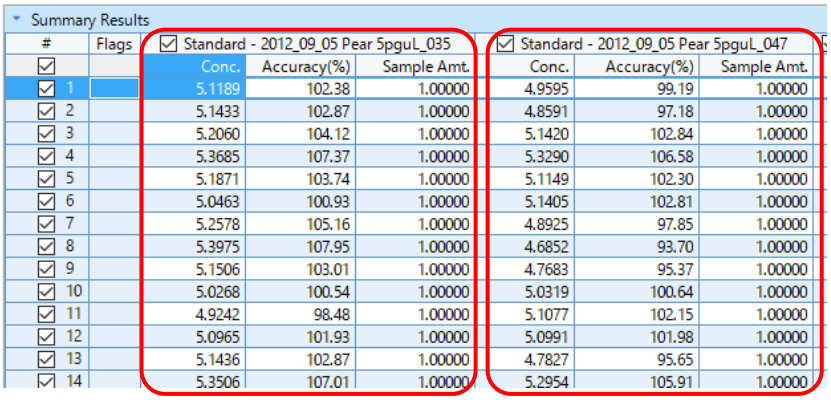
Use the up and down arrow buttons to change the order of the fixed columns. The column listed at the top appear leftmost and the bottom at the rightmost of the fixed part of the Summary table.



Configure which columns to compare results by.



A “block” of selected columns repeat for each sample or compound:



Summary Results

#	Flags	Standard - 2012_09_05 Pear 5pguL_035			Standard - 2012_09_05 Pear 5pguL_047		
		Conc.	Accuracy(%)	Sample Amt.	Conc.	Accuracy(%)	Sample Amt.
1		5.1189	102.38	1.00000	4.9595	99.19	1.00000
2		5.1433	102.87	1.00000	4.8591	97.18	1.00000
3		5.2060	104.12	1.00000	5.1420	102.84	1.00000
4		5.3685	107.37	1.00000	5.3290	106.58	1.00000
5		5.1871	103.74	1.00000	5.1149	102.30	1.00000
6		5.0463	100.93	1.00000	5.1405	102.81	1.00000
7		5.2578	105.16	1.00000	4.8925	97.85	1.00000
8		5.3975	107.95	1.00000	4.6852	93.70	1.00000
9		5.1506	103.01	1.00000	4.7683	95.37	1.00000
10		5.0268	100.54	1.00000	5.0319	100.64	1.00000
11		4.9242	98.48	1.00000	5.1077	102.15	1.00000
12		5.0965	101.93	1.00000	5.0991	101.98	1.00000
13		5.1436	102.87	1.00000	4.7827	95.65	1.00000
14		5.3506	107.01	1.00000	5.2954	105.91	1.00000

Use the left and right arrow buttons to move columns between the [Available columns] and [Selected columns] lists. Columns listed in the [Selected columns] list will appear side by side for each sample or compound column.

Use the up and down arrow buttons to change the order of the fixed columns. The column listed at the top appear leftmost and the bottom at the rightmost of the comparison part of the Summary table.

The summary table orientation can also be set here. Select [Samples vs. Compounds] to have samples going down and compounds going across. Select [Compounds vs. Samples] to have compounds going down and samples going across.

Setting [Filter by sample type] enables the user to narrow down the samples to display by the sample type. When the [Filter by sample type] checkbox is not selected, all samples are displayed.

When the checkbox is selected, only samples that fall under the selected sample type are displayed.

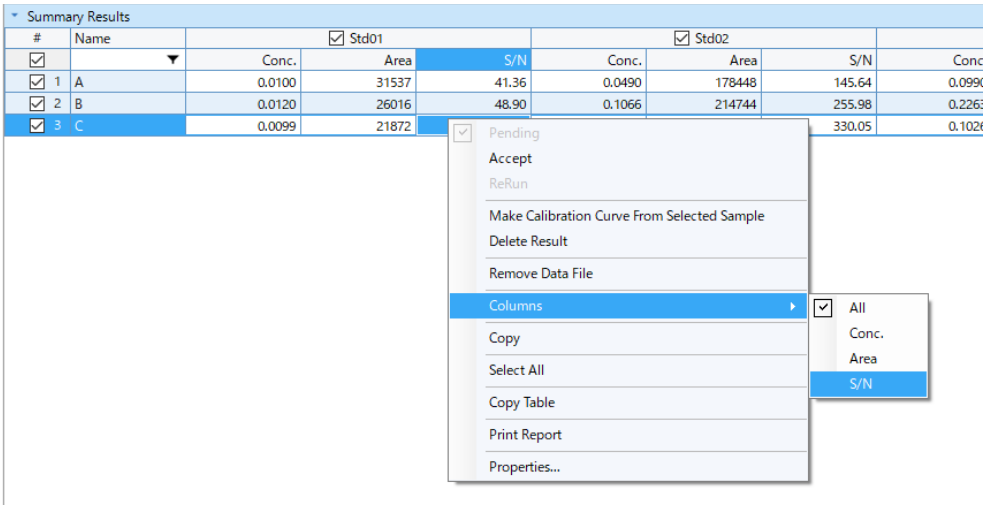
For [Sample identifier], the label of the samples to be displayed in Summary can be selected from among data file name, sample name, and sample ID.

Table cells relating to compounds that are not present in a particular sample are shown as such by the use of a series of dash characters (-----).

The [Sample List] operations available in [Compound View] are now accessed through right clicking on a cell in the [Summary] table.

3.13.2 Show Selected Columns

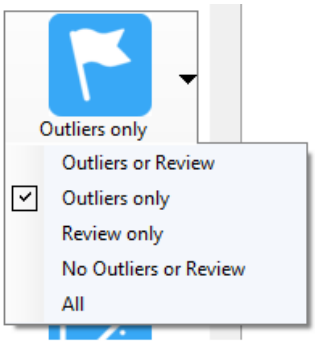
It is possible to show or hide columns being compared in the Summary table directly from the table. Right click on the table and select the [Columns] menu. The [Columns] menu lists the quantitation results that have been selected to be compared in the Summary Table. Select the required columns to be displayed as required. In order to show all columns, select [All].



3.14 [View] Flags Filter

Click on the second button (Flags Filter) in the View menu band and select filtering based on the flags from the drop down list that appears under the button.

The Flags Filter button is enabled only if there are flags defined.



When a Flags Filter is selected the contents of the lists currently being displayed will be immediately updated so that only samples and compounds that have the flags of the selected filter type will be shown.

Selecting the Flags Filter option overrides any filtering that has already been applied to the lists.

All existing column filtering will be removed.

Column filtering can subsequently be applied in the usual way.

Selecting the Flags Filter and selecting the ‘All’ option will turn the option off, all filtering will be removed and the entire (unfiltered) list of sample and compound results will be displayed in all views.

When a particular Flag Filter is active, the Flags Filter button will change to indicate which filter is currently selected:

All

Show all samples regardless of their flag status.

Outliers or Review

Show only those samples with Review or Outlier flags.

Outliers only

Show only those samples with Outlier flags.

Review only

Show only those samples with Review flags.

No Outliers or Review

Show only those samples with no flags.

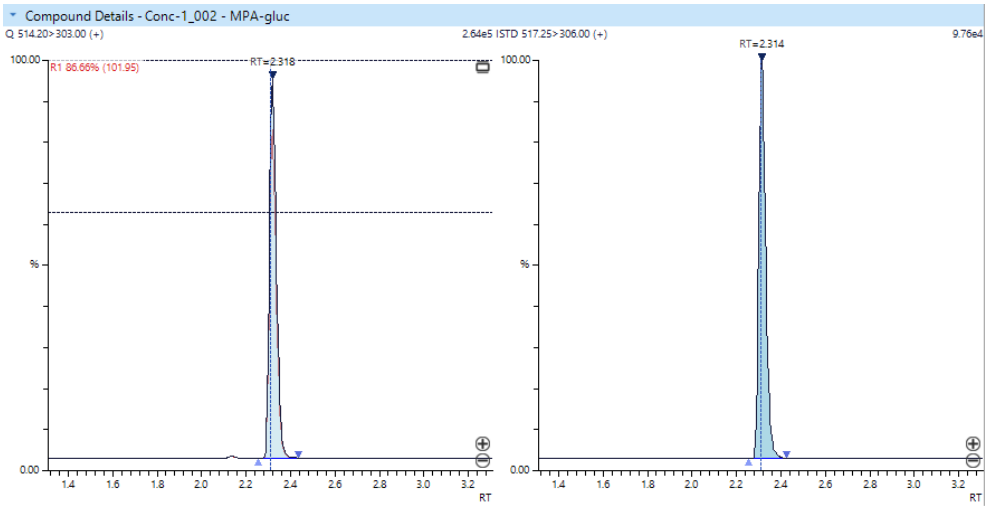
3.15 [View] Compound Details

The Compound Details pane can be displayed by pressing the Compound Details button in the View menu band.

If the Compound Details pane is not already shown when this menu button is clicked then a new pane is opened.

If the Compound Details pane is already created, but not showing on top, clicking on this button will bring Compound Details to the top.

If the Compound Details is showing on top, clicking on this button will close the pane.



The [Compound Details] pane can display chromatograms of the quantitative ions and reference ions for a selected compound. It can also display chromatograms of ISTD compounds when an ISTD group is specified.

For GCMS data, comparison chromatograms are appended to the bottom of the chromatograms. Please see sections 3.15.9 “Show Spectra (GCMS only)” and 3.15.10 “Show Comparison Chromatograms (GCMS only)” for details.

The items to be displayed in the [Compound Details] pane can be specified by right-clicking the mouse and selecting [Properties] in the menu displayed or selecting the [Settings] button in the [View] menu band.

See [3.19.2 Chromatogram] for details on the [Display Settings] dialog.

A popup menu can be accessed by right clicking in the graphs.

Undo Zoom	Undo the previous zoom.
Redo Zoom	Redo the last zoom.
Initialize Zoom	Initialize the zoom to default.
Copy	Copy the current graph as a graphic.
Paste	Paste the content of the clipboard.
ID Peak	Display the identified peak.
All Peaks	Display peaks in the entire data acquisition time.
Update	Retention Time and Reference Ion Ratios]：update the retention time to the specified time on the chromatogram and the reference ion ratios to the actual ratio.

	[Retention Time only]: update the retention time to the specified time on the chromatogram [Reference Ratios only]: update the reference ion ratios to the actual ratio.
Select Quant Ion	Select a transition (or mass) to be used as the target ion from among the transitions (or masses) specified for the reference ion and switch them. An asterisk (*) is added at the beginning of the transition (or mass) specified as the target ion.
Manual Identification	Manual peak identification indicator is displayed for peaks that have been identified. To identify a different peak as a compound peak, drag an indicator to the target peak using the mouse.
Clear Identified Peak	Delete peak identification results from the current chromatogram.
Delete All Peaks	Delete all peaks from the current chromatogram.
Manual Peak Integrate	Select Link Point, Horizontal or New Baseline and perform manual peak integration.
Apply Peak Integration To All Samples	Apply the manual peak integration process applied to the currently selected chromatogram to all samples.
Properties	Display the dialog box for chromatogram settings in display settings.

3.15.1 ID Peak / All Peaks

These are paired and toggled options.

1.6.2

ID Peak will display a window of data around the identified peak(s). All Peaks will display the entire acquisition duration to show all peaks.

3.15.2 Update RT / Ion Ratios 1.6.2

Select the set retention time on the graph area and update it. The current reference ion ratio can be applied as the set value.

Update

Retention Time and Ion Ratio*	Set the retention time and update the reference ion ratio at the same time.
Retention Time only*	The set retention time can be selected on the graph. Move the mouse cursor to move the bar and click the mouse at the retention time the user wants to set to update the set retention time.
Reference Ion Ratio only	Apply the measurement value of the current reference ion ratio as the set value.

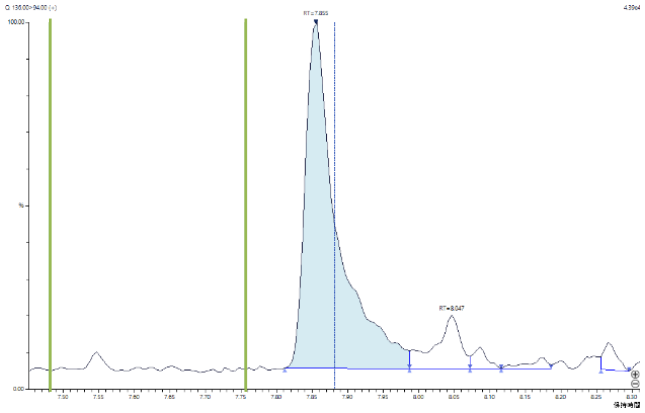
*For GCMS only, the event number is adjusted automatically when the retention time is changed.

3.15.3 Noise Range Setting (GCMS only)

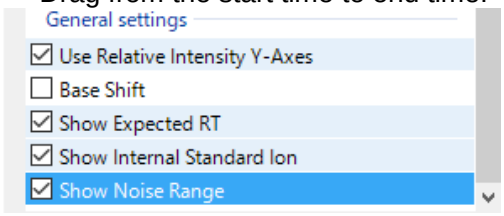
The start and end times of noise calculation can be selected and specified on the graph area.

Update

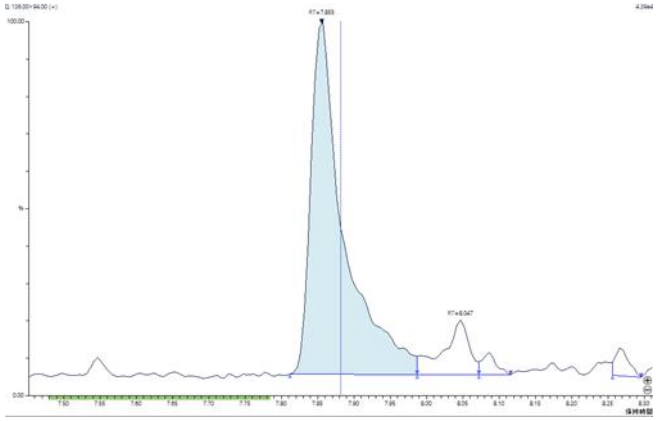
Noise Range Setting	The start and end times of noise calculation can be selected and specified on the graph area. Drag the time you want to set and update the start time and end time and the green bar will move.



Drag from the start time to end time.



When [Show Noise Range] is checked in Display Settings, the specified noise range and automatically calculated noise range can be checked on the chromatogram.



3.15.4 Select Quant. Ion

It is possible to swap a reference ion in for the quantitation ion. Click on this context menu item to show a list of available reference ions. Select the required reference ion to make it the new quantitation ion. Quantitation is performed automatically.

3.15.5 Manual Identification

There are 3 ways to do Manual identification. Manual identification can only be performed on the quantifier ion.

A) Using the context menu

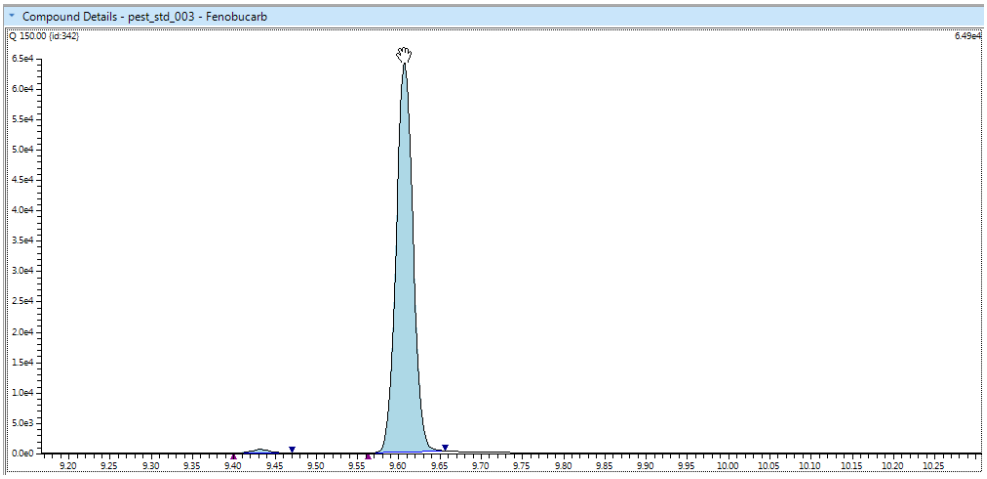
1. Right click in a chromatogram graph area in Compound Details pane to show the context menu.
2. Select Manual Identification. This brings up a vertical bar in the chromatogram.
3. Move the bar by moving the mouse cursor.
4. Click over or near a peak to be identified.
5. Data gets updated for that compound in the Compound Results pane and in the Compound Details pane and a triangle mark appears over the apex of the nearest peak.

B) Using the keyboard shortcut

1. Right click on a peak while holding the [Shift] and [Ctrl] keys down.
2. Data gets updated for that compound in the Compound Results pane and in the Compound Details pane and a triangle mark appears over the apex of the peak.

C) If there are multiple peaks picked and one of them has been identified (has a triangle at its apex) it is possible to reassign the identification to another peak by dragging the triangle to the new peak.

1. Move the mouse on to the apex of the identified peak. A hand cursor signifies it is possible to perform the change.
2. Click and hold down the left mouse button to “grab” the triangular mark, then drag the mark over to the apex of the new peak and release the mouse button to “let go” of the mark.



3. Data gets updated for that compound in the Compound Results pane and in the Compound Details pane and a triangle mark should appear over the apex of the newly identified peak.

If the exact peak apex is not selected, the nearest peak apex will be selected as the new peak.

Setting peak identification for a standard sample will result in a calibration point being displayed for the selected sample and compound.

3.15.6 Clear Identified Peak

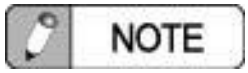
There are 2 ways of removing peak identification for a compound. Peak identification can only be deleted from a quantifier ion.

A) Using the context menu.

1. Right click in a chromatogram graph area in Compound Details pane to show the context menu.
2. Select 'Clear Identified Peak' in the context menu.
3. Click over an identified peak.
4. Data gets updated for that compound in the Compound Results pane and in the Compound Details pane and the arrow above the peak apex will be removed and there will be no peak identified for the selected compound.

B) Using the keyboard shortcut.

1. Double right click on an identified peak while holding the [Shift] and [Ctrl] keys down.
2. Data gets updated for that compound in the Compound Results pane and in the Compound Details pane and the arrow above the peak apex will be removed and there will be no peak identified for the selected compound.



Removing a peak identification in a standard sample results in removing the corresponding calibration point in the calibration curve for the selected sample and compound.

3.15.7 Delete All Peaks

Delete all peaks in the result chromatogram.

3.15.8 Manual Peak Integrate

If peaks cannot be detected normally by performing automated peak integration, peak integration can be performed manually. The following operations can be performed.

Manual Peak Integrate

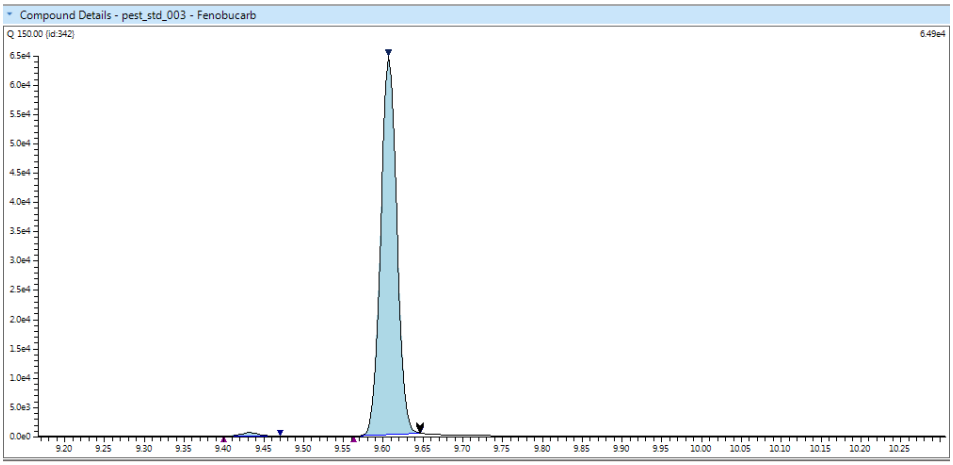
Link Point	Draws a baseline connecting two points of a chromatogram specified using the mouse to create a new peak.
Horizontal	Draws a horizontal baseline connecting two points specified on the x-axis using the mouse to create a new peak.
New Baseline	Draws a baseline connecting arbitrary 2 points by dragging the mouse.

These operations can be accessed from the context menu displayed by right-clicking the mouse on a chromatogram in Compound Details.

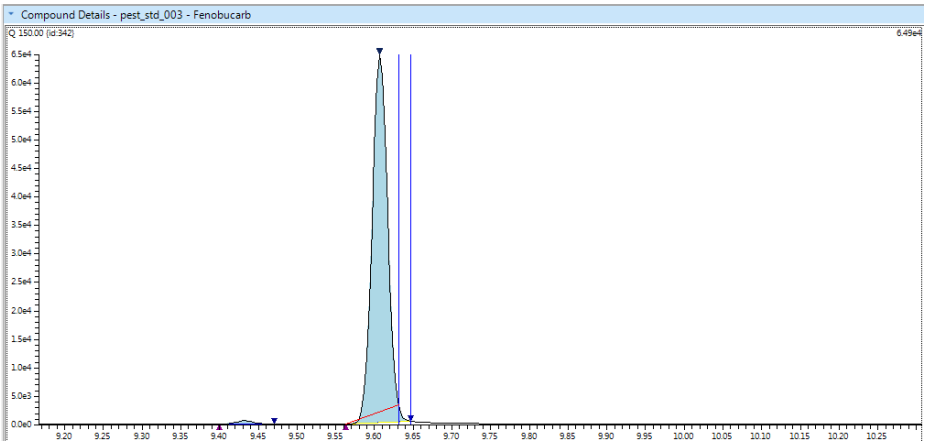
3.15.8.1 Manual Peak Integration – Adjusting existing baselines

It is possible to modify a peak by dragging its ends to a new location. For this

1. Select the chromatogram trace (bring to the top) whose peak is to be modified.
2. Bring the cursor over the baseline indicators marking the start or the end of a peak. As the cursor goes over the chromatogram at a peak baseline indicator end, it changes its default shape to an arrow to indicate possibility for a change.



3. While the new cursor is displayed, click and drag the mouse to a new location. Vertical lines show the start and end of the dragging. The new baseline is drawn that connects the intersection of the chromatogram at the destination of the dragging operation with the other end of the peak.



4. Release the mouse button to select the new location as the peak start or end position. Data gets updated for that compound in the Compound results pane and in the Compound Details pane.

This procedure can be done at either end of the peak.

3.15.8.2 Manual Peak Integration – Adding a peak 1.6.2

It is possible to define a new peak using either the context menu or via the keyboard shortcut. If the operation is done over an existing peak, it has the same effect as replacing the old peak with the new one.

A) Using the context menu.

1. Right click in a chromatogram graph area in Compound Details pane to show the context menu.
2. Select Manual Peak Integration followed by either Link Point, Horizontal or New Baseline.

   Link Point: Draws the baseline line as a straight line connecting the two points on the chromatogram.

   Horizontal: Draws the horizontal baseline from the x-values of the two points on the chromatogram. The y-axis value is taken from the start point of the peak.

   New Baseline Draw the baseline connecting the arbitrary 2 points.
3. Click on the left mouse button at the start of the new peak, then hold down and drag to the end of the new peak.
4. Release the mouse button to confirm the new peak.
5. Data gets updated for that compound in the Compound results pane and in the Compound Details pane.

B) Using the keyboard shortcut.

1. Hold down the [Shift] key or the [Ctrl] key.

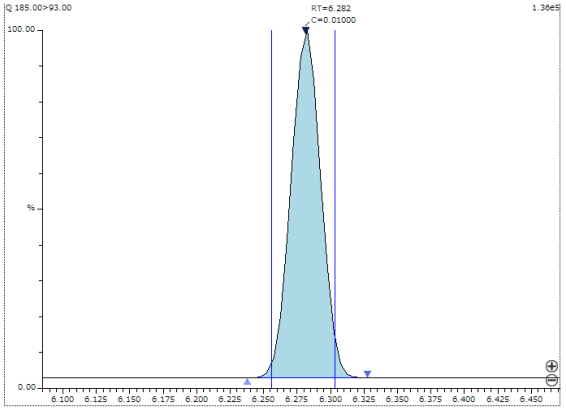
   [Shift] key: Same effect as selecting Link Point in the context menu.

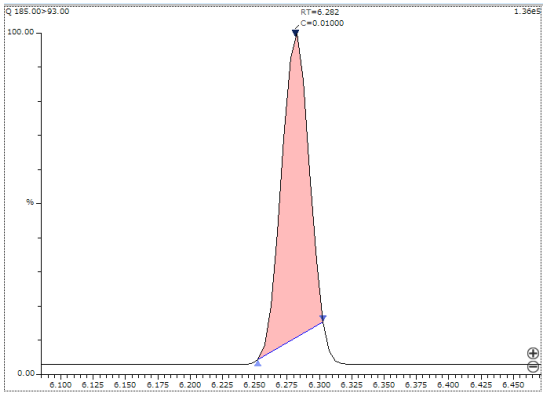
   [Ctrl] key: Same effect as selecting Horizontal in the context menu.

   [Alt] key: Same effect as selecting New Baseline in the context menu.
2. Right click with the mouse, drag the mouse and release it to mark the start and the end of a new peak. Vertical bars mark the start and end of the mouse drag.
3. Data gets updated for that compound in the Compound results pane and in the Compound Details pane.

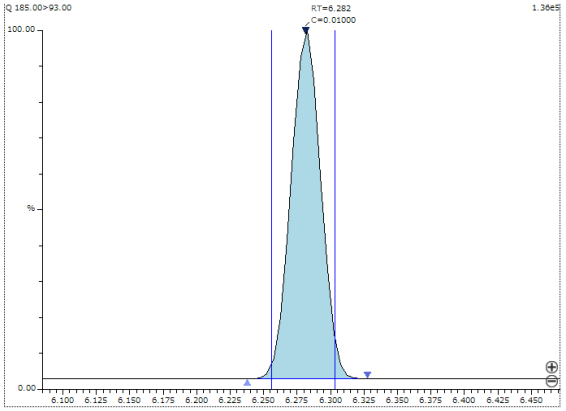
Below are examples showing the difference among Link Point, Horizontal and New Baseline options:

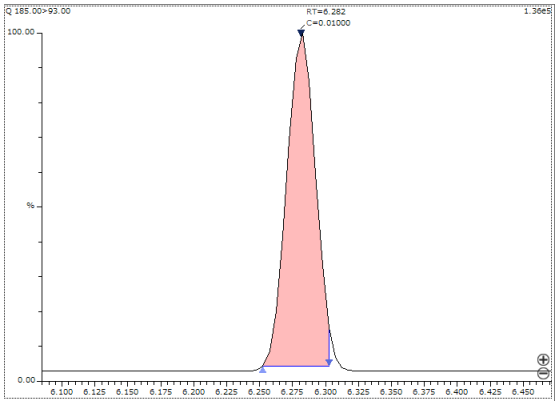
Link Point



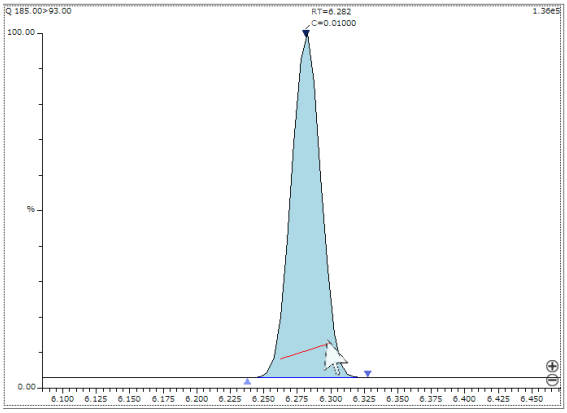


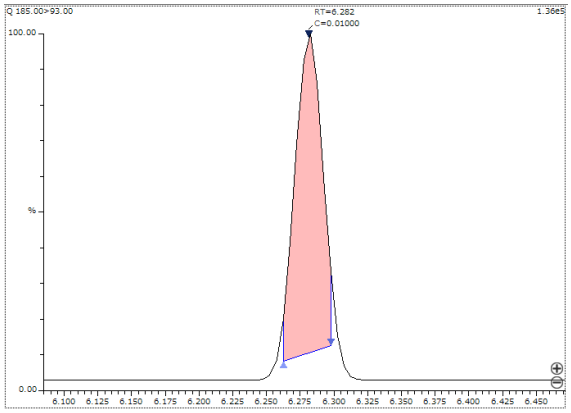
Horizontal





New Baseline



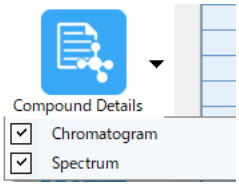


3.15.8.3 Apply Peak Integration to All Samples

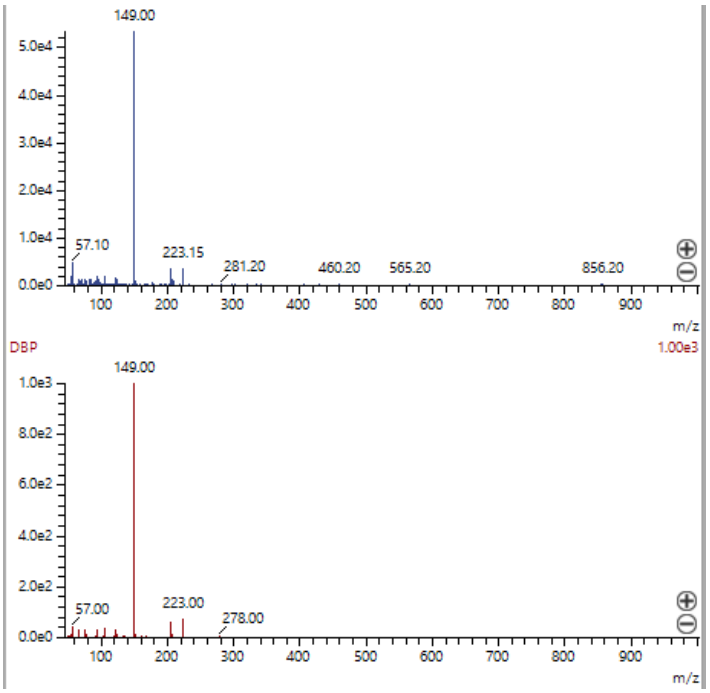
Apply the peak integration performed on the currently selected chromatogram to the chromatogram of the same compound of all samples.

3.15.9 Show Spectra (GCMS only)

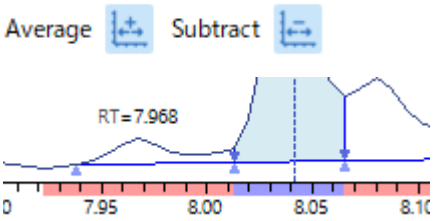
Normally, chromatograms are displayed in the Compound Details pane. For GCMS, it is possible to show spectra next to chromatograms. In order to show spectra, select Spectra from the drop down menu of the Compound Details button.



The Spectrum pane is split horizontally into two. The upper part shows the spectrum corresponding to the chromatogram currently displayed in the Compound Details pane. The lower part shows the standard spectrum registered for the compound currently being selected. The standard spectra are available in Shimadzu Method Packages and Database products.



The spectrum in the upper part is averaged and subtracted in the retention time range automatically calculated from the peak integration result of the current chromatogram. Spectrum Processing Tools can be used to obtain spectra from a specific retention time range. The averaged rage is shown in blue, and the subtracted range is shown in red along the retention time axis.



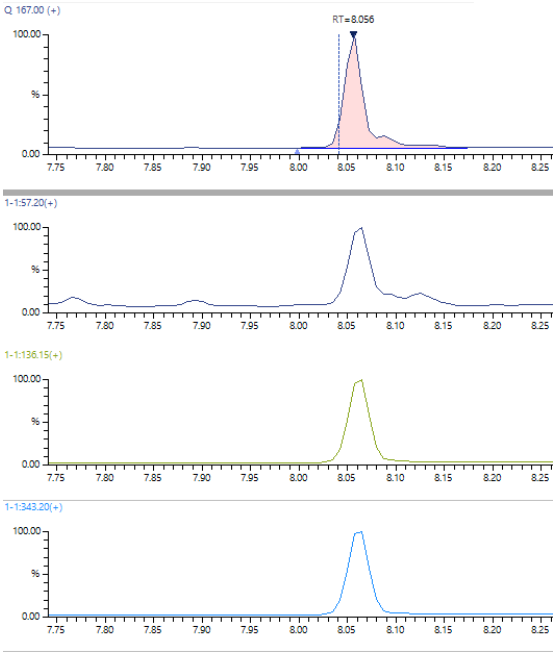
Right click context menu items specific or useful to this view are listed below:

Select	Select a spectrum peak for which to show the Comparison Chromatogram. The Comparison Chromatogram is added to the bottom of the Chromatogram Pane.
Copy	Copies the current spectrum to clipboard.
Picture (Enhanced Metafile)	Copies the spectrum as a picture.

Text	Copies the spectrum as text of m/z – intensity pairs and some header information.
Paste	Paste the content of the clipboard onto the spectrum view. The pasted item can be selected and edited or deleted.
Picture (Enhanced Metafile)	Pastes a picture on the spectrum.
bitmap	Pastes a picture on the spectrum.
Unicode Text	Paste the text in Unicode.
Text	Paste the text as is.
Export…	Export the current spectrum to file in JCAMP format. Name the file and save the exported JCAMP to the required location.
Properties	Configure the view settings for spectra.

3.15.10 Show Comparison Chromatograms (GCMS only)

It is possible to draw an XIC for the m/z of a spectrum peak obtained from the spectrum of the current chromatogram peak. Double clicking on the spectrum peak automatically displays the XIC. Up to 5 comparison chromatograms can be drawn, and they are displayed below the target chromatogram and reference ion chromatograms.

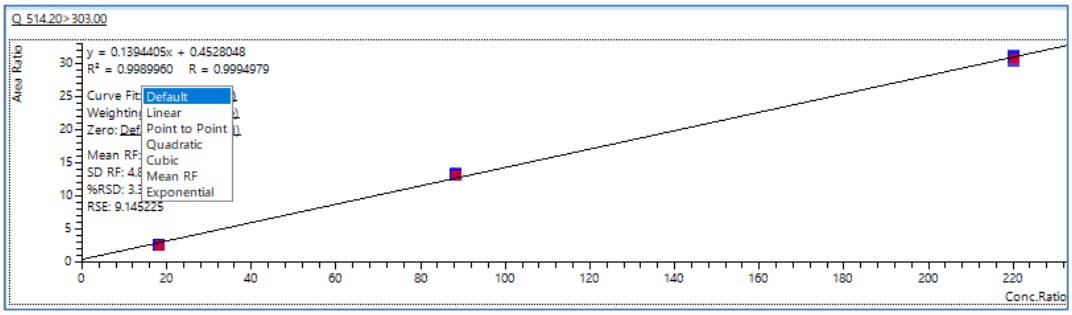


3.16 [View] Calibration Curve

To open the [Calibration Curve] pane, press the [Calibration Curve] button in the [View] menu band. If the [Calibration Curve] pane is not displayed when this menu button is clicked, a new pane opens.

3.16.1 Edit Calibration Curve

Parameters that can be changed are underlined in properties in the calibration curve sub-window.

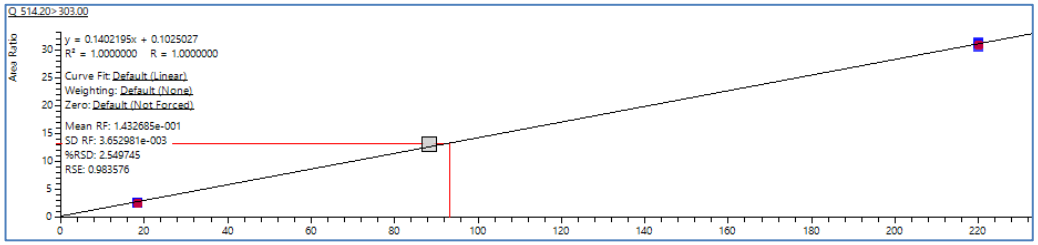


Curve Fit	Select the type of calibration curve to fit to the calibration points.
Default	Use the curve type selected in the method's quantitative parameters.
Linear	Draw a straight line through the calibration points.
Point to Point	Draw straight lines between each calibration point.
Quadratic	Draw a quadratic curve through the calibration points.
Cubic	Draw a cubic curve through the calibration points.
Mean RF	Use the mean of the response factors to determine the slope of the calibration curve. This curve always passes through the origin.
Exponential (LCMS only)	A linear calibration curve is drawn in a natural log-natural log graph.
Weighting	Select the type of weighting to employ in calculating the fit.
Default	Uses the weighting method selected in the method's quantitative parameters.
None	
1/C	Weighting by the concentration.
1/C^2	Weighting by the square of the concentration.
1/A	Weighting by the area (or height when height is used).
1/A^2	Weighting by the square of the area (or height when height is used).
Zero	Select how to handle the origin.
Default	Use the zero through option selected in the method's quantitative parameters.
Not Zero Forced	Do not force the calibration curve through the origin.
Zero Forced	Force the calibration curve through the origin.
Line to Level #1 (GCMS only)	Draw a straight line from the origin to the first calibration point regardless of the type of calibration curve. The selected type of calibration curve is drawn from the 1st calibration point to the last calibration point.

Calibration points can be excluded or included from the calibration curve.

Sample Type	Cal Point
	☐
Standard	☑
Standard	☑
Standard	☐
Standard	☑
Standard	☑
Standard	☑

Disabled calibration points are shown in grey.



3.16.2 About the Calibration Curve

Calibration involves the preparation of a set of standards containing a known amount of an analyte of interest, measuring the instrument response for each standard and establishing the relationship between the instrument response and analyte concentration in the form of a graph called calibration curve. Analyte concentrations in unknown samples are evaluated by using regression results obtained from calibration curves.

The calibration curve models supported here are:

- Linear
- Quadratic
- Cubic
- Point to Point
- Mean Response Factor
- Exponential (LCMS only)

The method of least squares is the technique used for fitting a polynomial (linear, quadratic and cubic) curve through a set of data points.

The procedure assumes that the errors in the y values are substantially greater than the errors in the x values. This condition is usually true in a calibration curve in which the experimental response (y values) is less certain than the quantity of analyte (x values).

A second assumption is that the uncertainties (standard deviations) in all the y values are similar. For the polynomial curves variations of these models can be obtained by forcing the curve through the (0,0) point and/or by introducing weights in the curve fit.

The assumption in no weight least square is that each data point provides equally precise information for the curve fit. This favours numbers of larger value over numbers of smaller value.

Other possibilities for weights are: 1/C where C is the concentration (does not favour high concentrations), 1/C2 (favours smaller concentrations), 1/A where A is the response measured as are or height (does not favour higher response values), and $1/A^2$ (favours smaller response values). The main advantage of weighted least squares is the ability to handle regression situations in which the data points are of varying quality. The correlation coefficient R^2 is displayed as a measure of the strength of the degree of correlation between the concentration and response. A positive result close to 1 indicates a direct correlation.

In point-to-point calibration the calibration curve is a linear interpolation between any two consecutive calibration points.

In mean response factor curves, a line is calculated passing through each individual point and the origin, then the mean of the coefficients of the slopes is calculated and used to set a line with that slope passing through the origin.

Three useful statistics are calculated and displayed for the calibration data: mean response factor, standard deviation of the response factor and relative standard deviation of the response factor.

In addition to the calibration curve a graph plot of the residuals from a fit can be displayed as it can highlight problems with the calibration data fit. Ideally, the residuals should be spread randomly around the zero.

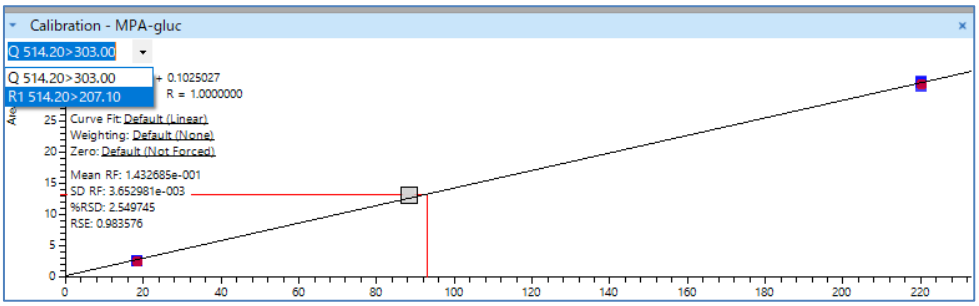
In edit mode both graphs allow calibration points to be excluded from a curve fit. The calibration curve graph still displays excluded points so that they can be included again should the user choose to do so.

Repeated measurements per concentration are allowed and their average response used to form a calibration point.

3.16.3 Reference Ion Calibration Curves

Insight automatically calculates the reference ion calibration curve if the reference ion peak has been integrated. Quantitation results obtained using the reference ion calibration curves are displayed in the results table as [Ref n conc.]. Reference ion calibration curves can be selected from the drop-down list at the top left of the calibration curve pane.

The calibration curve parameters are common to target ions and reference ions.



3.17 [View] Survey

The Survey view is accessed through the [Survey] button in the View menu band.

If the Survey pane is not already shown when this menu button is clicked, then a new pane is opened.

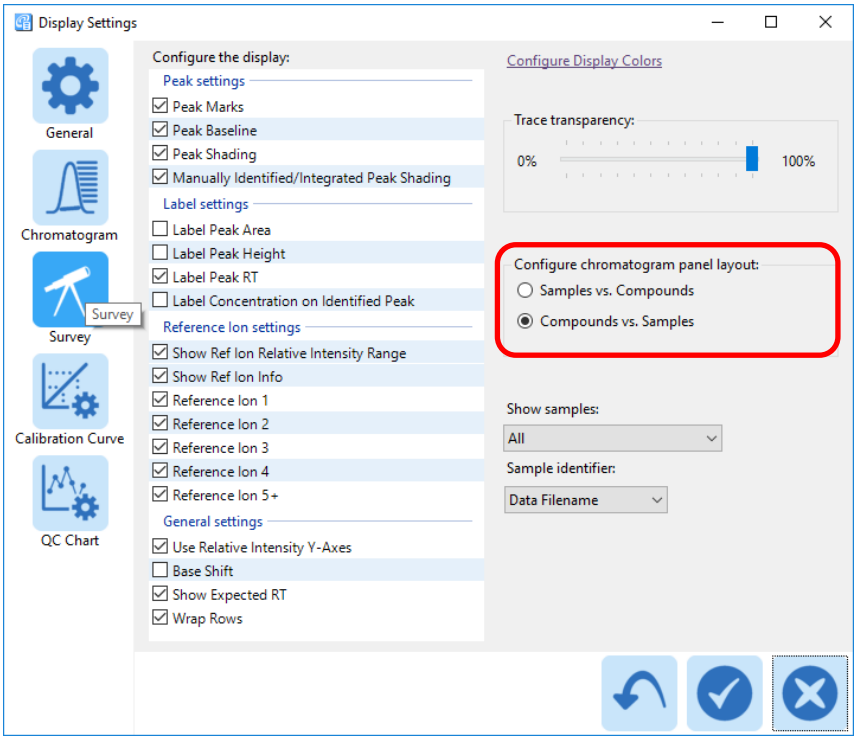
If the Survey pane is already created, but not showing on top, clicking on this button will bring Survey to the top.

If the Survey pane is showing on top, clicking on this button will close the pane.

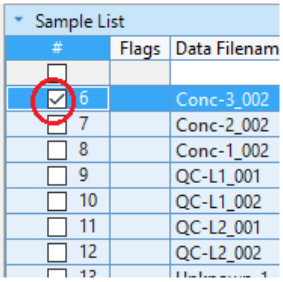
The purpose of the [Survey] pane is to present a grid of measured ion chromatograms. The chromatograms can be shown as compounds against samples or samples against chromatograms.

Access the Survey [Display Settings] by selecting the [Properties…] caption menu option. Set the orientation of the Survey View by selecting the appropriate button in [Configure chromatogram panel layout:]. See 3.19.4 Survey for details on the rest of the display options for the Survey View.

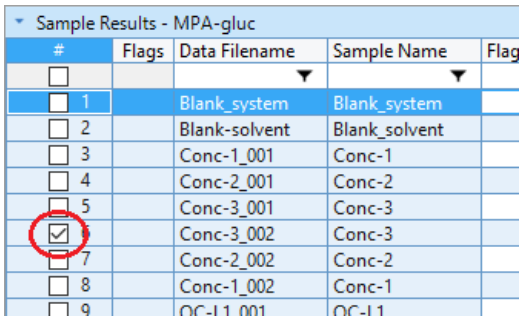
It is also possible to select which compounds and samples to show the chromatograms for.



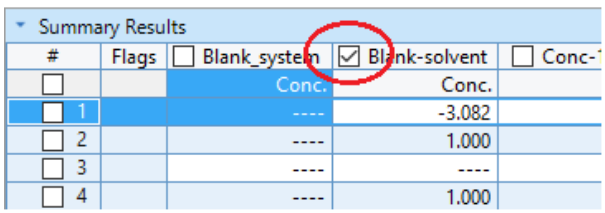
The samples to be shown in the Survey view are specified by checking/unchecking the sample selection checkbox for each sample in the Sample List, Sample Results or Summary table.



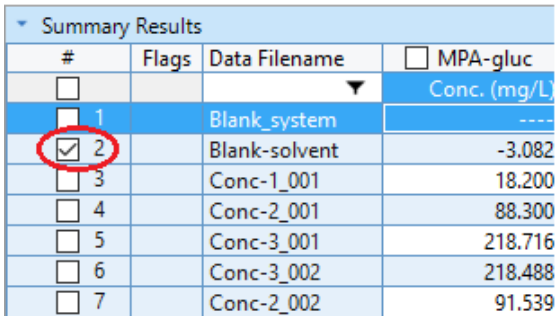
Compound View
Sample selection checkbox is in the [Sample List].



Sample View
Sample selection checkbox is in the [Sample Results] table.



Summary View
(Compounds vs Samples)
Sample selection checkbox is in the header next to each sample name.



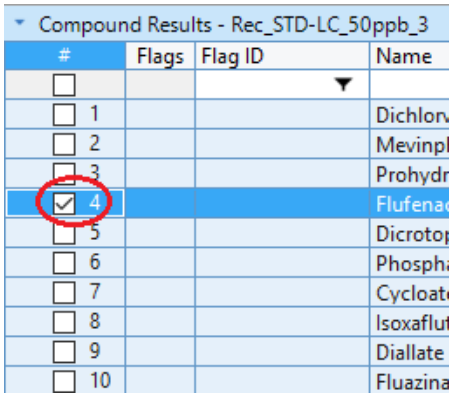
Summary Results

#	Flags	Data Filename	MPA-gluc
			Conc. (mg/L)
1		Blank_system	----
2		Blank-solvent	-3.082
3		Conc-1_001	18.200
4		Conc-2_001	88.300
5		Conc-3_001	218.716
6		Conc-3_002	218.488
7		Conc-2_002	91.539

(Samples vs Compounds)

The selection checkbox is next to the sample ID (#).

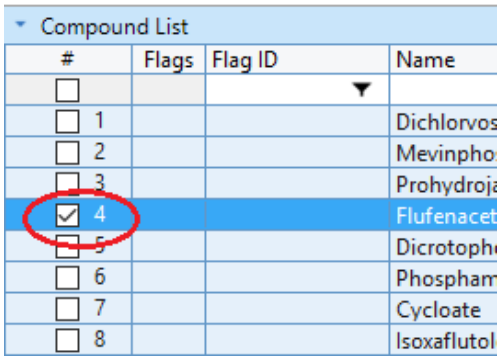
Similarly, compounds to be shown in the Survey view are specified by checking/unchecking the compound selection check box for each compound in the Compound Results, Compound List or Summary table.



Compound Results - Rec_STD-LC_50ppb_3

#	Flags	Flag ID	Name
1			Dichlorv
2			Mevinpl
3			Prohydr
4			Flufenac
5			Dicrotop
6			Phospha
7			Cycloat
8			Isoxaflut
9			Diallate
10			Fluazina

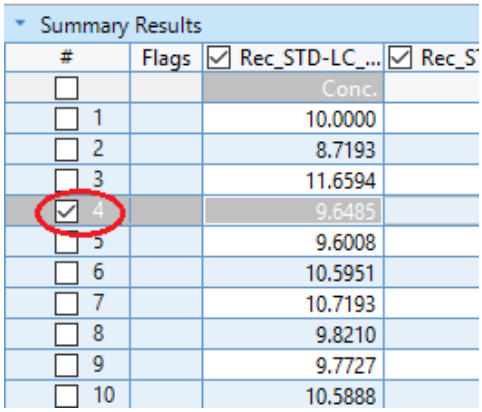
Compound View
Compound selection checkbox is in the Compound Results table.



Compound List

#	Flags	Flag ID	Name
1			Dichlorvos
2			Mevinpho
3			Prohydroja
4			Flufenacet
5			Dicrotoph
6			Phospham
7			Cycloate
8			Isoxaflutol

Sample View
Compound selection checkbox is in the Compound List.



Summary Results

#	Flags	Rec_STD-LC_...	Rec_S
		Conc.	
1		10.0000	
2		8.7193	
3		11.6594	
4		9.6485	
5		9.6008	
6		10.5951	
7		10.7193	
8		9.8210	
9		9.7727	
10		10.5888	

Summary View
(Compounds vs. Samples)
Compound selection check box is found next to the Compound ID (#).

(Samples vs. Compounds)

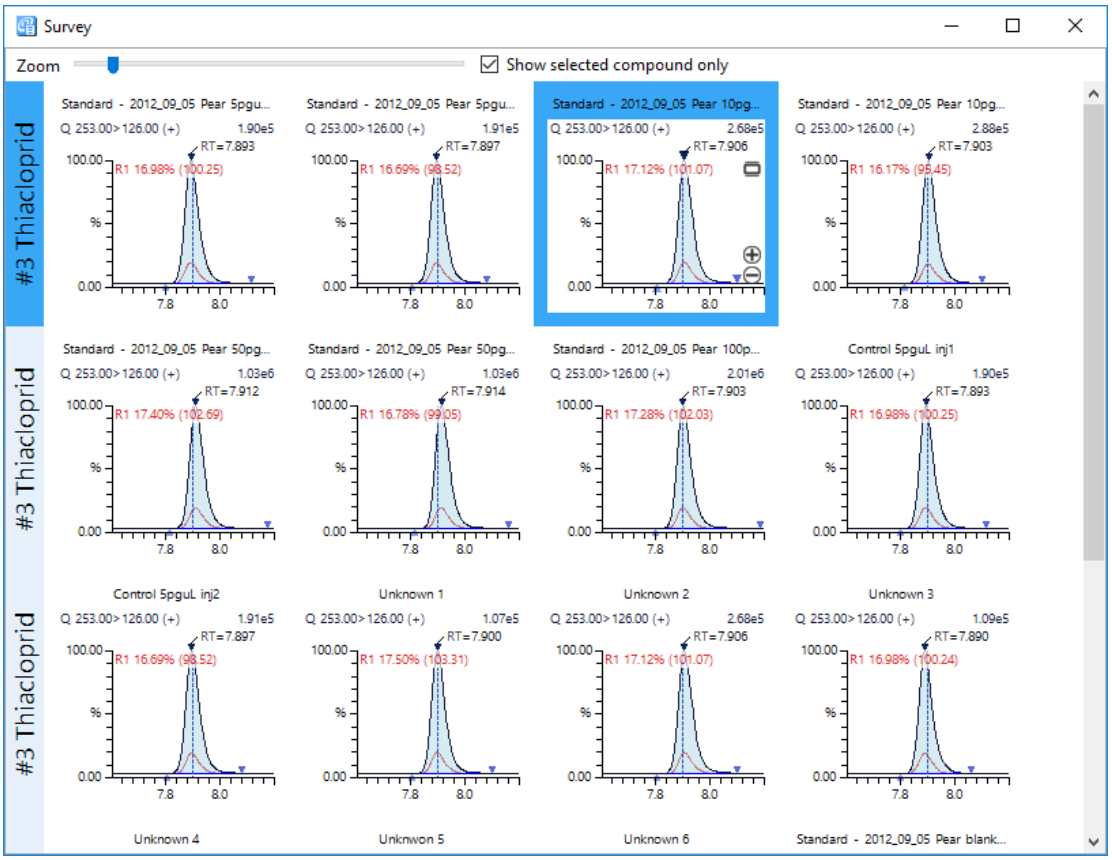
Summary Results

#	Flags	Data Filena...	Dichlo...	Mevin...	Prohy...	Flufenacet
			Conc. (p...	Conc. (p...	Conc. (p...	Conc. (ppb)
1		Rec_STD-L...	10.0000	8.7193	11.6594	9.6485
2		Rec_STD-L...	50.0000	50.2561	49.6681	50.0703
3		Rec_Cucu...	12.1518	12.3191	13.3125	11.3199
4		Rec_Cucu...	11.7214	11.6882	12.4720	10.8412
5		Rec_Cucu...	12.0569	12.0525	15.5644	10.6429

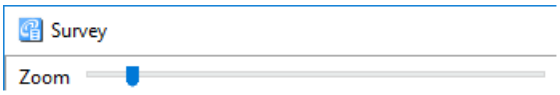
Compound selection checkbox is in the header next to each compound name.

Filtering is applied to Lists and Results are also applied to [Survey]. Only those samples showing in the List or Results table are shown in Survey.

Once samples and compounds are selected for showing in [Survey], their chromatograms are drawn as shown below:

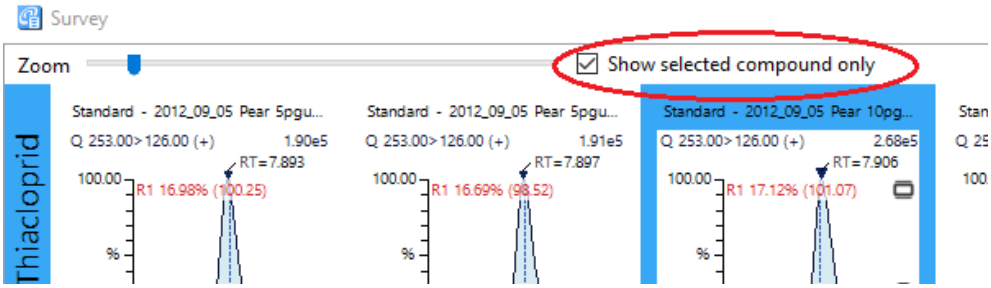


The Survey view supports chromatogram zooming functionality by means of a slider control at the top of the view:



The level of zoom set using this control is applied to all chromatograms displayed in the Survey view.

There is an option to show the selected compound or sample only:



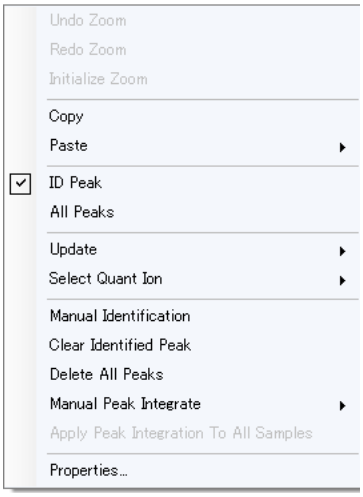
When checked the compound selected in the [Compound List] is the only row to be shown.

Selecting [Show selected sample only] provides a similar result where only the selected samples are shown.

When [Show selected compound only] is selected, only the compound row selected in the Compound List is displayed. Selecting [Show selected sample only] provides same results.

Right click in a chromatogram graph to show the context menu below.

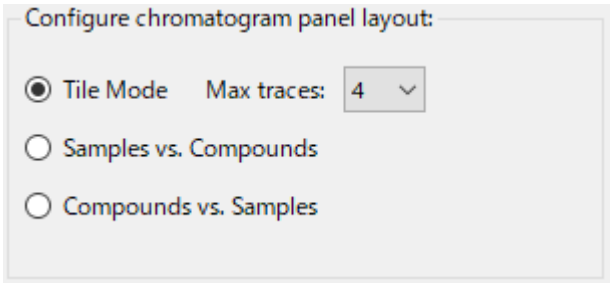
Select the appropriate zooming operation as required.



3.17.1 Tile Mode

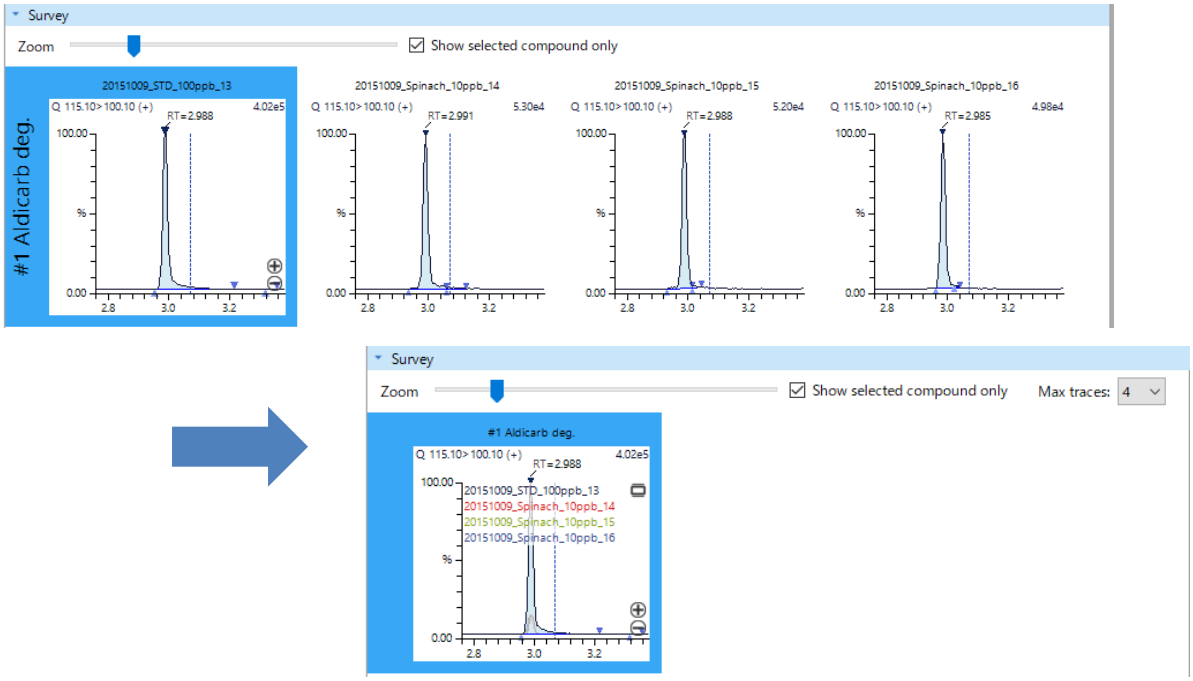
The chromatogram for each compound and sample is shown in the [Survey] view. In the Tile Mode, the chromatogram of multiple samples can be shown in 1 pane for the specified compound and can be compared with ease. In LabSolutions Insight, it is called “Tile”.

In Display Settings in the [Survey] view, select [Tile Mode] in Configure chromatogram panel layout. Refer to 3.18［View］-[Settings]‐[3.18.3 Survey] regarding how to set.

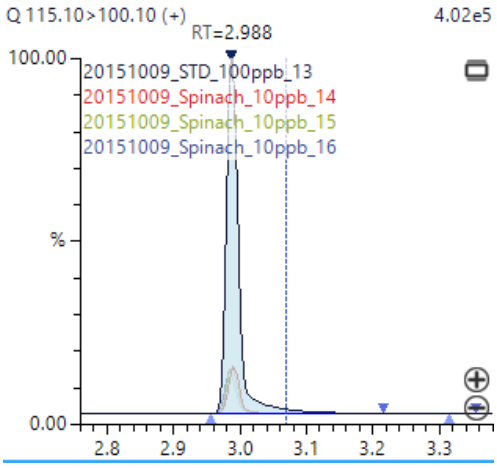


In the Tile Mode, the multiple chromatogram specified in [Max traces] is shown in 1 tile.

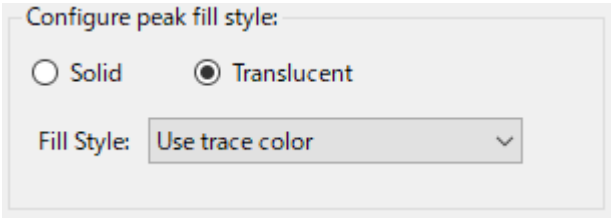
The following example shows 4 chromatogram is shown in 1 tile.



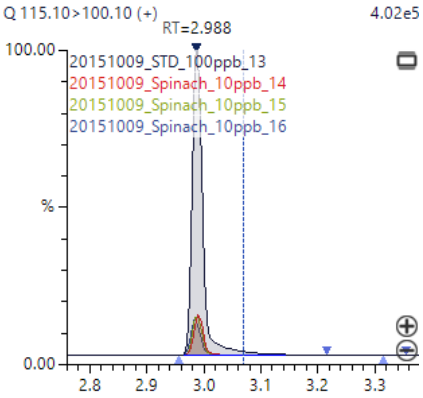
4 chromatogram is shown in 1 tile. The compound name is shown on the top. The label(file name and color) at the upper left shows the corresponding data.



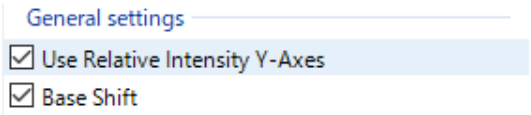
In the Tile mode, it is easy to confirm what data has the largest peak area when the filling chromatogram color is different among each data. It is recommended to set the peak fill style as follows.

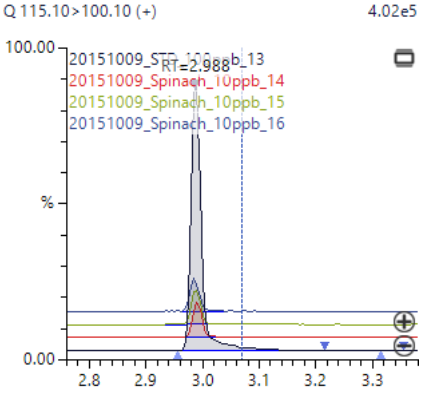


In Configure peak fill style, set [Translucent] and [Use trace color] and the chromatogram as shown in the above sample is shown as follows.

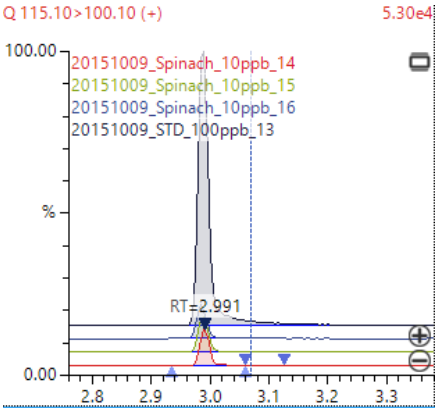


When [Base Shift] is checked, it is easy to confirm the peak starting and end points.

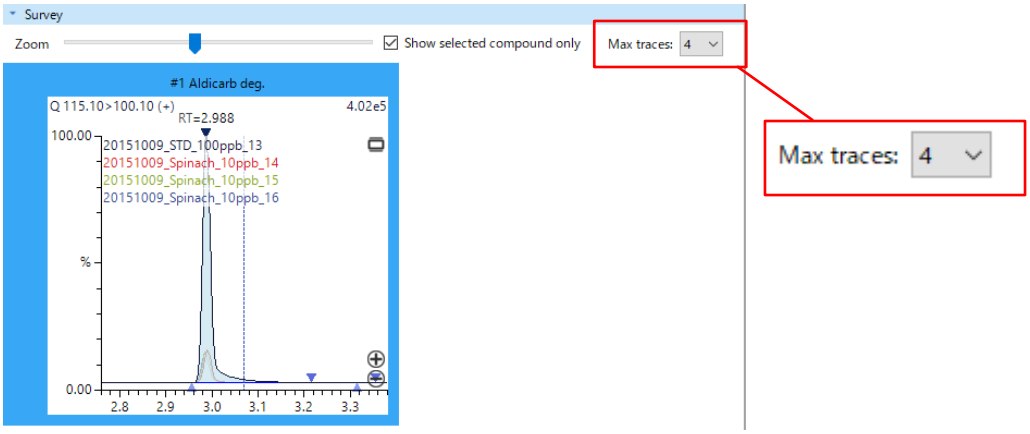




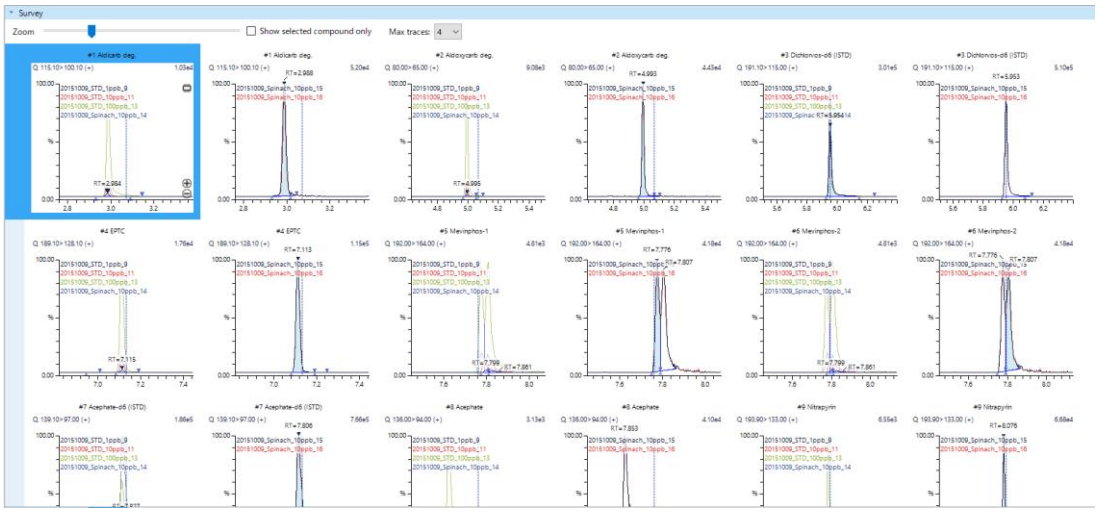
The manual peak integration is possible for the overlay chromatogram and available for the top most chromatogram. The top on the label at the left top shows the top most data. Click to switch the data. When it is clicked, the top most chromatogram will be changed as follows.



The number of the samples shown in 1 tile can be changed by changing the parameter on the [Survey] view.



1 tile is shown in the above example. When [Show selected compound only] is not checked, the tiles for all the compounds will be shown.

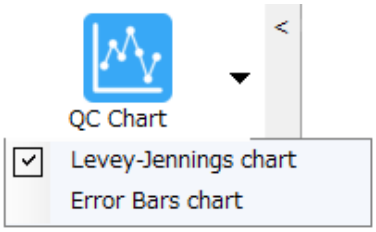


3.18 [View] QC Chart 1.6.2

The [QC Chart] pane can be opened from the [QC Chart] button in the [View] menu band. If the [QC Chart] pane is not displayed when this menu button is clicked, a new pane opens.

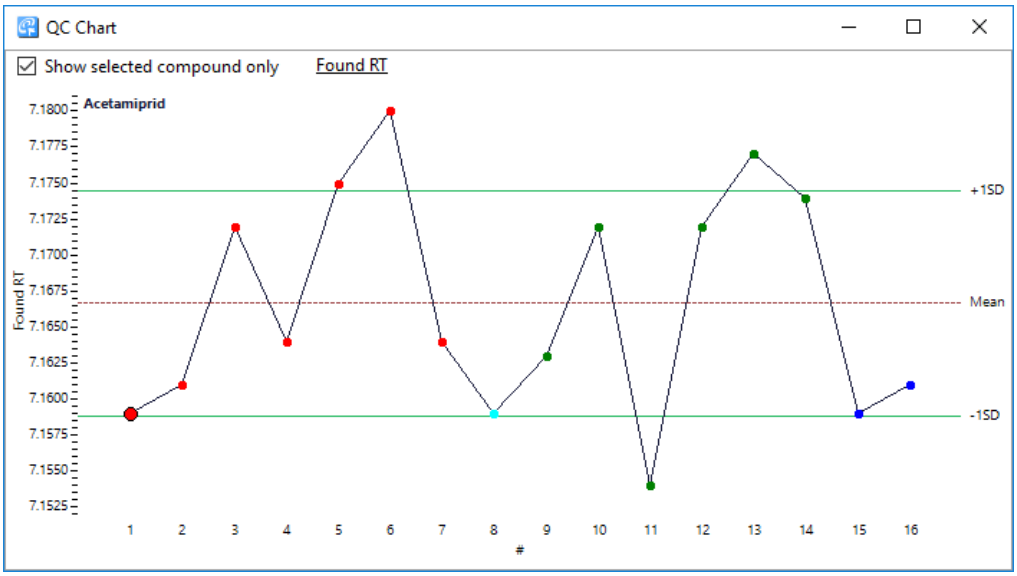
If the [QC Chart] pane has already been created but not activated, clicking this button activates [QC Chart]. If the button is clicked when the [QC Chart] pane is active, the pane closes.

Select the graph to display in the [QC Chart] pane from the drop down list of the [QC Chart] button.



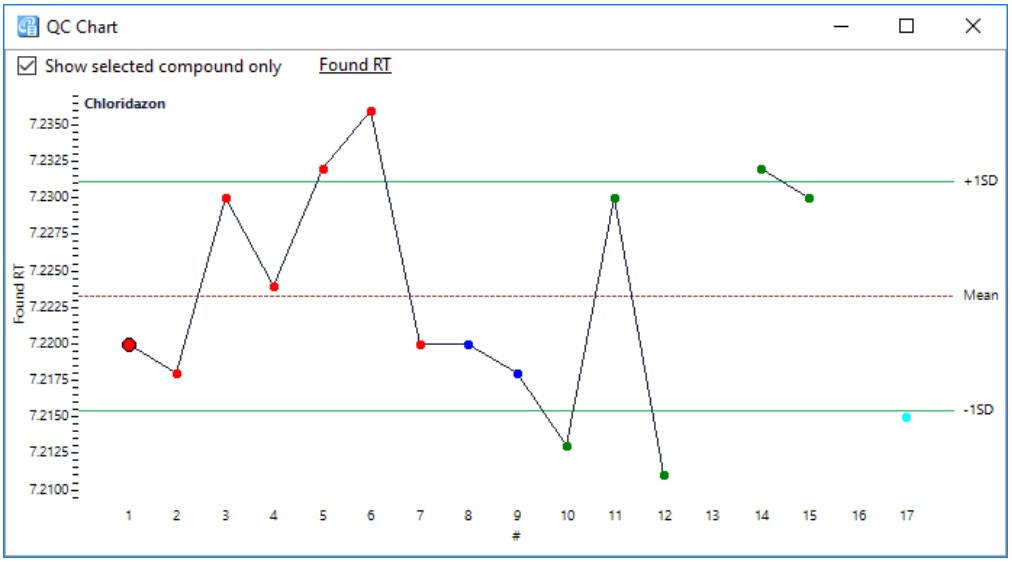
3.18.1 Levey-Jennings chart

In the Levey-Jennings chart, quantitative values of the compound selected on the table in each sample are plotted on the vertical axis and sample IDs on the horizontal axis on the graph in the order that they are displayed in [Sample List], [Sample Results] or [Summary].

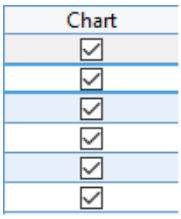


Data points corresponding to the currently selected sample are displayed slightly larger than other data points. Samples corresponding to the data points selected on the chart are also selected on the table.

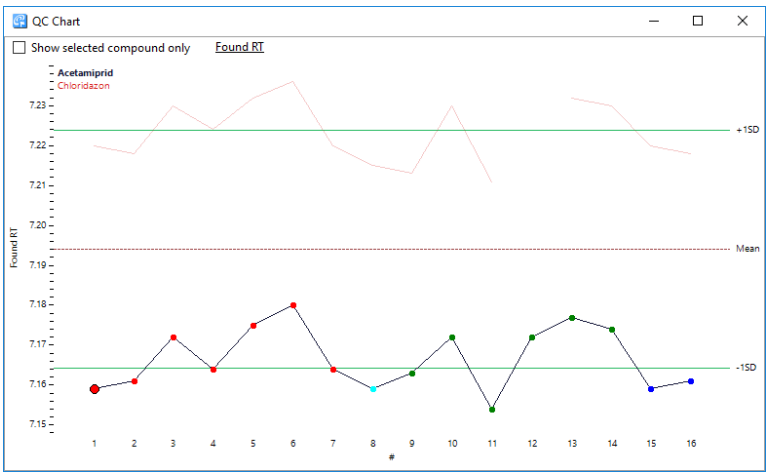
When there is no corresponding quantitative value for a sample because no peak has been identified or for any other reason, the point is skipped and the chart becomes discontinuous.



The samples to be displayed in the [QC Chart] pane can be specified by selecting the checkbox in the [Chart] item for each sample in [Sample List], [Sample Results], or [Summary].



When the [Show selected compounds only] checkbox is cleared, the graphs of all compounds for which the checkbox for the [Chart] item is selected are displayed. At this time, data points are displayed only for the selected compound. The list of the displayed compound names is shown in the upper left area of the chart.



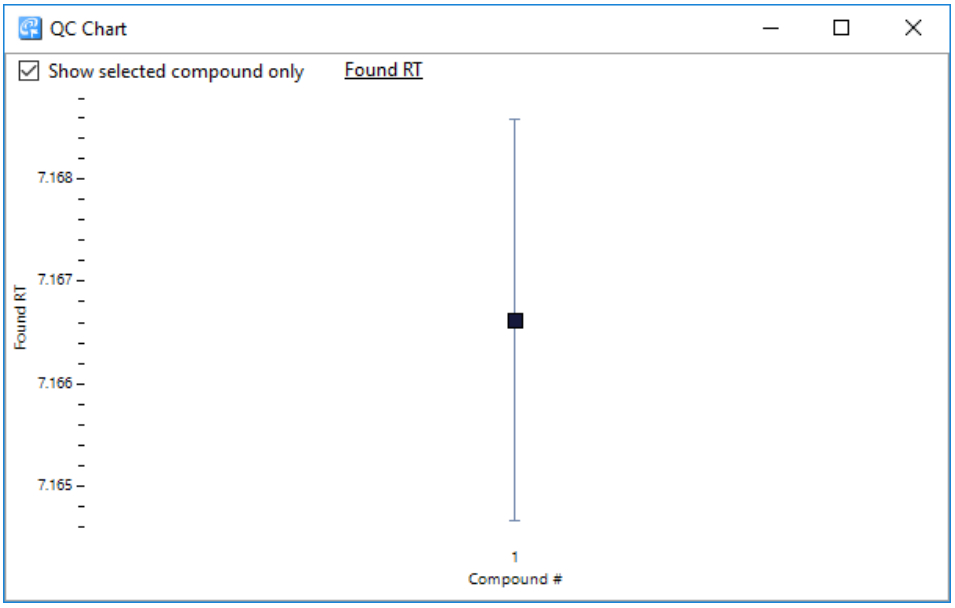
The following quantitative values can be displayed in the [QC Chart].

%Conc. Outside Curve　　ISTD %Diff (Stds.) Area　　Ref 1-5 Std Ratio %Diff

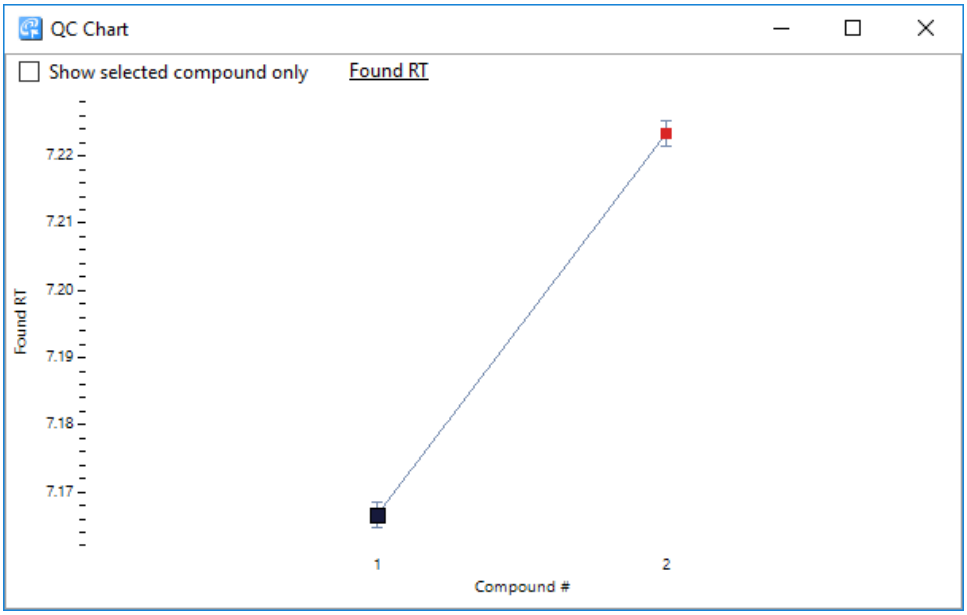
%Dev RRT	ISTD Amount	Ref. RRT
%Diff	ISTD Area	RF
%RSD (Area)	ISTD Height	RF %RSD (curve)
%RSD (Conc)	ISTD RT	RF %RSD (level)
Accuracy (%)	ISTD RT Diff	RF Deviation
Actual Ret. Index	Mass Error (mDa)	RF Mean (curve)
Area	Mass Error (ppm)	RF Mean (level)
Area Ratio	Mass Error Score	RF RSE (curve)
Asymmetry	Noise	RF SD (curve)
Average Conc.	Peak End	RF SD (level)
Average Conc. (R1, R2)	Peak Start	RRT
Conc.	Quant. Limit (QL)	RT %Diff
Conc. (no Dil.)	Recovery	RT %Diff Score
Confidence	Ref 1-5 Actual Ratio	RT Diff
Custom Calc. Result 1 – 5	Ref 1-5 Conc.	S/N
Detect. Limit (DL)	Ref 1-5 Found Mz	Sample Amt.
Dil. Factor	Ref 1-5 Mass Error (mDa)	Score
Found Mz	Ref 1-5 Mass Error (ppm)	Std RT Diff
Found RT	Ref 1-5 Measured	Tailing F (10%)
Height	Ref 1-5 Noise	Tailing F.
Height Ratio	Ref 1-5 RRT	Width (50%)
ISTD %Diff (Controls) Area	Ref 1-5 S/N	

3.18.2 Error Bars chart

The Error Bars chart displays the error bar for the quantitative value of all samples for each compound.



When the [Show selected compounds only] checkbox is cleared, the graphs of all compounds for which the checkbox for the [Chart] item is selected are displayed.



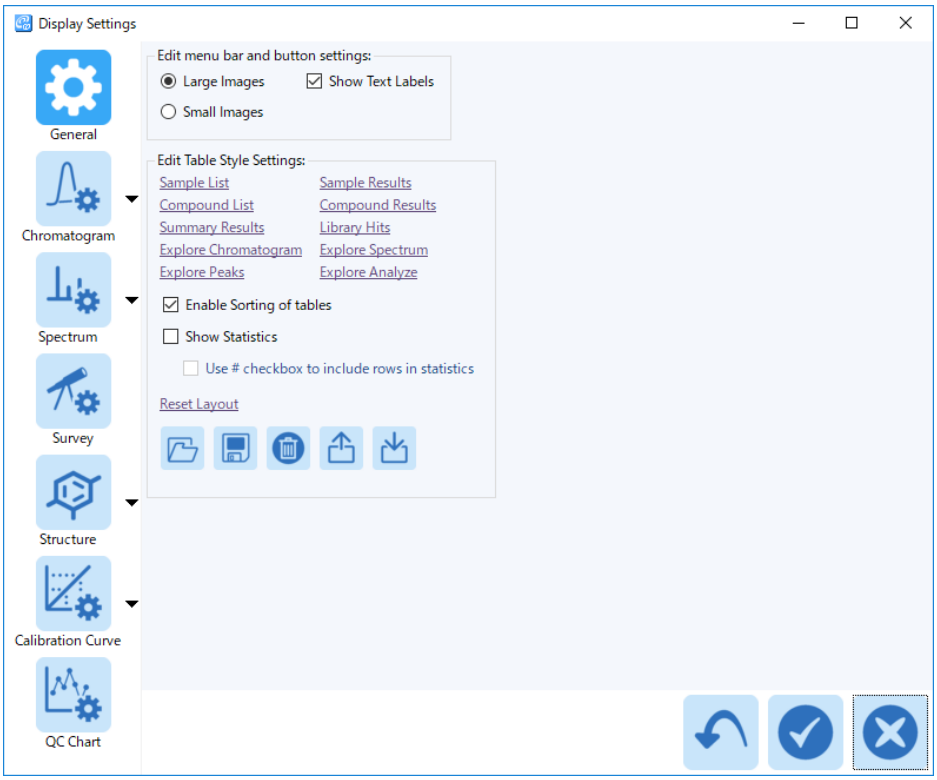
3.19 [View] Settings

Click on the [Settings] button in the [View] menu band to show the [Display Settings] dialog.

Set each of the five types of settings as appropriate:

3.19.1 General

Configure general settings for Insight.



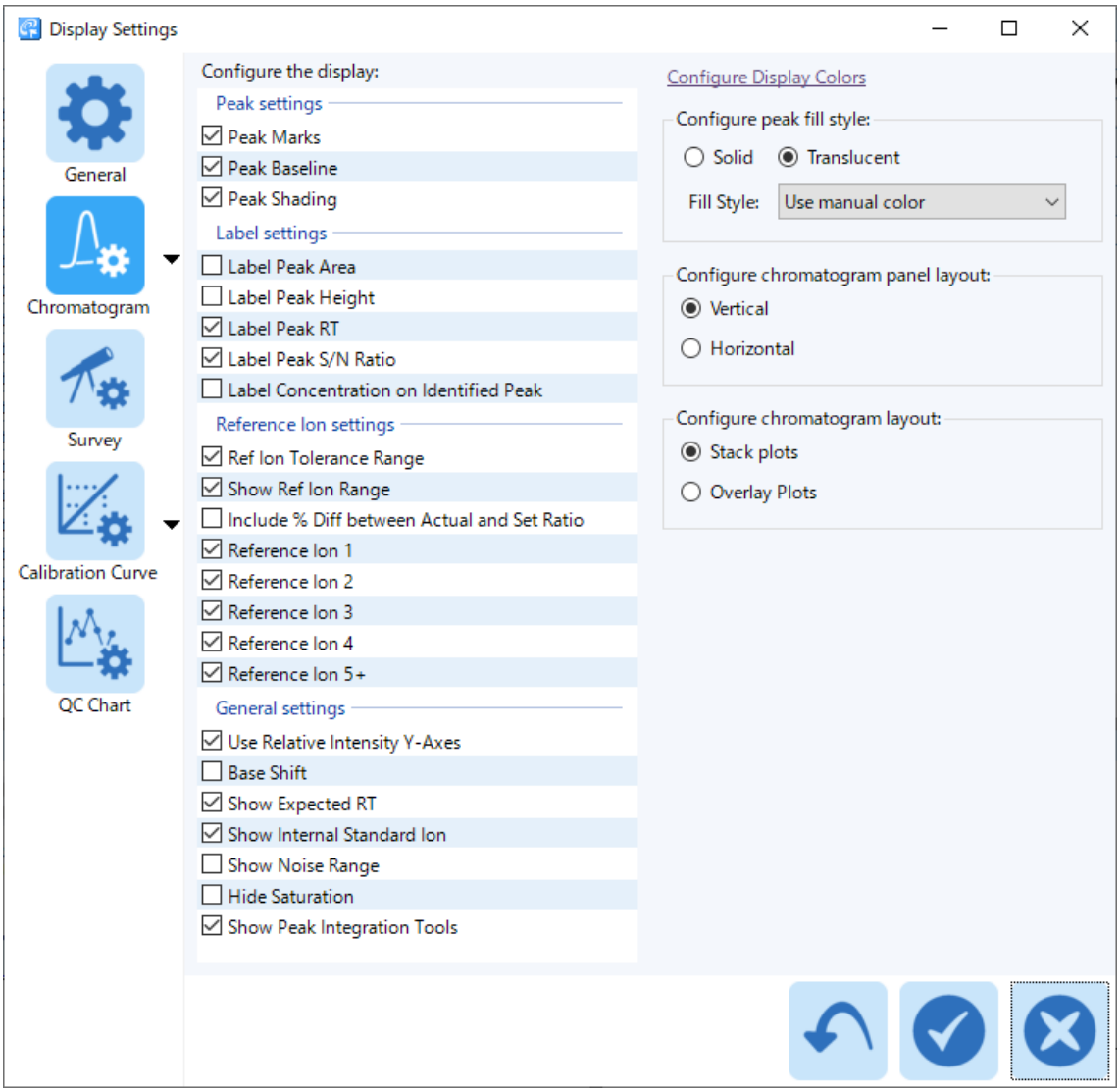
Edit toolbar and button settings

Large Images	Make the menu bar icons large.
Small Images	Make the menu bar icons small.
Show Text Labels	Tick to show text labels for each icon in the menu bar.
Edit Table Style settings	Click on each underlined item to configure the table styles. See the sections on each View to see details about each table style.
Enable sorting	When sorting is enabled, clicking on the table column heading sorts the contents in ascending or descending order.
Show statistics table	Show the statistics table below the results table.
Use checked rows for statistics calculation	Use only the rows with the check box in the [#] column checked to calculate the statistics.
Reset Layout	Reset layout options to factory default.

Load Layout	Select a saved layout and apply to the current table.
Save Layout	Save the current table style as layout.
Export Layout	Write saved layout to file.
Import Layout	Load layout from file.

3.19.2 Chromatogram

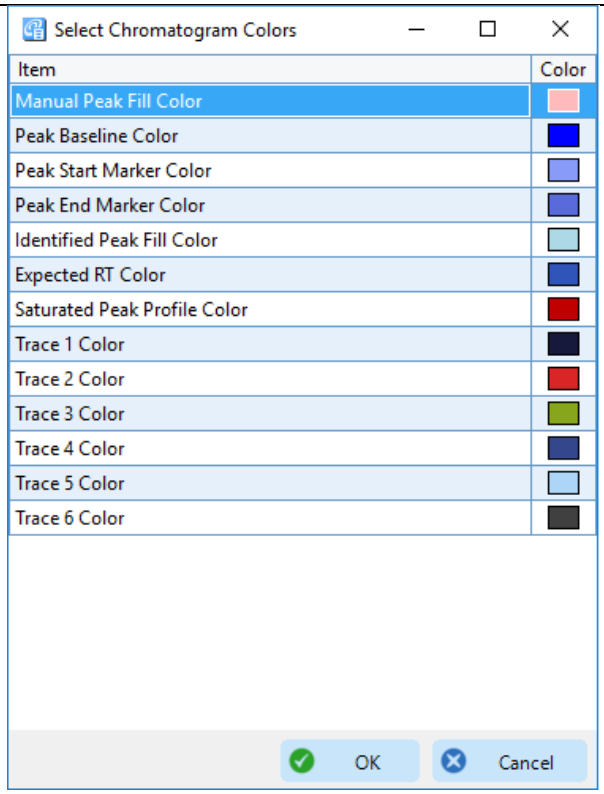
Configure settings for displaying chromatograms.



Peak settings	
Peak Marks	Show a ▼ mark at the peak start and end times.
Peak Baseline	Show the peak baseline.
Peak Shading	Fill the identified peaks. They are filled in blue by default.
Label settings	
Label Peak Area	Show the area at the peak top.

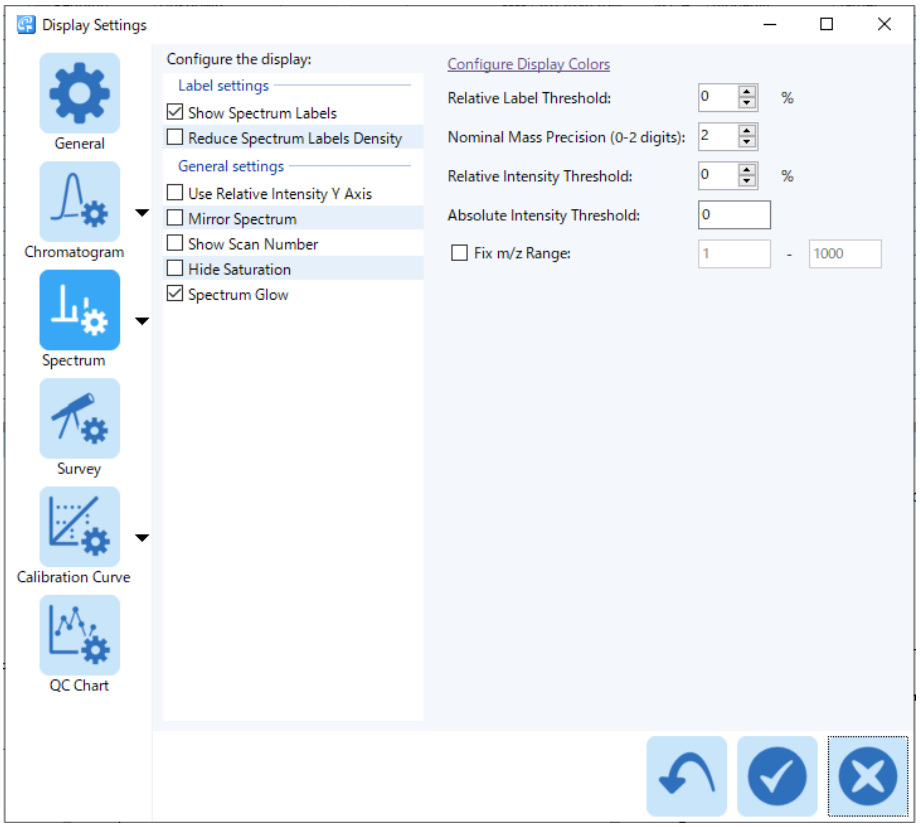
Label Peak Height	Show the height at the peak top.
Label Peak RT	Show the retention time at the peak top.
Label Peak S/N Ratio	Show the S/N at the peak top.
Label Concentration on Identified Peak	Show the concentration at the peak top of identified peaks.
Reference ion settings	
Show Ref Ion Tolerance Range	Show the allowable range of the reference ion on the chromatogram with two lines.
Show Ref Ion Range	Show the reference ion range on the top left of the chromatogram.
Include % Diff between Actual and Set Ratio	Show the difference between the set reference ion ratio and the actual reference ion ratio as a percentage. The value is displayed only when [Show Ref Ion Range] option is enabled.
Reference Ion 1 ~ 5+	Show reference ions 1 to 5.
General settings	
Use Relative Intensity Y-Axes	Display the y-axis in %.
Base Shift	Shift the base of overlaying chromatograms upward.
Show Expected RT	Show a dotted line at the position of the specified retention time on the chromatogram.
Show Internal Standard Ion	Show the internal standard chromatogram in the Compound Details pane.
Show Noise Range	The noise start end time is shown as a green line on the time axis.
Hide Saturation	Do not use red coloured chromatogram peak.
Show Peak Integration Tools	Show the peak integration tools on Compound Details pane and Survey Pane.
Show Product Ion Chromatograms	Show the product ion scan chromatogram in a similar way to target and reference ion chromatograms.

Configure Display Colors	Change the color used to display the chromatogram.

<table>
<tr><td></td><td> 
</td></tr>
<tr><td>Configure peak fill style</td><td>Specify the transparency to fill the chromatogram.
Solid Filled with color with no transparency
Translucent Filled with color with transparency
Fill Style
Use single color Fill all chromatograms with the same color. The color specified in [Identified Peak Fill Color] is used in the Display Settings.
Use manual color Fill the manual integrated chromatogram with another color. In Display Settings, the color specified in [Manual Peak Fill Color] is used for the manually integrated chromatogram.
Use trace color Fill with the same color as the color of the line that shows the chromatogram. For the line color of the chromatogram, the color specified in [Trace 1 to 6 Color] is used in Display Settings.</td></tr>
<tr><td>Configure chromatogram panel layout</td><td>Specify the direction to place the chromatograms in the Compound Details pane.</td></tr>
<tr><td>Configure chromatogram layout</td><td>Specify either to overlay chromatograms or place them side by side in the Compound Details pane.</td></tr>
</table>

3.19.3 Spectrum (GCMS only)

Configure settings for spectra shown in Compound Details for GCMS.



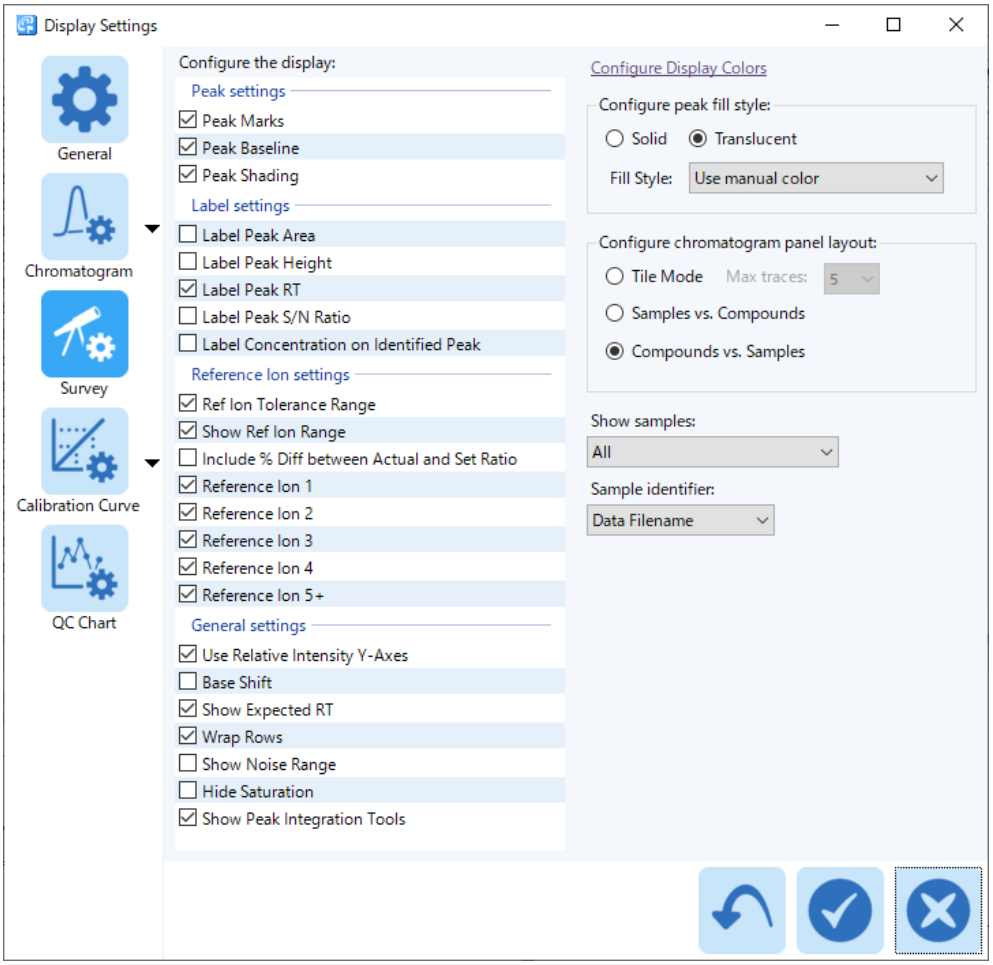
The settings are described below. Items that are already described for Chromatogram settings are omitted:

Label settings	
Show Spectrum Labels	Display labels against spectrum peaks.
Reduce Spectrum Labels Density	Reduce the number of labels when there are many peaks in a particular area.
General settings	
Mirror Spectrum	Plot comparison spectrum mirrored against the target spectrum.
Show Scan Number	Show the scan number at the top left of the spectrum.
Hide Saturation	Do not change saturated peak colour to red.
Spectrum Glow	Highlight spectrum peak that is recognised as being pointed at by the mouse cursor.
Other settings	
Relative Label Threshold	Peaks whose relative intensities, with respect to the tallest peak in the spectrum, exceed this threshold will be labelled.

Nominal Mass Precision (0-2 digits)	Configure the number of decimal places to be used for the peak labels. The number of decimal places can be 0, 1 or 2.
Relative Intensity Threshold	Peaks whose relative intensities, with respect to the tallest peak in the spectrum, are below this threshold will not be shown.
Absolute Intensity Threshold	Peaks whose intensities are less than this threshold will not be shown.
Fix m/z Range	Turning this option ON will set the m/z axis range for the spectrum to what is specified in the two edit boxes. Enter the start m/z and end m/z for the axis range.

3.19.4 Survey

Configure settings for the survey view.

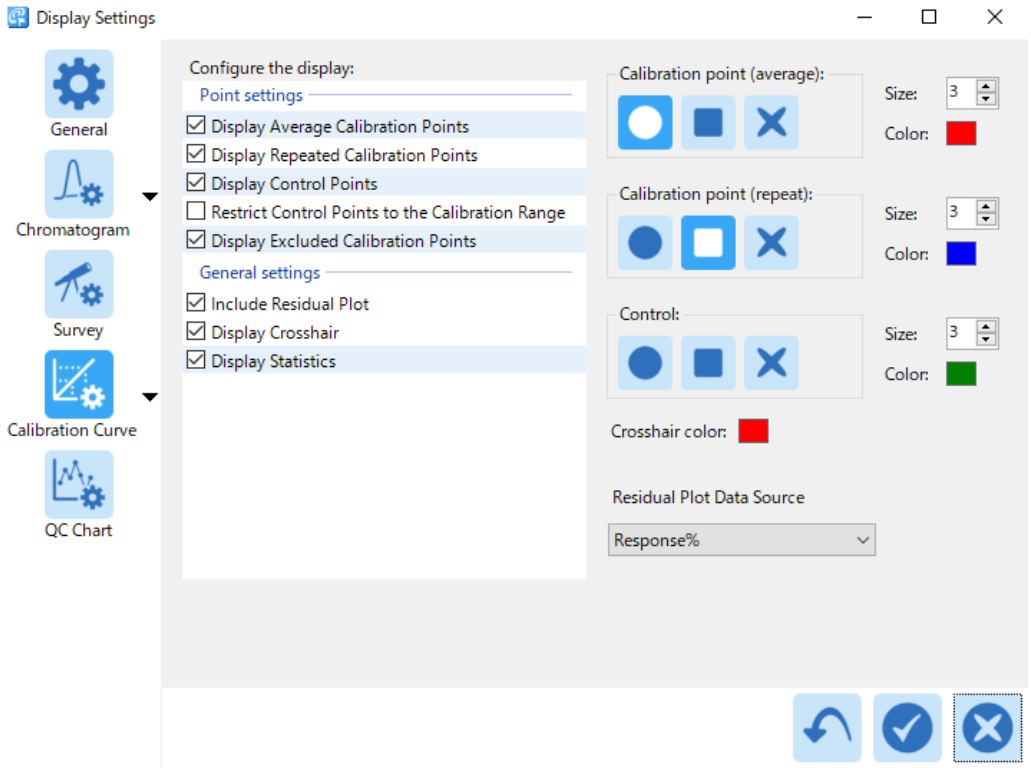


Explanation is omitted for settings that are common for chromatogram settings.

Wrap Rows	Specify either to display chromatograms in multiple rows dividing them at the right end of the screen or display them in a single row with a horizontal scroll bar in the Survey pane.
Configure chromatogram panel layout	Specify the item to be displayed on the vertical and horizontal directions in the Survey pane. • Tile Mode：The chromatogram is shown in the Tile Mode. For details, see 3.16.1. Tile Mode. • Sample-compound: Samples are displayed in the vertical direction and compounds in the horizontal direction. • Compound-sample: Compounds are displayed in the vertical direction and samples in the horizontal direction.
Show samples	Specify how the samples to be displayed in the Survey pane are narrowed down. • All: All samples are displayed. • Filtered and Flagged: Samples extracted by a filter and flagged samples are displayed. • Filtered only: Only samples extracted by a filter are displayed.
Sample identifier	Select the characters to be displayed on the title of the Survey pane. Specify the data file name, sample name, or sample ID.

3.19.5 Calibration Curve

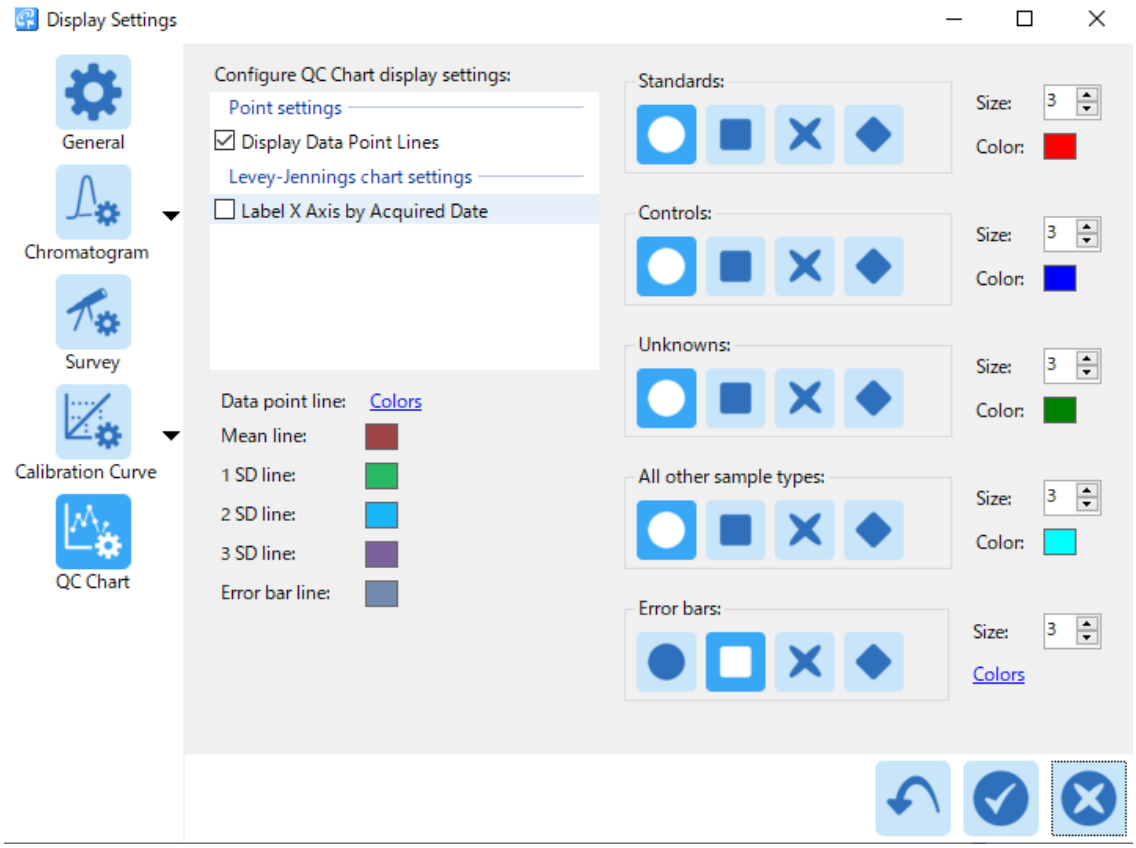
Configure settings for the calibration curve view.



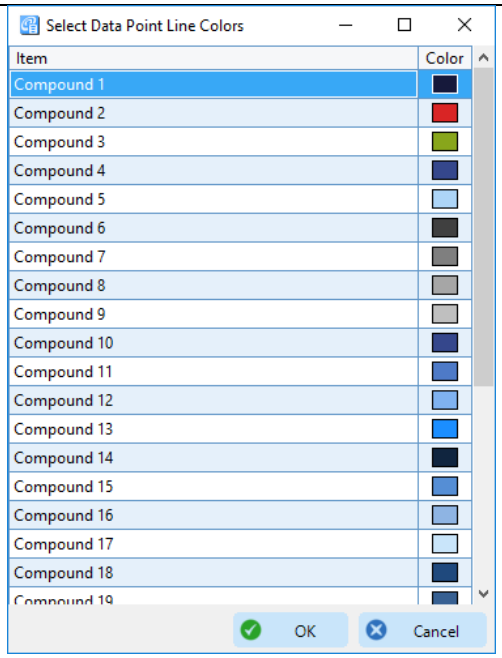
Display Average Calibration Points	Show the average point of the calibration points of the same level.
Display Repeated Calibration Points	Show all calibration points of the same level.
Display Control Points	Show the points from the control sample on the calibration curve.
Restrict Control Points to the Calibration Range	Only show control points that fall within the calibration range. Check the Display Control Points check box above to make full use of this functionality.
Display Excluded Calibration Points	Show excluded calibration points in gray.
Include Residual Plot	Show a residual plot below the calibration curve.
Display Crosshair	Show the auxiliary line for the currently selected sample on the calibration curve.
Display Statistics	Show the average RF, SD RF, and %RSD on the calibration curve.
Calibration point (average)	Select a marker type, size and color. To set the color, click on the colored rectangle to show a palette to select a color from.
Calibration point (repeat)	
Control	
Crosshair color	Select the color of the crosshair. Click on the colored rectangle to show a palette to select a color from.

3.19.6 QC Chart

Configure settings for the QC Chart view.



Display Data Point Lines	Show neighboring data points connected with a line.
Label X Axis by Acquired Date	Display the x-axis by the acquisition date of each data item.
Data point line	Click on Colors to show the color selector for each compound:

	 Click on the colored rectangles to show a palette to select a color from.
Mean line	Select a color for the mean line. Click on the colored rectangles to show a palette to select a color from.
1 SD line	Select a color for 1 standard deviation (SD) line. Click on the colored rectangles to show a palette to select a color from.
2 SD line	Select a color for 2 standard deviations (SD) line. Click on the colored rectangles to show a palette to select a color from.
3 SD line	Select a color for 3 standard deviations (SD) line. Click on the colored rectangles to show a palette to select a color from.
Error bar line	Select a color for the error bar line. Click on the colored rectangles to show a palette to select a color from.
Standards Controls Unknowns All other sample types	Select a marker type, size and color. Click on the colored rectangle to show a palette to select a color from.
Error bars	Select a marker type, size and color. Color can be selected for each compound in the same way as the Data Point Line described above.

3.19.7 Saving and Loading Layouts

It is possible to save table styles as a layout template. It is also possible to write the layout to file and to import from an exported layout so that the same layout can be shared across all systems.

- Save Layout (internal)

  Save the current layout. Click on the Save button and enter a name for the layout.

- Load Layout (internal)

  Select a saved layout and load. Click on the Open button and select a layout from a list of saved layouts.

- Delete Layout (internal)

  Select a saved layout and delete.

- Export Layout (to file)

  Output saved layout to file. Click on the Export button and select a layout to export, then enter a file name. The layout can be written to a folder of choice as an Insight Browser Layout (*.ibl) file.

- Import Layout (from file)

  Load layout from a Layout file. Click on the Import button and select an Insight Browser Layout (*.ibl) file. In order to apply the imported layout, it is necessary to then Load the imported layout.

3.20 [View] Audit Trail

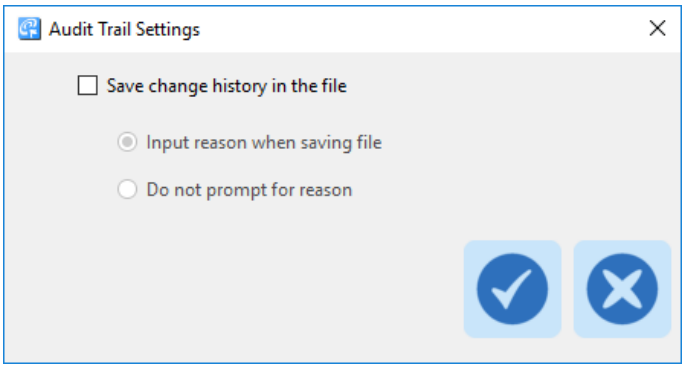
Insight can record changes made to projects.

3.20.1 Audit Trail Settings

Audit trail can be set in both Data mode and Processing mode for the current files.

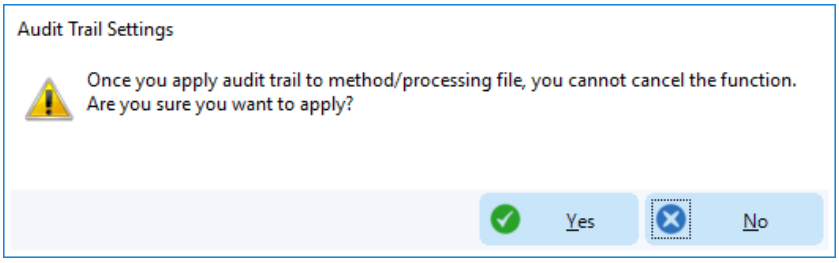
In Processing mode, the Audit Trail Settings apply to processing files. If the current data set was opened without using a processing file, then the Audit Trail Settings below will apply when the data set is first saved as a processing file.

Click on the [Audit Trail] menu button to show the settings window.



Check the [Save change history in the file] check box to enable audit trail.

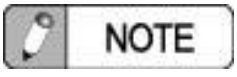
The following warning message is displayed.



Click on [Yes] to enable audit trail.

Once audit trail is enabled, select whether to be prompted to input reasons for any changes made.

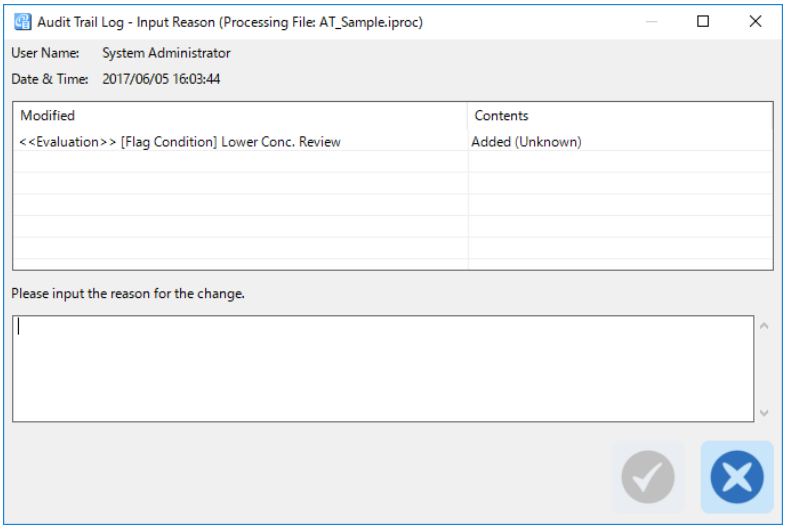
Click on the  button to confirm the settings.



Once the [Save change history in the file] check box is ticked, it cannot be unticked. However, whether to input a reason when saving can be changed at any time.

3.20.2 Entering the Reason for Change

If [Input reason when saving file] was selected in the Audit Trail Settings window, then Insight will prompt for a reason when saving.



The reason given here can be seen in the [Reason for the Change] field in the Audit Trail Log.

In Data mode, Insight will not prompt for reasons if only flag settings or compound selection have changed.

3.20.3 Viewing the Audit Trail Log in Data Mode

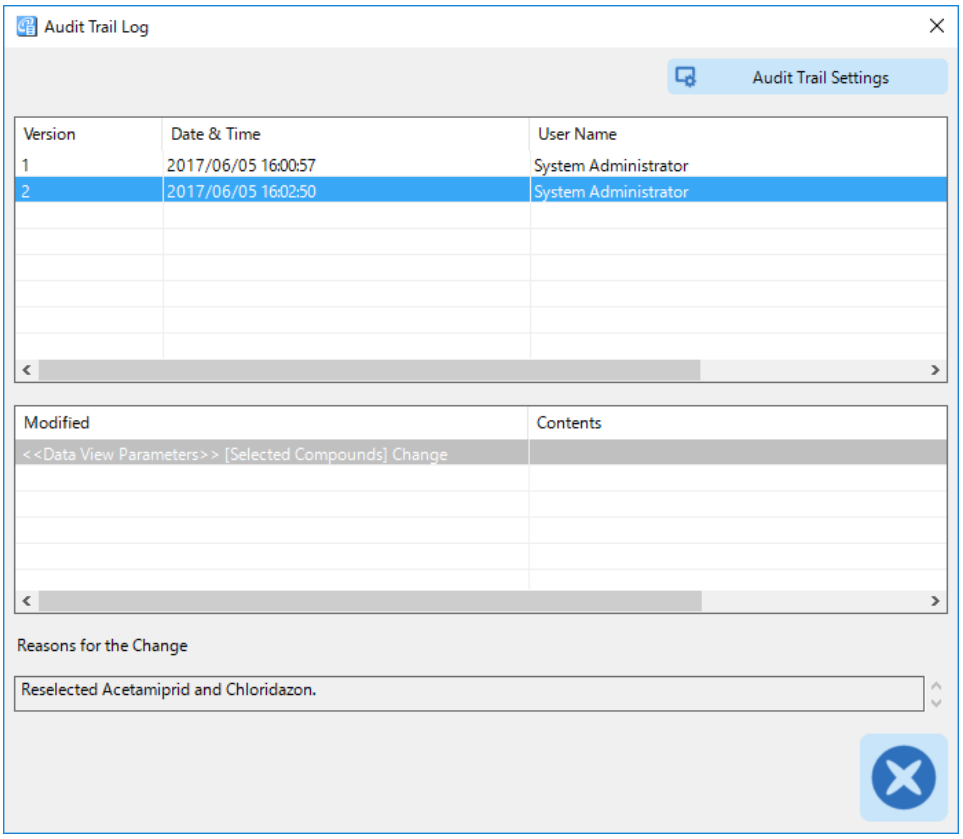
In Data Mode, the audit trail log can be viewed in LabSolutions LCMS or GCMSsolution.

Open the relevant file in LabSolutions LCMS or GCMSsolution Postrun and select [Show Audit Trail Log…] from the [File] menu.

Refer to the LabSolutions LCMS and GCMSsolution instruction manuals for details.

3.20.4 Viewing the Audit Trail Login Processing Mode

Once audit trail is enabled, clicking on the [Audit Trail] menu button will display the audit trail log.



Click on the [Audit Trail Settings] button to display the Audit Trail Settings window again.

Whether to input reason for changes made to the project can be changed, but whether to perform audit trail at all cannot be changed.

3.21 [Edit] Edit Method

Click on the Edit Method button in the Edit menu band to show the Edit Method window.

The behaviour differs depending on whether GCMS or LabSolutions data is being used.

NOTE

Insight only supports Internal Standard, External Standard or Standard Addition for the Quantitative Method settings, even though other selections are possible .

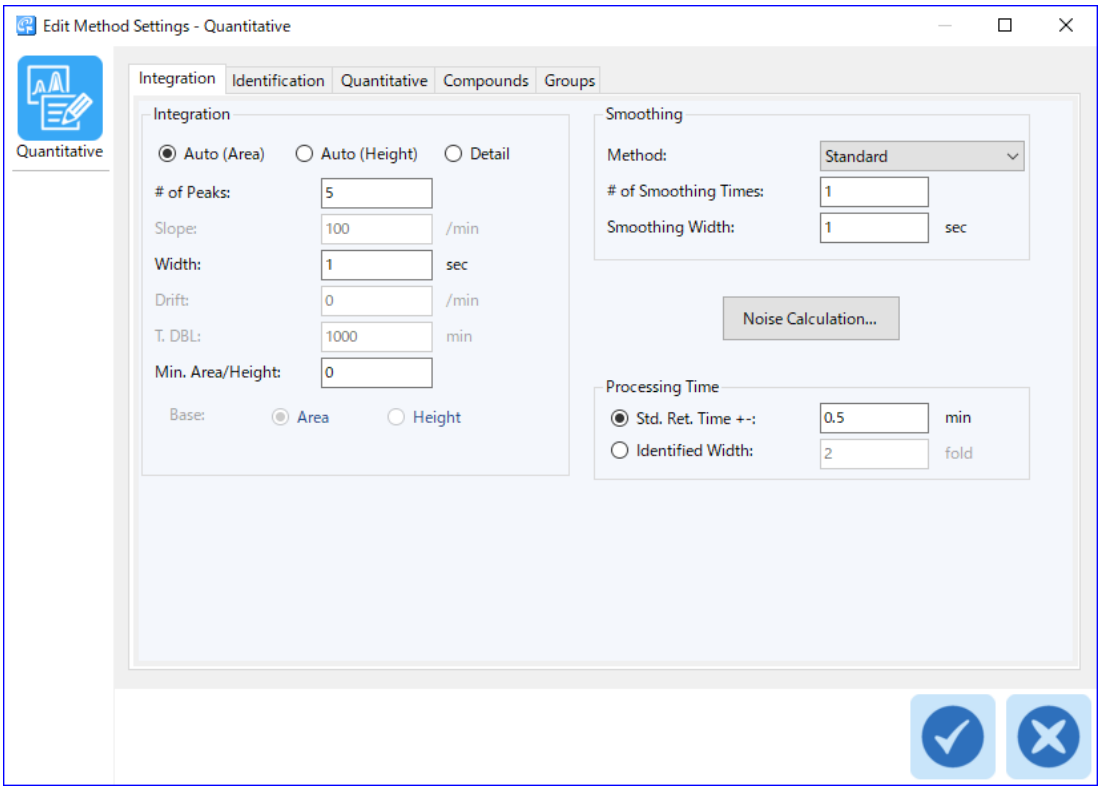
Hint

If the method editor is "Read Only" but it is required that the method is edited, please check the following:

- User rights
  - Make sure you have the right to edit methods
- Windows functionality
  - Make sure the method file is not set to Read Only using the Windows File Explorer
  - Make sure the method file is not saved in a region on the PC with access restriction
  - Make sure you are logged in to Windows as a user with editing rights
  - Make sure there are no other applications using the method file
- Insight functionality
  - Remove any samples in the sample list that says "Not available"
  - You cannot edit GCMS semi-quantitation methods
  - Processing file may have failed to open correctly. Please restart Insight and open the processing file in question again

3.21.1 GCMS parameters

In Insight GCMS, the Quantitative dialog similar to GCMSsolution appears.

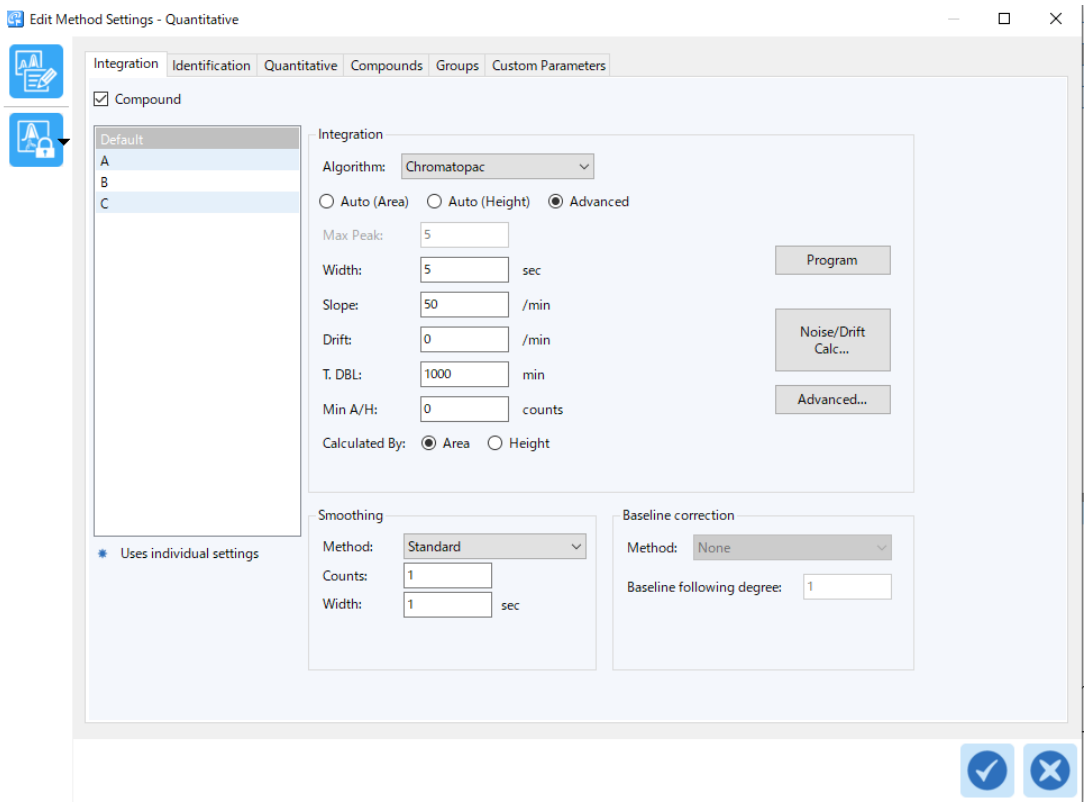


See GCMSsolution instruction manual or online manual on how to set each parameter.

After Quantitative Parameters are modified, Insight will automatically perform quantitative calculations on all samples and compounds. However, Insight will not perform peak integration operations even if peak integration and identification parameters are changed. In order to apply these changes to the results, choose one of the Integrate options: Integrate Compound, Integrate Sample or Integrate Batch.

3.21.2 LCMS parameters

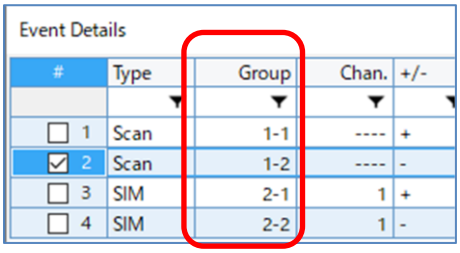
In Insight LCMS, the Quantitative dialog similar to LabSolutions LCMS appears.



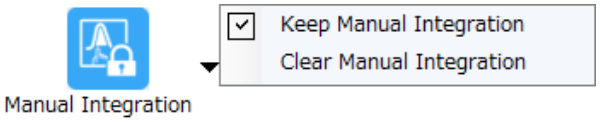
See LabSolutions LCMS instruction manual or online manual on how to set each parameter.

NOTE

For LCMS-2020 methods, the Group column in the Event Details dialog opened from the Compound tab in the Method Editor shows the segment and the event numbers combined.

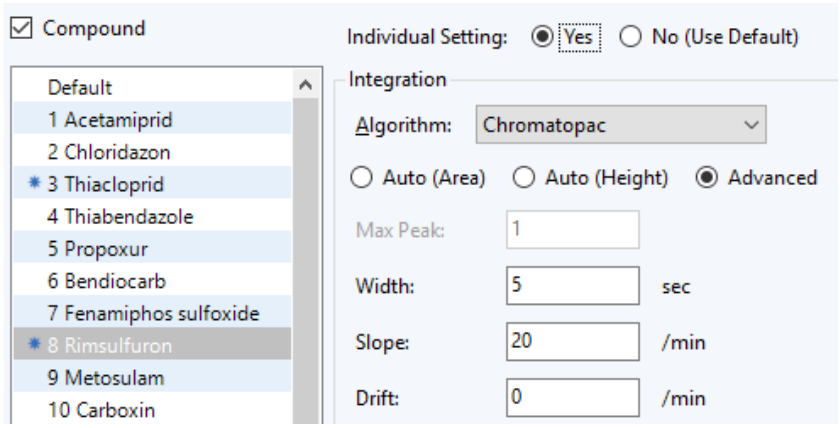


In Insight LCMS, integration and quantitative calculation are automatically performed for all samples and compounds when the method setting window is closed. To keep the manual peak integration results, select [Keep Manual Integration] from the drop down list shown below. To delete all manual peak integration results and overwrite them with the automatic peak integration results, select [Clear Manual Integration].



	Keep Manual Integration	Manual peak integration results will be kept without any modification.
	Clear Manual Integration	All manual peak integration results will be overwritten with automatic peak integration results.

Hint

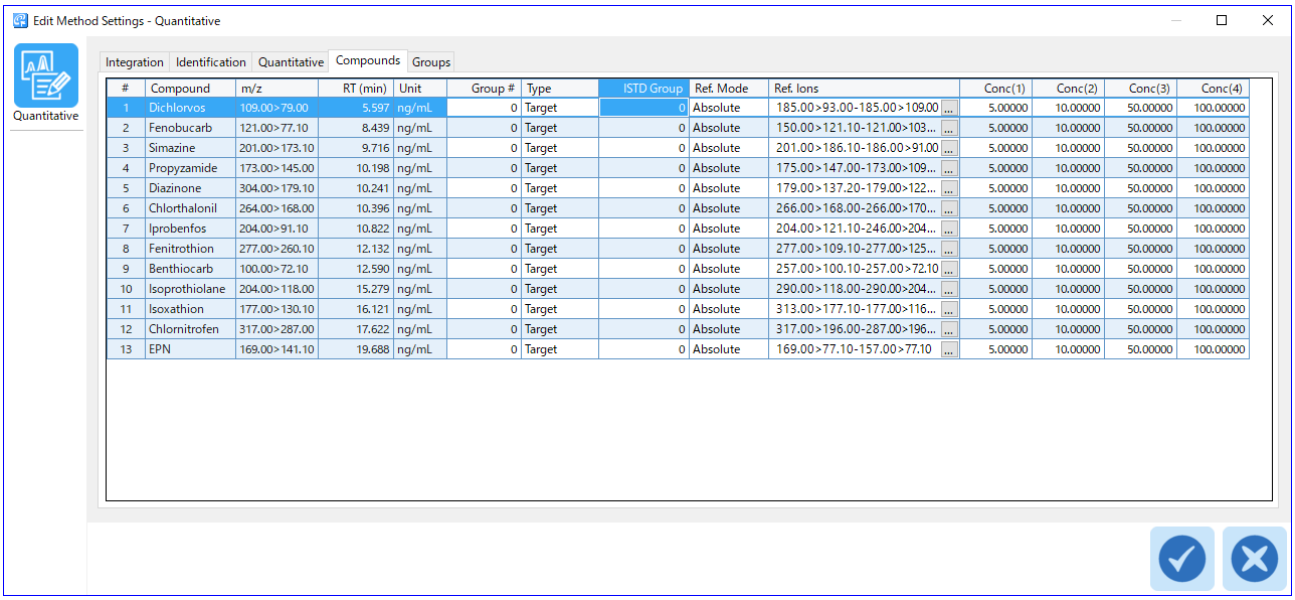


When a compound is set to use individual parameter settings, rather than the default settings, a marker (*) is shown in front of the compound.

In order to make all compounds use the default parameters, select “Default” then click on the underlined “Use default for all compounds”.

3.21.3 Compound Table

Some of the parameters in the compound table can be edited in the [Compounds] tab.

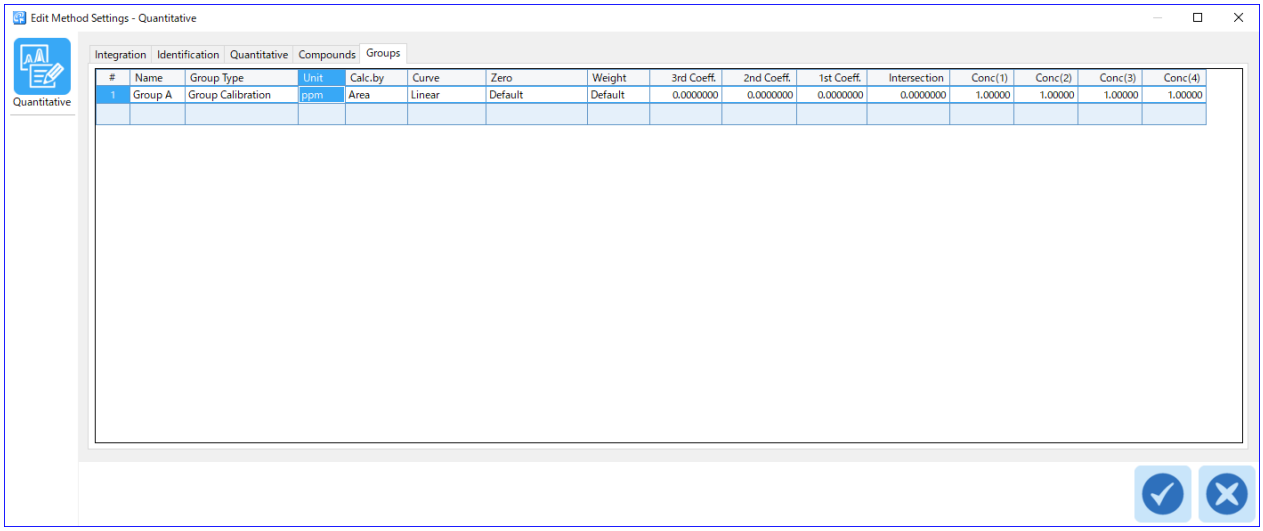


#	Compound	m/z	RT (min)	Unit	Group #	Type	ISTD Group	Ref. Mode	Ref. Ions	Conc(1)	Conc(2)	Conc(3)	Conc(4)
1	Dichlorvos	109.00>79.00	5.597	ng/mL	0	Target	0	Absolute	185.00>93.00-185.00>109.00	5.00000	10.00000	50.00000	100.00000
2	Fenobucarb	121.00>77.10	8.439	ng/mL	0	Target	0	Absolute	150.00>121.10-121.00>103...	5.00000	10.00000	50.00000	100.00000
3	Simazine	201.00>173.10	9.716	ng/mL	0	Target	0	Absolute	201.00>186.10-186.00>91.00	5.00000	10.00000	50.00000	100.00000
4	Propyzamide	173.00>145.00	10.198	ng/mL	0	Target	0	Absolute	175.00>147.00-173.00>109...	5.00000	10.00000	50.00000	100.00000
5	Diazinone	304.00>179.10	10.241	ng/mL	0	Target	0	Absolute	179.00>137.20-179.00>122...	5.00000	10.00000	50.00000	100.00000
6	Chlorthalonil	264.00>168.00	10.396	ng/mL	0	Target	0	Absolute	266.00>168.00-266.00>170...	5.00000	10.00000	50.00000	100.00000
7	Iprobenfos	204.00>91.10	10.822	ng/mL	0	Target	0	Absolute	204.00>121.10-246.00>204...	5.00000	10.00000	50.00000	100.00000
8	Fenitrothion	277.00>260.10	12.132	ng/mL	0	Target	0	Absolute	277.00>109.10-277.00>125...	5.00000	10.00000	50.00000	100.00000
9	Benthiocarb	100.00>72.10	12.590	ng/mL	0	Target	0	Absolute	257.00>100.10-257.00>72.10	5.00000	10.00000	50.00000	100.00000
10	Isoprothiolane	204.00>118.00	15.279	ng/mL	0	Target	0	Absolute	290.00>118.00-290.00>204...	5.00000	10.00000	50.00000	100.00000
11	Isoxathion	177.00>130.10	16.121	ng/mL	0	Target	0	Absolute	313.00>177.10-177.00>116...	5.00000	10.00000	50.00000	100.00000
12	Chlornitrofen	317.00>287.00	17.622	ng/mL	0	Target	0	Absolute	317.00>196.00-287.00>196...	5.00000	10.00000	50.00000	100.00000
13	EPN	169.00>141.10	19.688	ng/mL	0	Target	0	Absolute	169.00>77.10-157.00>77.10	5.00000	10.00000	50.00000	100.00000

See GCMSsolution or LabSolutions LCMS instruction manual or online manual on the detail of each parameter.

3.21.4 Compound Group

The grouping parameters can be edited in the [Groups] tab.



#	Name	Group Type	Unit	Calc.by	Curve	Zero	Weight	3rd Coeff.	2nd Coeff.	1st Coeff.	Intersection	Conc(1)	Conc(2)	Conc(3)	Conc(4)
1	Group A	Group Calibration	ppm	Area	Linear	Default	Default	0.0000000	0.0000000	0.0000000	0.0000000	1.00000	1.00000	1.00000	1.00000

See GCMSsolution or LabSolutions LCMS instruction manual or online manual on the detail of each parameter.

The quantitative results for the compound group added here are added to the end of Compound List or Compound Result.

Compound List

#	Flags	Flag ID	Name	Status	Type
1			Dichlorvos	Pending	Target
2			Fenobucarb	Pending	Target
3			Simazine	Pending	Target
4			Propyzamide	Pending	Target
5			Diazinone	Pending	Target
6			Chlorthalonil	Pending	Target
7			Iprobenfos	Pending	Target
8			Fenitrothion	Pending	Target
9			Benthiocarb	Pending	Target
10			Isoprothiolane	Pending	Target
11			Isoxathion	Pending	Target
12			Chlornitrofen	Pending	Target
13			EPN	Pending	Target
14			Group A		Target

When the compound group is selected on the table, the quantitation result and the calibration curve (only for Group Calibration) and the chromatogram is blank. Also, the quantitation result is limited to values that can be calculated as the result of the group. (Concentration, Area, etc.)

The quantitation result of the compound group can be exported as well as the quantitation result of the compounds.

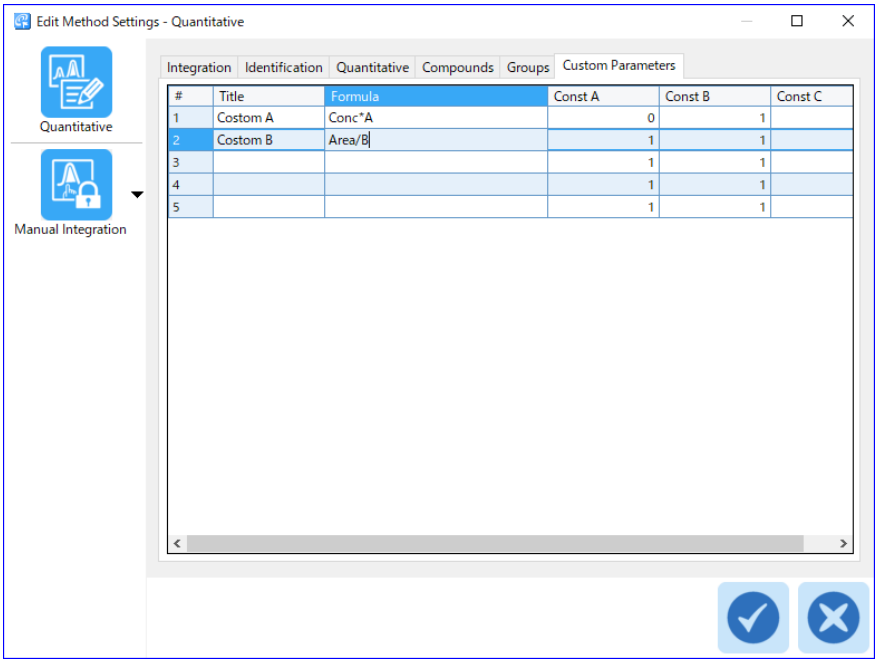
NOTE

Although Group Quantitation using Internal Standards is supported for GCMS data in Insight, GCMSsolution does not support this method of quantitation.

Please DO NOT open data that has been quantitated using Group Quantitation with Internal Standards in Data Mode in GCMSsolution.

3.21.5 Custom Parameters (LCMS Only)

The custom parameter can be edited in the [Custom Parameters] tab. This is available for LCMS only.



The results calculated according to the calculation formula entered here can be shown in the quantitation result (Compound and Sample) and the Summary view. The calculation formula is described by a combination of a character string indicating a preset constant and several operators. When an undefined character string is used, or when an operator that is not available is used, if an expression does not hold as an expression, an appropriate value will not be calculated.

The calculation formula is described in the following format.

• Quantitative Result

Retention time	RetTime
Area	Area
Height	Height
Concentration	Conc
Standard Concentration	StdConc

Compound Table Retention Time	RetTimeCompTable
ISTD Compound's Retention Time	RetTimeISTD
ISTD Compound's Compound Table Retention Time	RetTimeCompTableISTD

- Constant

Constant A	A
Constant B	B
Constant C	C

- Operator

Addition	+
Subtraction	-
Multiplication	*
Division	/ （It does not calculate when the denominator is 0）
Power	e （Only integers can be specified for the exponent part）

- Parenthesis

  Parentheses () allows you to define the order of calculation.

- Special function

Square root	sqrt()

3.21.6 Spectrum (LCMS Only)

Spectrum processing parameters can be configured in the Spectrum tab. This feature is only available for LCMS.

Spectrum processing parameters are used for calculating spectra under the processed chromatogram peaks. Please refer to the LabSolutions user manual for details on the meaning of the parameters.

3.22 [Edit] Integrate Batch

Select Integrate Batch from the Edit menu band to perform automated peak integration and quantitative calculations on all compounds in all samples.

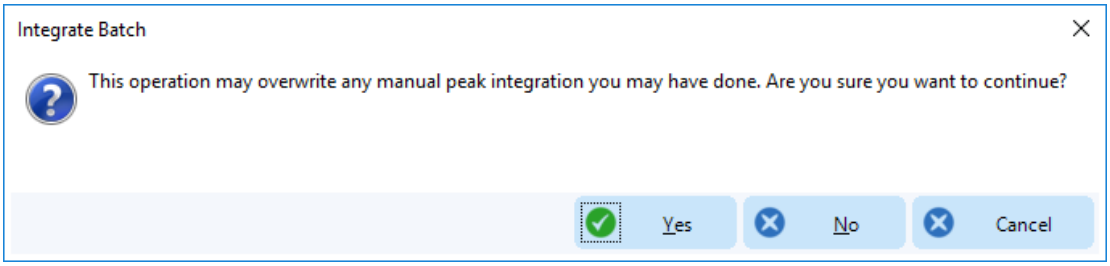
Flags and filters will be reassigned and reapplied as appropriate.

This operation cannot be carried out by a user who does not have edit rights.

This operation cannot be carried out if any of the data files are read-only.

NOTE

When [Integrate Batch] is applied for GCMS data, the following message will appear.



When [Yes] is selected, the manual peak integration result will be deleted and automatic peak integration will be performed. When [No] or [Cancel] is selected, it will not be deleted aborting the automatic peak integration.

3.23 [Edit] Integrate Sample

When [Integrate Sample] in the [Edit] menu band is selected, the automatic peak integration and quantitative calculation are performed for all compounds of the currently selected sample.

When the sample type of the selected sample is Standard, the calibration curves for all compounds are recalculated and all sample results are updated. The flagging and filtering will be applied again.

Users without editing privileges cannot perform this operation. Also, this operation cannot be performed when one of the data files is read-only.

When [Integrate Sample] is applied to GCMS data, the message confirming deleting the manual peak integration result will appear like [Integrate Batch].

3.24 [Edit] Integrate Compound

When [Integrate Compound] in the [Edit] menu band is selected, the automatic peak integration and quantitative calculation are performed for the selected compounds of the currently selected sample.

When the sample type of the selected sample is Standard, the calibration curves for all compounds are recalculated and all sample results are updated. The flagging and filtering will be applied again.

Users without editing privileges cannot perform this operation. Also, this operation cannot be performed when one of the data files is read-only.

When [Integrate Compound] is applied to GCMS data, the message confirming deleting the manual peak integration result will appear like [Integrate Batch]

3.25 [Edit] Integrate Result

When [Integrate Result] in the [Edit] menu band is selected, the automatic peak integration and quantitative calculation are performed for the selected sample of the currently selected compound.

When the sample type of the selected sample is Standard, the calibration curves for all compounds are recalculated and all sample results are updated. The flagging and filtering will be applied again.

Users without editing privileges cannot perform this operation. Also, this operation cannot be performed when one of the data files is read-only.

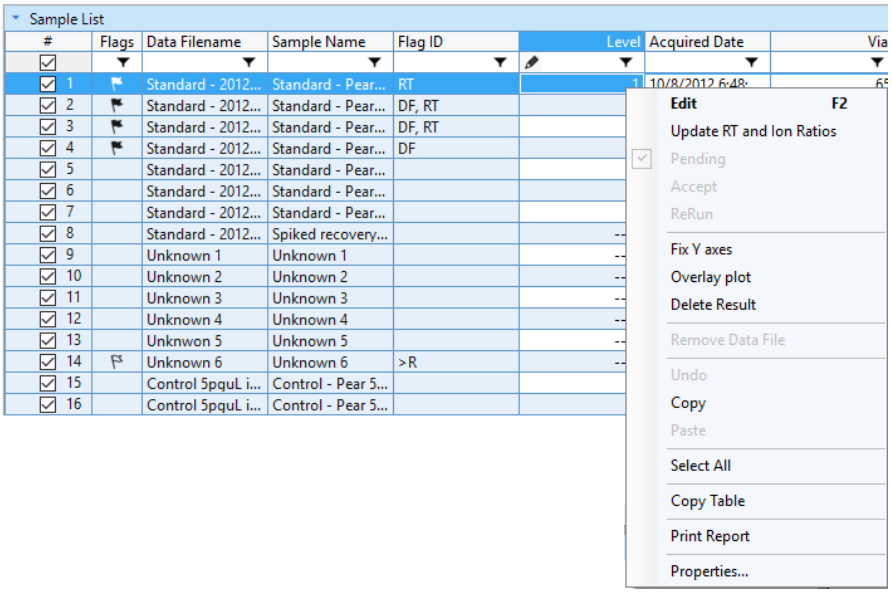
When [Integrate Result] is applied to GCMS data, the message confirming deleting the manual peak integration result will appear like [Integrate Batch].

3.26 [Edit] Edit Tables

Edit Tables mode can be invoked by clicking on the Edit Tables button in the Edit menu band. When the Edit Table button is turned ON (turned dark blue) the Edit Tables mode is activated. Clicking on the Edit Tables button again turns it off (turns light blue)

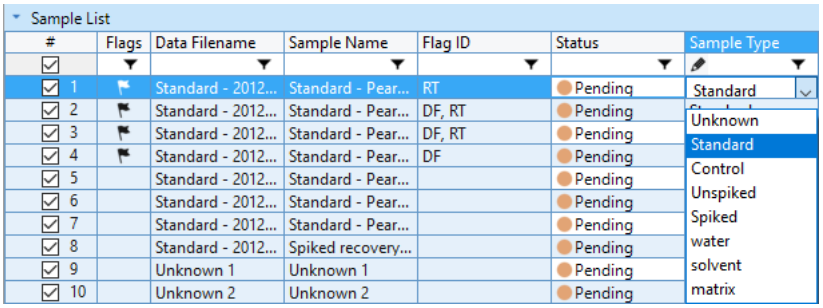
Sample levels and/or sample types in the Sample List or Sample Results can be edited in Edit Tables mode.

Right click on the item that needs to be changed and display the Edit context menu.



Alternatively, double click in the field to be edited.

A drop down list is shown using either method.



Select the sample type to change to.

The sample level, retention time and Ref1-5 Set Ratio can be set in a similar way.

The pencil mark shown below is shown for items that can be edited.

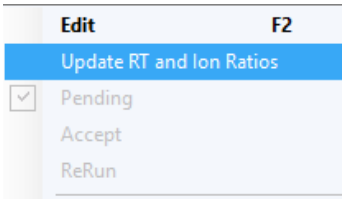
3.26.1 Update RT and Ion Ratios

In the Edit Tables mode, the set values for the retention time and reference ion ratio can be changed based on the measured values.

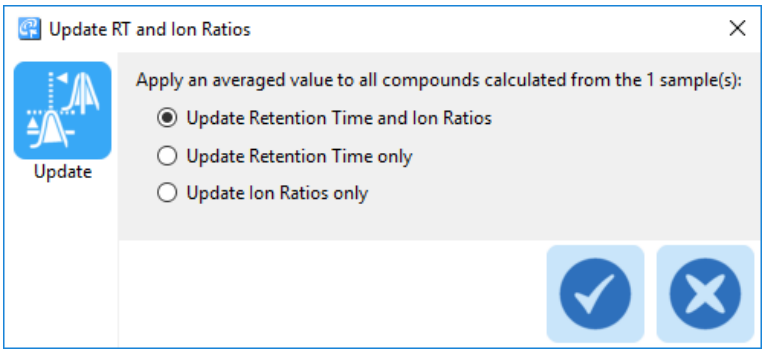
Using the [Update RT and Ion Ratios] menu, the measured value of a single sample can be simply copied or the average of the measured value of multiple samples can be used as the set value.

1. To use the measured value of a single sample as the set value

Turn ON the Edit Tables mode, select a single sample in [Sample List], [Sample Results], or [Summary], right-click the mouse, and then click [Update RT and Ion Ratios]. 1.6.2



The [Update RT and Ion Ratios] window is displayed.



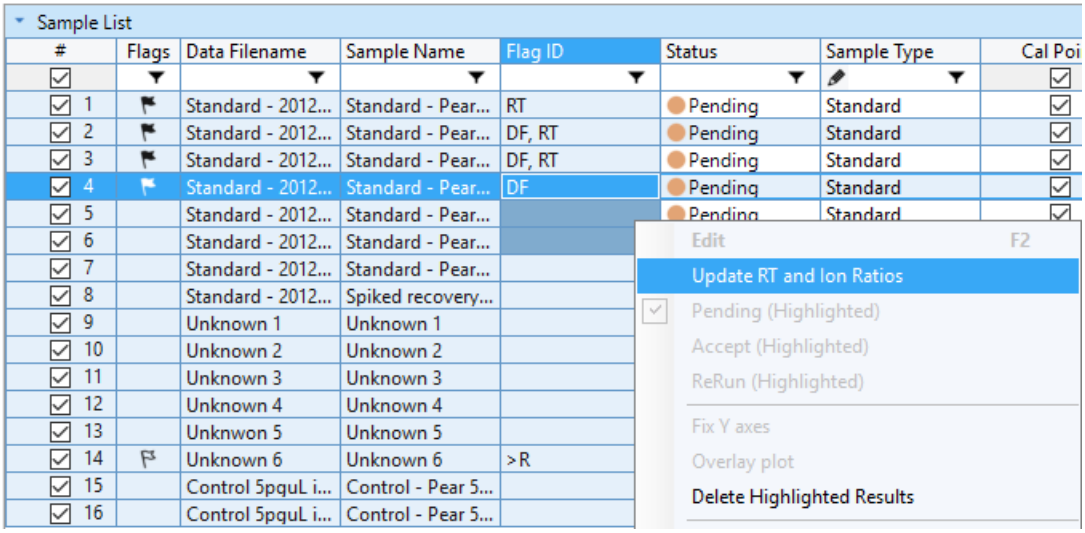
If the user selects a single sample and selects the menu from the right-click menu, [Apply an average value to all compounds calculated from the 1 sample(s);] is displayed as shown above. In this case, [Found Ret. Time] and [Ref 1-5 Actual Ratio] of the currently selected sample are simply copied to [Ret. Time] and [Ref 1-5 Set Ratio].

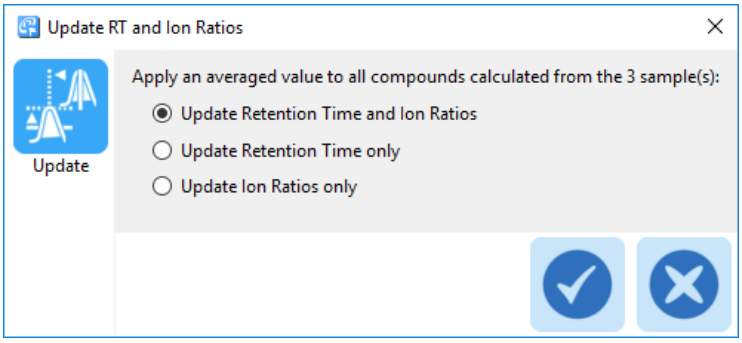
Update Retention Time and Ion Ratios*	Change [Ret. Time] and [Ref 1-5 Set Ratio].
Update Retention Time only*	Change [Ret. time].
Update Ion Ratios only	Change [Ref 1-5 Set Ratio].

* For GCMS only, the event number is adjusted automatically when the retention time is changed.

2. To use the average of the measured value of multiple samples as the set value

Highlight multiple samples and select [Update RT and Ion Ratios] from the right click menu.

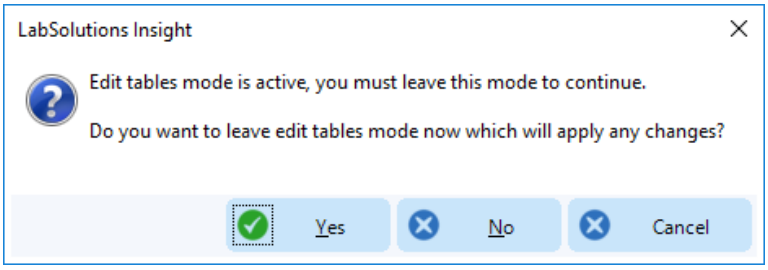




If the user selects multiple samples and selects the menu from the right-click menu, [Apply an averaged value to all compounds calculated from the ## sample(s):] is displayed as shown above. In this case, the average value of [Found Ret. Time] and [Ref 1-5 Actual Ratio] of the selected samples is set for [Ret. Time] and [Ref 1-5 Set Ratio].

On exiting the Edit Tables mode, the calibration curve(s) will be updated as necessary and quantitation results updated.

Closing current files and exiting the application cannot be done whilst in the Edit Tables mode.

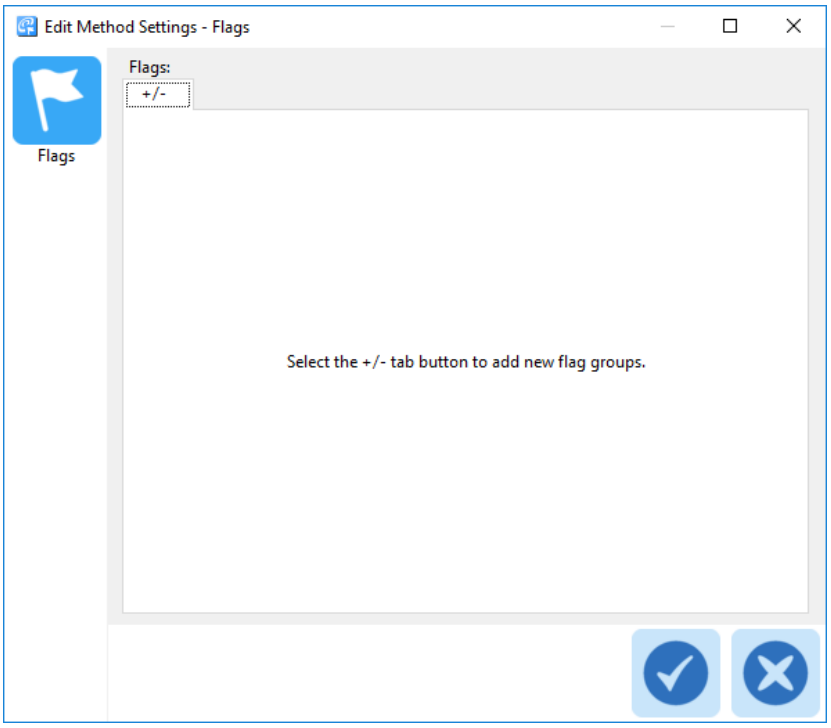


Select Yes to exit Edit Tables mode to perform other operation.

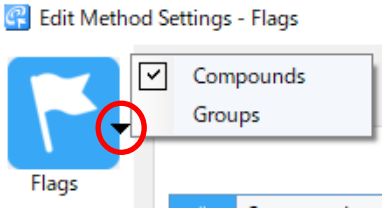
Select No or Cancel to stay in Edit Tables mode and continue editing the tables.

3.27 [Edit] Edit Flags

Select Edit Flags from the Edit menu band to launch the Edit Method Settings – Flags dialog. Flag criteria can be set here.

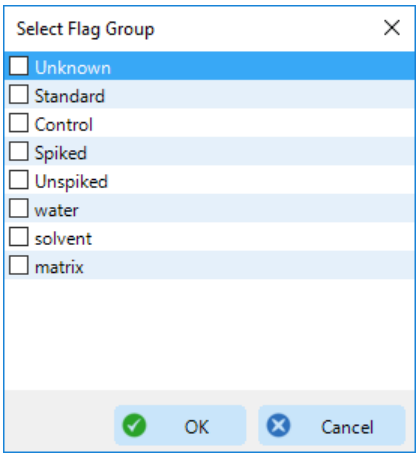


When Group Quantitation is being used, a small triangle will be shown next to the Flags button. Clicking on this button will show a drop down list to select between compounds and groups.



3.27.1 Setting flag groups

Click on the +/- tab to add new flag groups. The flags are not applied to ISTD.



The available flag groups are:

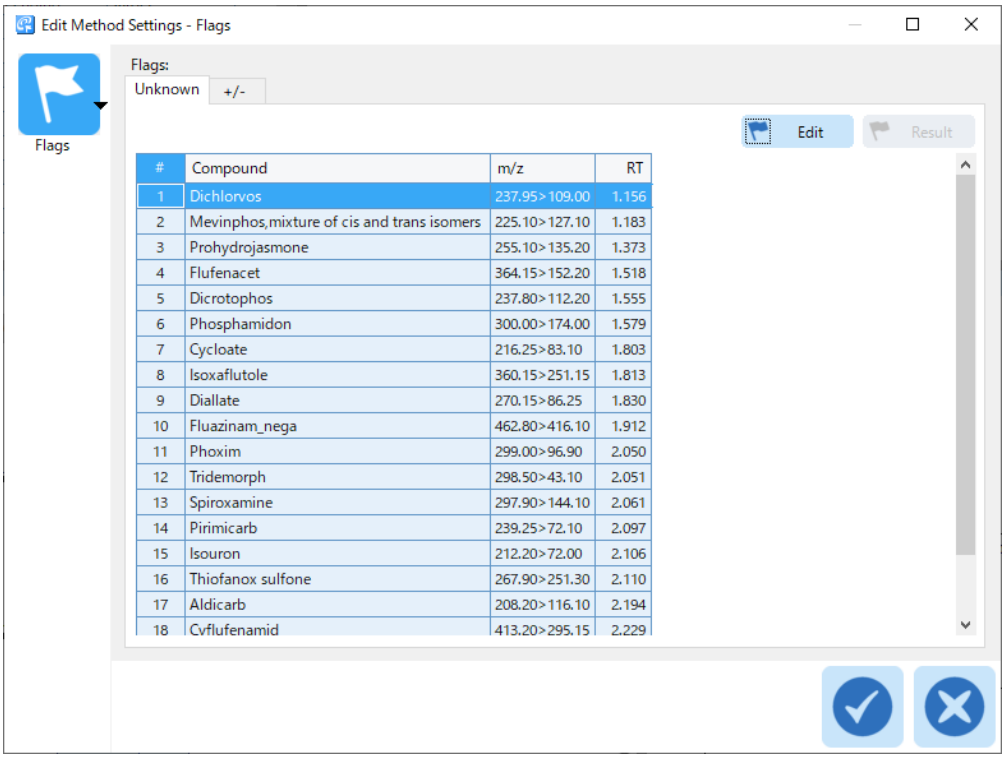
Unknown	Flags set in this group only apply to Unknown sample types.
Standard	Flags set in this group only apply to Standard sample types.
Control	Flags set in this group only apply to Control sample types.
Spiked	Flags set in this group only apply to Spiked sample types.
Unspiked	Flags set in this group only apply to Unspiked sample types.
water	Flags set in this group only apply to blank samples that have been identified as “water”. This blank type is available by default.
solvent	Flags set in this group only apply to blank samples that have been identified as “solvent”. This blank type is available by default.
matrix	Flags set in this group only apply to blank samples that have been identified as “matrix”. This blank type is available by default.

Check the appropriate flag group to show the flag criteria table for the flag group, or uncheck the boxes to hide the flag groups. Right click context menu is available to set or unset flag groups all at once:

Select All	Highlight all items.

When a new sample type tab is added it will contain a flags table containing the read only compound identification columns and an Edit flags button. The compound identification columns are:

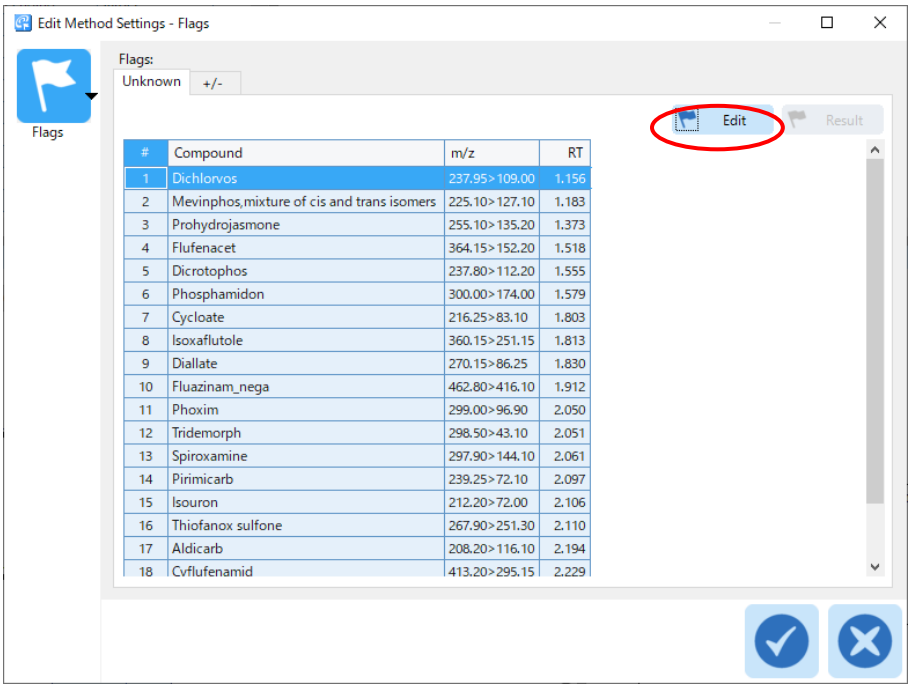
#	Row number.
Compound	Compound name.
m/z	m/z of the compound, or for MRM experiments, the MRM transition for the compound.
RT	Retention time of the compound.



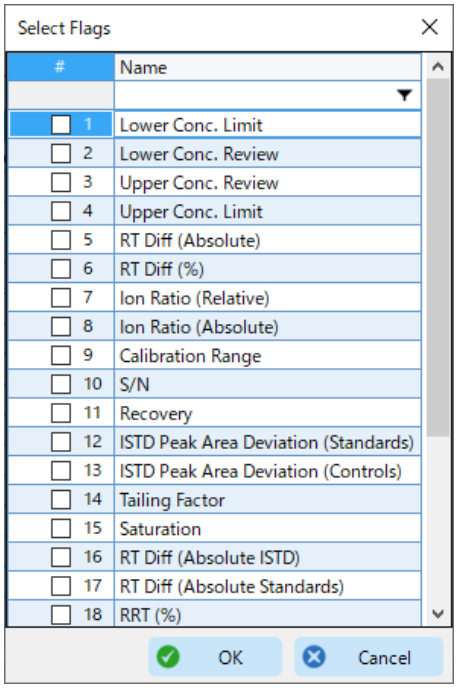
#	Compound	m/z	RT
1	Dichlorvos	237.95>109.00	1.156
2	Mevinphos,mixture of cis and trans isomers	225.10>127.10	1.183
3	Prohydrojasmone	255.10>135.20	1.373
4	Flufenacet	364.15>152.20	1.518
5	Dicrotophos	237.80>112.20	1.555
6	Phosphamidon	300.00>174.00	1.579
7	Cycloate	216.25>83.10	1.803
8	Isoxaflutole	360.15>251.15	1.813
9	Diallate	270.15>86.25	1.830
10	Fluazinam_nega	462.80>416.10	1.912
11	Phoxim	299.00>96.90	2.050
12	Tridemorph	298.50>43.10	2.051
13	Spiroxamine	297.90>144.10	2.061
14	Pirimicarb	239.25>72.10	2.097
15	Isouron	212.20>72.00	2.106
16	Thiofanox sulfone	267.90>251.30	2.110
17	Aldicarb	208.20>116.10	2.194
18	Cyflufenamid	413.20>295.15	2.229

3.27.2 Setting flags

Click on the Edit button to add and remove flag criteria columns.



Check the boxes for the flags required and press OK.

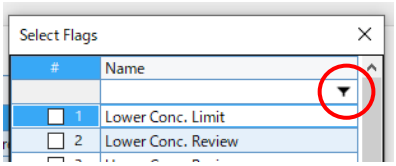


Any deselected flags will be removed from the flag table and any newly selected flags will be added to the flag table. Newly added flags will be displayed with no values set. If a flag is deselected and then reselected then it is displayed with its previously set value. Flags can be selected or unselected all at once using the right click context menu:

Select All	Highlight all items.

Hint

Since there are many flags, it may be a challenge to find the one that is needed.



Use the filter button at the top right to help find the required flag.

Please refer to Section 3.11.1 for details.

The flags that can be selected depend on the flag group. Please see 2.6.3 Flag ID for details.

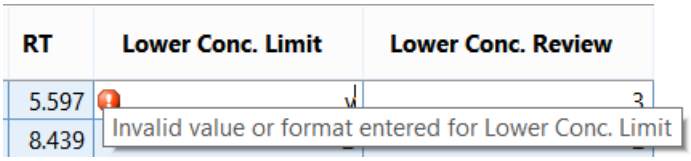
3.27.2.1 Setting flag criteria

Each flag criterion can be typed in directly or set using the right click context menu items:

Clear	Clears the current cell value.
Fill Down	Sets the value of all rows of this flag type below this row to this row's value.
Use Default	Uses the flag's default value for this cell value.
Use Default (All Rows)	Sets the value of all rows of this flag column to the default value.

Default values are shown in different color text to custom values.

If an invalid value is entered in the flag criteria, it is highlighted using a red "!" mark. Hover the mouse pointer over the red "!" mark to get a tooltip that explains the reason for the "!". The problem must be corrected before any other fields can be edited.



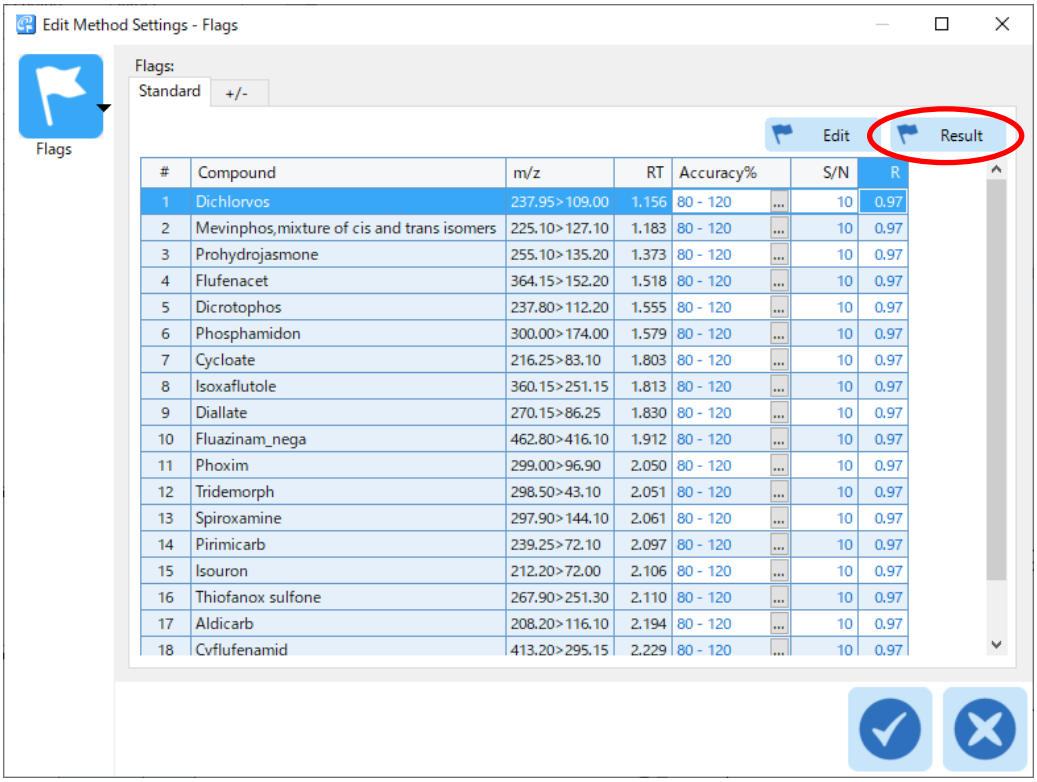
Hint

Highlight multiple rows in the flag criteria to copy and paste.

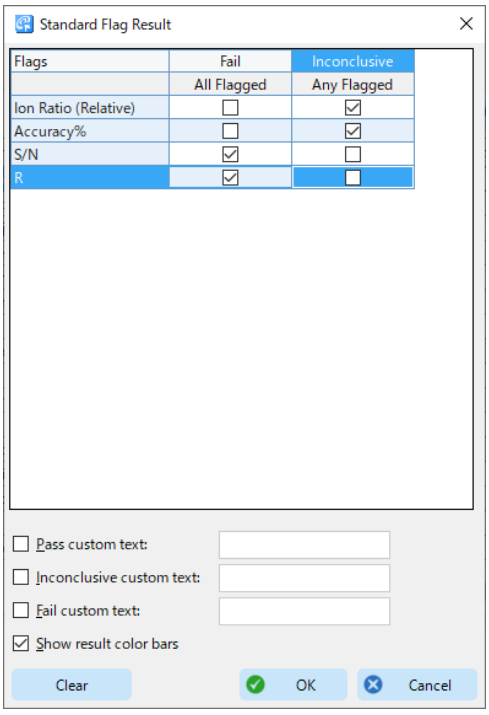
3.27.3 Flag Results

A combination of flags can be used as criteria for obtaining flagged results.

Click on the Result button at the top right of the Flag Editor.



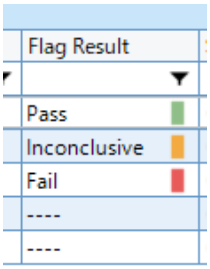
The results can be labelled Pass, Fail or Inconclusive using a combination of the flags.



Flags — List of flags currently in use.

Fail — When flags selected here apply, the result will be labelled “Fail”.
Clicking on “All Flagged” and “Any Flagged” will toggle between the two.

Inconclusive	When flags selected here apply, the result will be labelled “Inconclusive”. Clicking on “All Flagged” and “Any Flagged” will toggle between the two.
Pass custom text	Results that are neither Fail nor Inconclusive are labelled “Pass” by default. Tick this option and enter a custom text to show in place of “Pass”.
Inconclusive custom text	Tick this option and enter a custom text to show in place of “Inconclusive”.
Fail custom text	Tick this option and enter a custom text to show in place of “Fail”.
Show result color bars	Show color bars in the Flag Result column.



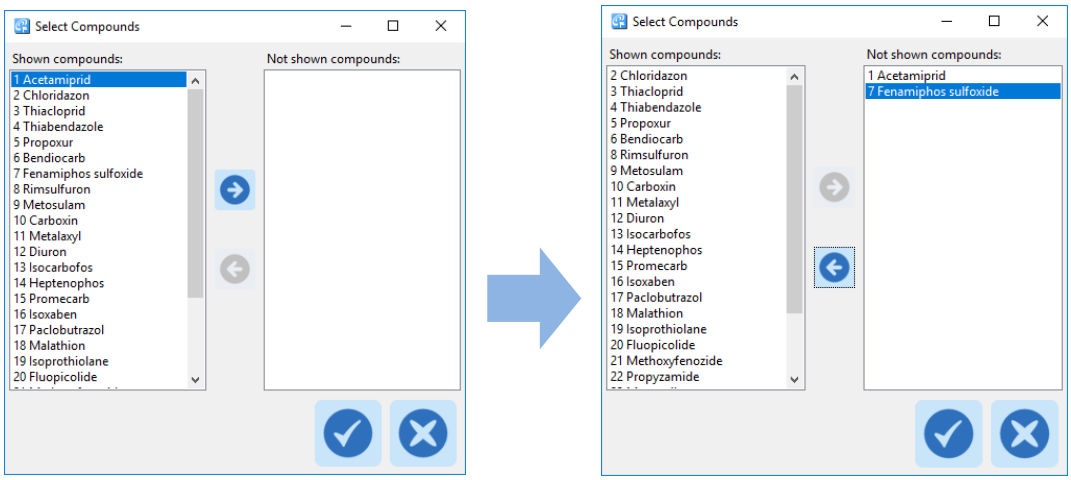
The colors can be configured in Application Configuration.

Please see Section 1.15 for details.

3.28 [Edit] Select Compounds

Selected compounds can be hidden.

Select [Select Compounds] in the [Edit] menu band to display the [Select Compounds] window.



The [Shown compounds] list displays all compounds that are currently visible in the [Compound List], [Compound Results] or [Summary].

Select compounds that should not be visible in the [Compound List], [Compound Results] or [Summary] and click on the  button to move the compounds to the [Not shown compounds] list.

Similarly, select compounds in the [Not shown compounds] list and click on the  button to move the compounds to the [Shown compounds list.

Click on the  button to reflect the changes to the [Compound List], [Compound Results] or [Summary].

3.29 [Review] Review Status

Review Status is set for each compound contained in samples. Setting the Status enables recording of the status of processes for all analysis targets. In Data mode, the status is saved in the DAMLP file. In Processing mode, the status is saved in the processing file.

Status is registered to the table of all Compound, Sample, and Summary Views. The [Status] column can be enabled from the [Table Style] configuration dialog.

[●Pending] is preset for all statuses. The following statuses can be set.

●Pending	Indicates that the respective quantitative result is in the [Pending] status.
●Accept	Indicates that the respective quantitative result is in the [Accept] status.
●Rerun	Indicates that the respective quantitative result is in the [Rerun] status.
●Review	Indicates that both [Pending] and [Accept] are included in the status of the compounds contained in the target sample or samples containing the target compound. Note: It indicates that the [Accept] process is being carried out or that the [Pending] status is intentionally maintained.
●Accepted	Indicates that the [Accept] status of the standard sample has been sent.
●Rerun Complete	Indicates that the [Rerun] status has been sent.
●Sent	Indicates that the [Accept] status has been sent. (Except for standard samples)
●Complete	Indicates that [Sent] or [Accepted] process has been completed for the status of all compounds contained in the target sample or the status of all samples containing the target compound.

NOTE

Review status cannot be set for compounds in internal standard substances (ISTD).

NOTE

The status of standard type samples cannot be set to [Rerun].

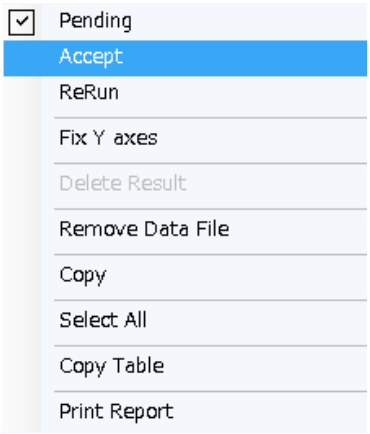
3.29.1 [Review] Accept

Click the [Accept] button in the [Review] menu band to change the status of the currently selected quantitative result to [Accept]

- When the Compound View is displayed, the status of the compound currently selected on [Compound Results] is changed. After the change, the next compound whose status is [Pending] is selected.
- When the Sample View is displayed, the status of the sample currently selected on [Sample Results] is changed. After the change, the next sample whose status is [Pending] is selected.
- When the Summary View is displayed, the status of the sample (compound) currently selected on [Summary] is changed. After the change, the next sample (compound) whose status is [Pending] is selected.

The status can be changed by the procedures below as well as by using the [Accept] button in the [Review] menu band.

- When Compound View is displayed, right-click the mouse on [Compound Results] and select [Accept].
- When Sample View is displayed, right-click the mouse on [Sample Results] and select [Accept].
- When Summary View is displayed, right-click the mouse on [Summary] and select [Accept].



- Use the keyboard shortcut.

  Press the [A] key, for “Accept”, on the keyboard.

When all compounds for a sample are either [Pending] of [Accept], the sample in the [Sample List] is marked as [Review]. When all samples for a particular compound are either [Pending] or [Accept], the compound in the [Compound List] is marked as [Review].

NOTE

The status of all compounds in a sample can be changed by right clicking on a sample in the [Sample List]. The status of all compounds in [Compound Results] changes at once.

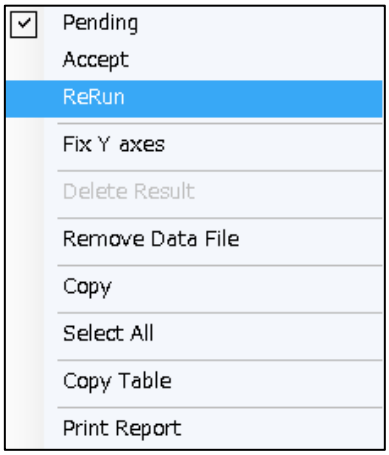
3.29.2 [Review] Rerun

Click the [Rerun] button in the [Review] menu band to change the status of the currently selected quantitative result to [●Rerun].

- When Compound View is displayed, the status of the compound currently selected on [Compound Results] is changed. After the change, the next compound whose status is [● Pending] is selected.
- When Sample View is displayed, the status of the sample currently selected on [Sample Results] is changed. After the change, the next sample whose status is [●Pending] is selected.
- When Summary View is displayed, the status of the sample (compound) currently selected on [Summary] is changed. After the change, the next sample (compound) whose status is [● Pending] is selected.

The status can be changed by the procedures below as well as by using the [Rerun] button in the [Review] menu band.

- When Compound View is displayed, right-click the mouse on [Compound Results] and select [Rerun].
- When Sample View is displayed, right-click the mouse on [Sample Results] and select [Rerun].
- When Summary View is displayed, right-click the mouse on [Summary] and select [Rerun].



- Use the keyboard shortcut.

  Press the [R] key for “Rerun” on the keyboard.

If there is at least one [●Rerun] compound in a sample, the sample is marked as [●Rerun] in the [Sample List]. If there is at least one [●Rerun] sample for a particular compound, the compound is marked as [●Rerun] in the [Compound List].

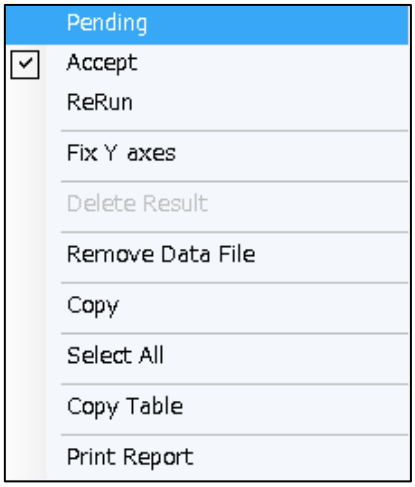
3.29.3 [Review] Pending

Click the [Pending] button in the [Review] menu band to change the status of the currently selected quantitative result to [●Pending].

- When Compound View is displayed, the status of the compound currently selected on [Compound Results] is changed. Clicking the [Pending] button does not change the selected target.
- When Sample View is displayed, the status of the sample currently selected on [Sample Results] is changed. Clicking the [Pending] button does not change the selected target.
- When Summary View is displayed, the status of the sample (compound) currently selected on [Summary] is changed. Clicking the [Pending] button does not change the selected target.

The status can be changed by the procedures below as well as by using the [Pending] button in the [Review] menu band.

- When Compound View is displayed, right-click the mouse on [Compound Results] and select [Pending].
- When Sample View is displayed, right-click the mouse on [Sample Results] and select [Pending].
- When Summary View is displayed, right-click the mouse on [Summary] and select [Pending].

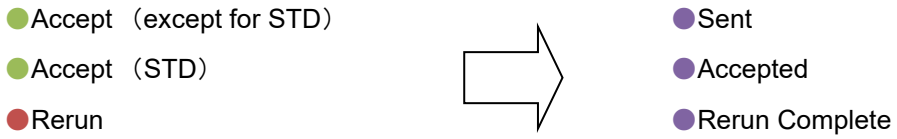


Note: There is no keyboard shortcut for this function.

3.29.4 [Review] Send

Clicking the [Send] button in the [Review] menu band changes the currently set status to indicate that the [Send] process has been completed. The status is also saved in the DAMLP file for Data mode and processing file for Processing mode.

Clicking the [Send] button changes the statuses as shown below.



When the [Sent] or [Accept] process is completed for the status of all compounds contained in the target sample or the status of all samples containing the target compound, the status of the sample becomes [Complete].

NOTE

The Status can be changed using the keyboard shortcut.

[A]: Change to [Accepted] and move to the next [Pending] sample.

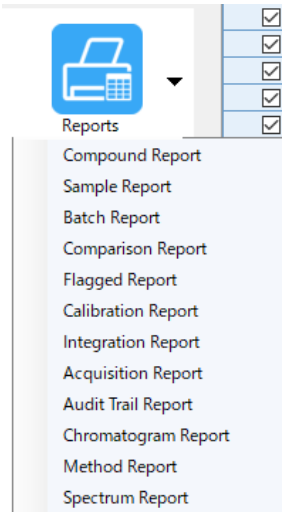
[R]: Change to [Rerun] and move to the next [Pending] sample.

[P]: Move to the previous [Pending] sample.

[N]: Move to the next [Pending] sample.

3.30 [Report] Reports

When [Reports] is clicked in the [Report] menu band, the report templates set in Application Configuration are shown in the drop-down list.

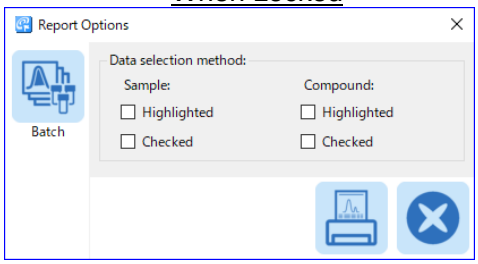


The report formats can be configured using the Report Configuration application. Please refer to the Report Configuration user manual for details.

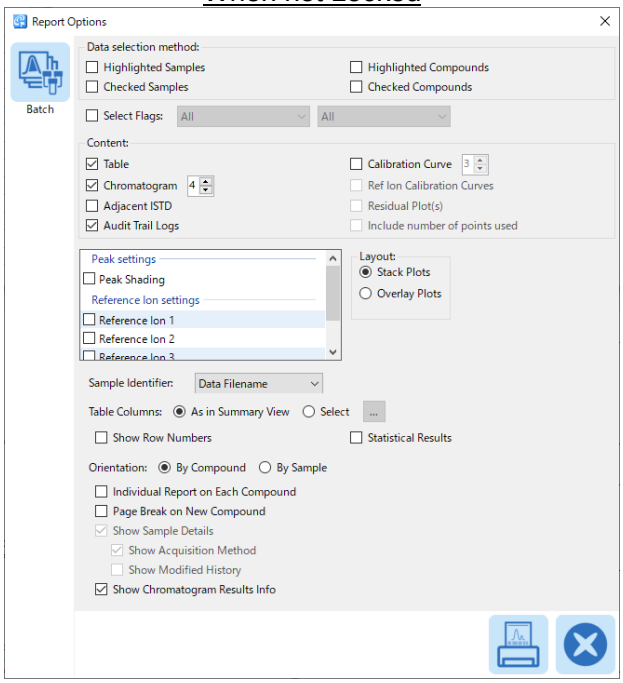
3.30.1 Report options

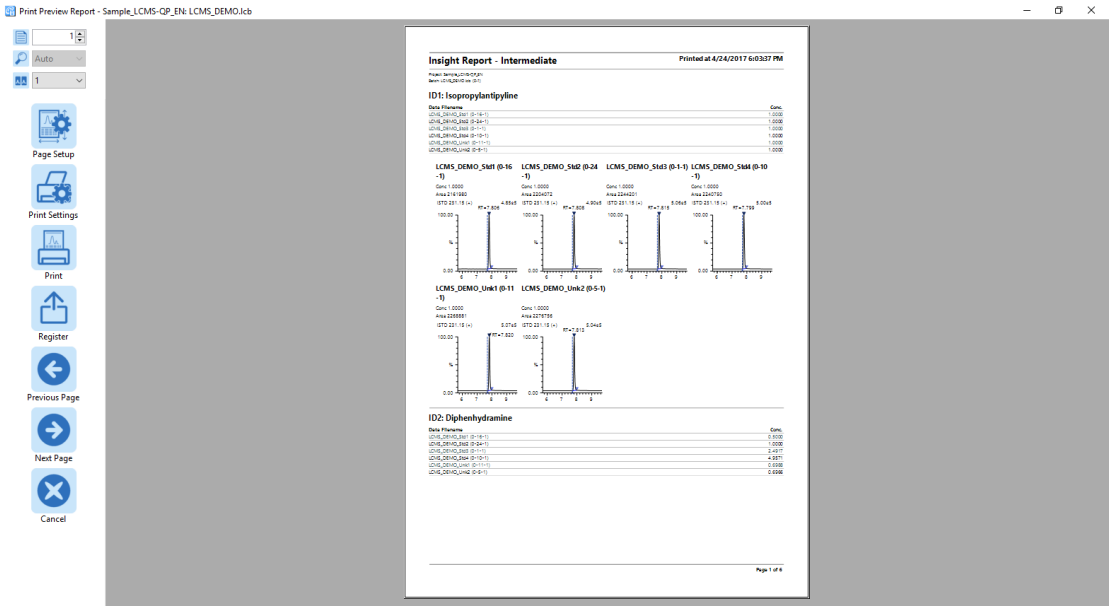
Depending on the “Locked” status of the selected template, the following dialog appears. For details of the report options, see 1.17 Report template management.

When Locked



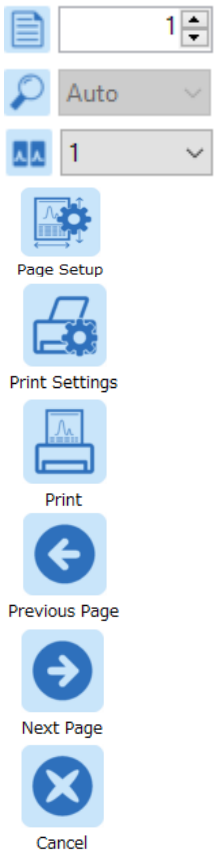
When not Locked





3.30.2 Print preview

Click on the button to show the print preview. The print layout and content can be previewed and Page Setup and Print Settings (printer) can be adjusted before choosing to send as a print job.



Select the page number to show in the preview.

Select the level of zooming of the preview.

Select the number of pages to show side by side in the preview.

Open the [Page Setup] dialog for the default printer.

Open the [Print Settings] dialog for the default printer.

Print to the default printer.

Show the previous page.

Show the next page.

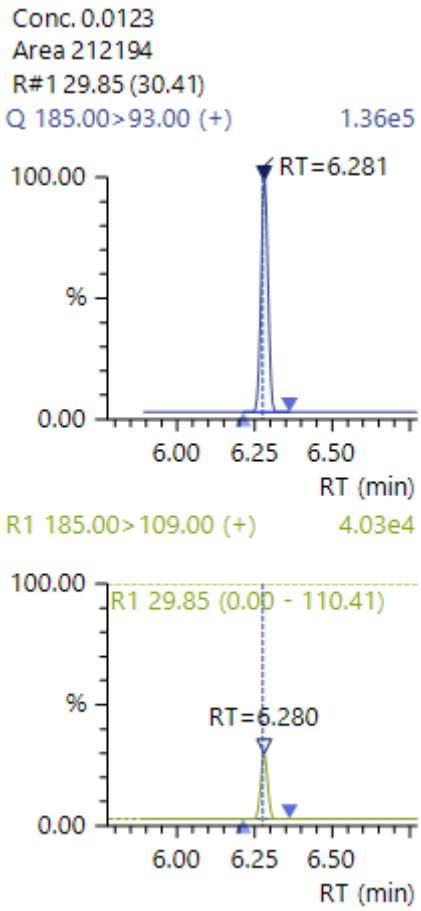
Cancel print preview.

3.30.3 Basic format of chromatograms with Reference Ions options

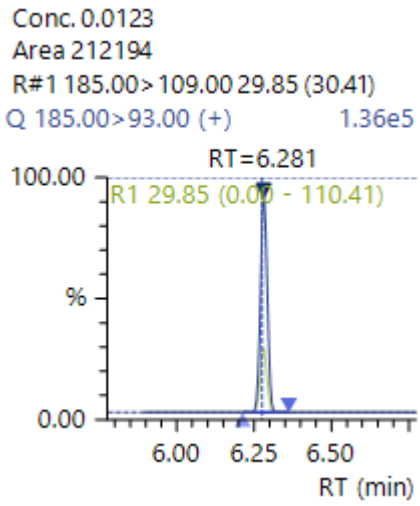
Retention time and area (or height) values are printed on the top of a chromatogram. If these labels are turned off in Display Settings, then they will be printed outside of the data view rectangle (as shown below).

Ion Ratio is displayed above the graphs. If the Ion Ratio is out of range, then an asterisk is added.

Stack



Overlay



3.30.4 General report layout

When all contents are to be reported, at the top of the report is a result table. Chromatograms of each compound for all samples are shown below the table.

When reporting per compound, each chromatogram for the compound in a sample is placed next to each other under the title line for the compound. Line feeds are used when there are too many chromatograms. After all chromatograms for a compound are displayed another line feed (end of paragraph) is issued and next compound title is written followed by the chromatograms for each sample. When reporting per sample, the same principle applies, except that now, compound chromatograms are reported per sample.

Data Filenames are printed without path or extension.

Hint

Compounds and samples that have been filtered out in the main Insight view are not included on the report.

3.31 [Report] Report

This function is available when GCMSsolution or LabSolutions LCMS is installed and [Data Mode] is slected.

It is also not available in Processing mode.

If a report format file is specified in a batch table before sample acquisition, the result of the data file can be printed in LabSolutions Insight.

Click on the Report button in the Report menu band to print a GCMSsolution or LabSolutions report. The report can be printed from the right click context menu in the following locations:

There is no intermediate dialog to choose any settings. The report will be sent to the default printer to be printed, immediately.

Hint

If GCMSsolution or LabSolutions report is printed without saving files, analysis result is not reflected in the printed report. Be sure to save analysis result before printing.

NOTE

If a PDF creator or other converter program is configured as the default printer, its dialogs can get hidden behind Insight. Use [Alt] + [Tab] key strokes to bring the relevant window to the top.

3.32 User Rights

What operations can be carried out depends on the user rights. Below is a table summarizing the relationship between LabSolutions user rights, Insight user rights and Insight operations.

1.6.2

	Read Only	Edit Result	Edit Method Part	Read Write
LabSolutions Right	None	Perform Postrun Analysis	Perform Postrun Analysis & Edit Method(RT and Conc)	Perform Postrun Analysis & Edit Method(data processing parameters)
Insight Features	Limitations			
Open	Yes	Yes	Yes	Yes
Wizard	No	Yes	Yes	Yes
Wizard – Create Method	No	No	No	Yes
Update	No	No	No	Yes
Load Method	No	No	No	Yes

Load Flags	No	Yes	Yes	Yes
Import	No	Yes	Yes	Yes
Save	No	Yes	Yes	Yes
Save As	No	No	Yes	Yes
Save Flags	No	Yes	Yes	Yes
Export (Text)	Yes	Yes	Yes	Yes
Export (Method)	No	No	No	Yes
Close	Yes	Yes	Yes	Yes
Edit Method	Yes	Yes	Yes	Yes
Edit Method - Except for Compound Tab	No	No	No	Yes
Edit Method - Compound Table	No	No	No	Yes
Edit Method - Compound Table (Std. Conc.)	No	No	Yes	Yes
Integrate Batch	No	Yes	Yes	Yes
Integrate Sample	No	Yes	Yes	Yes
Integrate Compound	No	Yes	Yes	Yes
Integrate Result	No	Yes	Yes	Yes
Integrate Batch - Integration	No	No	No	Yes
Integrate Sample - Integration	No	No	No	No
Integrate Compound - Integrate	No	No	No	Yes
Integrate Result - Integrate	No	No	No	No
Edit Table	No	Yes	Yes	Yes
Edit Table > Sample Name	No	Yes	Yes	Yes
Edit Table > Sample ID	No	Yes	Yes	Yes
Edit Table > Sample Amt.	No	Yes	Yes	Yes
Edit Table > Dil. Factor	No	Yes	Yes	Yes
Edit Table > Sample Type	No	No	No	Yes
Edit Table > Level	No	No	No	Yes
Edit Table > m/z	No	No	No	Yes
Edit Table > Ref 1~5 m/z	No	No	No	Yes
Edit Table > RT	No	No	Yes	Yes

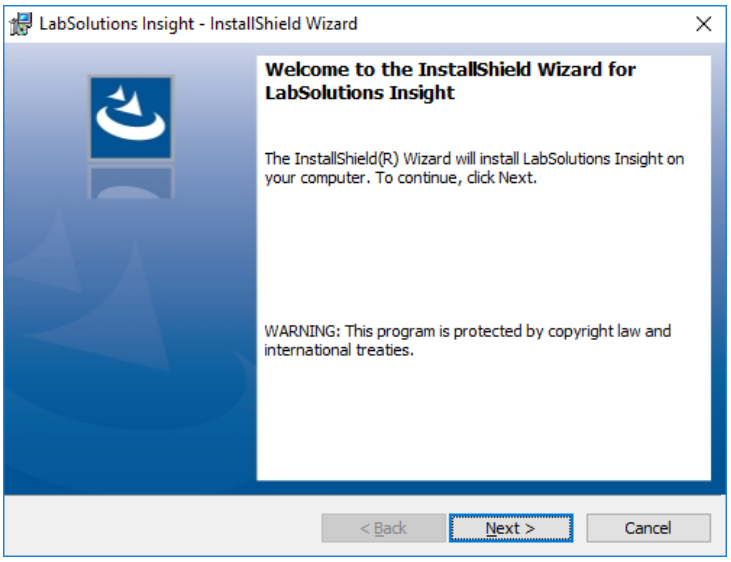
Edit Table > Update RT and Ref. Ions	No	No	Yes 1.6.2	Yes
Remove Data	No	Yes	Yes	Yes
Delete Result	No	Yes	Yes	Yes
Review	No	Yes	Yes	Yes
Chromatogram > Update RT and Ref. Ions	No	No	Yes	Yes
Chromatogram > Select Quant Ion	No	No	No	Yes
Chromatogram > Manual Identification	No	Yes	Yes	Yes
Chromatogram > Clear Identified Peak	No	Yes	Yes	Yes
Chromatogram > Delete All Peaks	No	Yes	Yes	Yes
Chromatogram > Manual Peak Integration	No	Yes	Yes	Yes
Calibration Point - Include / Exclude	No	No	No	Yes
Calibration Pane - Calibration Parameters	No	No	No	Yes
Edit Flags	No	Yes	Yes	Yes
Show Compounds	No	Yes	Yes	Yes
Print Report	Yes	Yes	Yes	Yes

4 Installation and Uninstallation

This section describes how to prepare Insight for use, and how to terminate its usage.

4.1 Installation

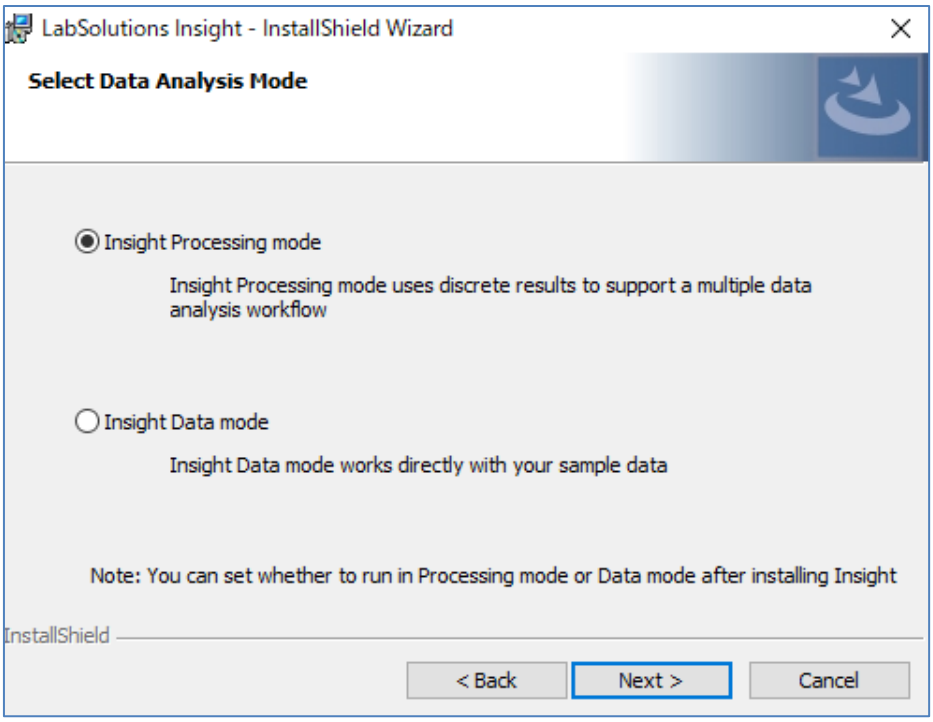
To install the LabSolutions Insight software, run Setup.exe in the installation disk.



Follow the onscreen prompts to install LabSolutions Insight software.

Select the operation mode as appropriate. See section 2.1 "Operation modes" for details.

Note that the prompt will provide useful information according to the current installation environment.



Hint

It is recommended that the following folders are excluded from the anti-virus software scanning routine if any are installed:

- C:\ProgramData\Shimadzu
- C:\Program Files (x86)\Shimadzu
- C:\Program Files (x86)\MSOLicense
- C:\Users\(Windows Username)\AppData\Local\Temp
- C:\Users\(Windows Username)\AppData\Roaming\Shimadzu

4.2 License

In order to use LabSolutions Insight, an appropriate license must be installed. The license is available in the form of an electronically authenticated software license or a USB dongle.

One license is needed to run one instance of Insight. That is to say, if 5 licenses are available and 5 instances of Insights are running, an instance must be closed before another instance may be started. Only one instance of Insight may run on a PC.

LabSolutions Insight has the capability to search for licenses on a network. Any license installed on the same subnet can be shared amongst installations of Insight. However, only the local licenses can be viewed using the Application Configuration License Server Information window; licenses installed on other PCs on the network will not be listed.

An exception to the license sharing capability is when Shared Insight is enabled. When Shared Insight is enabled, licenses can be shared across subnets. Please see 4.3 Shared Insight on details about Shared Insight.

4.2.1 Using an Electronically Authenticated License

When using this type of license, authentication over the internet is required. Access the Shimadzu software license management system using a web browser and activate the software license.

See the “Software License Authentication Manual” shipped with Insight for instructions on how to authenticate a Shimadzu license. The instruction manual explains how to authenticate a LabSolutions license. Replace “LabSolutions” with “LabSolutions Insight” and follow the same instructions.

NOTE

When LabSolutions LCMS is not installed, run "Software License Management Tool" described in Software Activation Procedure from the following location on the start menu.

Windows 10
Windows button→Shimadzu License Management Tool | Software License Management Tool

Windows 11
All Apps | Shimadzu License Management Tool | Software License Management Tool

NOTE

An existing Shimadzu Software License Management System account for authenticating LabSolutions products can be used to authenticate the Insight license.

NOTE

The same Shimadzu Software License Management System account for authenticating LabSolutions DB LCMS/CS can be used to authenticate the Insight license.

NOTE

There is no need to connect the PC with LabSolutions installed to the internet. However, license authentication is easier if it is.

The license becomes activated once the PC is rebooted after authenticating the license.

4.2.2 Using a USB Dongle

Insert the dongle on a PC after installing LabSolutions Insight. Reboot the PC for the license to take effect. If multiple dongles are inserted on a single PC, the licenses are added up. See section 1.12 "Licensor Server Information" on how to view the number of licenses available on the system.

4.3 Shared Insight

When Shared Insight is enabled, one installation of Insight can be shared by multiple PCs that do not have Insight installed on them. The PC on which Insight is installed is called the Server and the other PCs accessing this Server are called Clients.

NOTE

There is no need to install Insight on Clients, however all PCs wishing to run Insight and handle GCMS data must have one of the forms of GCMSsolution installation described in Section 0.

4.3.1 Setting up Shared Insight

4.3.1.1 Server Setup

First, install Insight on the Server PC.

Create a new folder to be used as the shared folder. This should be somewhere accessible by other users such as C:\LabSolutionsInsight\Shared.

Please see Section "1.11Shared LabSolutions Insight browser" on how to set up the shared folder and network details.

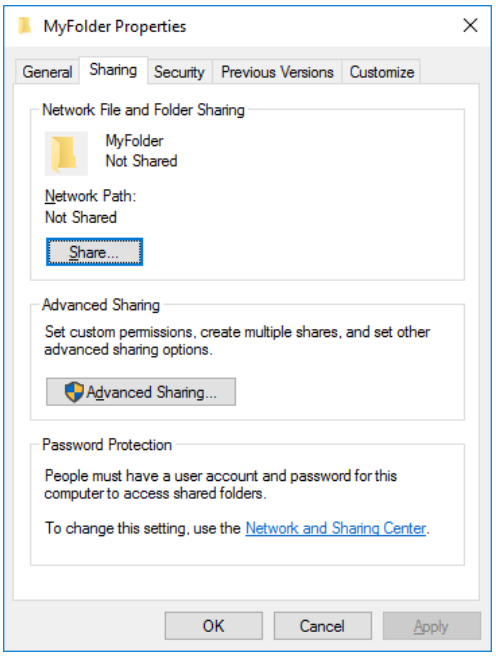
Hint

If the Server PC has more than one IP address, the Network Settings must be changed to specify which IP address should be used by Insight. Please see section 1.9 “Network Settings” for details.

If all the licenses are to be managed on the Server, the Advanced settings for the Shared Browser setting should be changed to specify the license server from which the Clients should obtain the licenses. Please see section 1.11 “Shared LabSolutions Insight browser” for details.

After setting up Shared Insight on the Server using Application Configuration, share the Shared Insight folder over the network using the standard Windows operation.

In Windows Explorer right click on the folder to be shared, select Properties and select the Sharing tab. Press the Share… button. Select who to share the folder within the File Sharing dialog and press Share.



Please consult your site IT or Network manager for details as security policies differ from site to site.

NOTE

For handling GCMS data, all user databases on the Server and Clients must be identical. Safe and correct behaviour of Insight is not guaranteed if user databases are changed on individual PCs.

When LabSolutions LCMS or GCMS solution is installed on the server, LabSolutions user management database is also used by Insight. When LabSolutions LCMS or GCMS solution is not installed on the server, Insight uses its own user management database.

Hint

Make sure to exclude the shared folder from the anti-virus software scanning routine.

4.3.1.2 Client Setup

However, when printing reports of GCMSsolution and LabSolutions LCMS from Insight, installation of GCMSsolution and LabSolutions LCMS or its secondary usage license is required.

On each of the Clients' desktop, create a shortcut to SharedInsightLauncher.exe on the Server located in the path set up in Section "4.3.1Server Setup". For convenience, rename the icon to LabSolutions Insight.

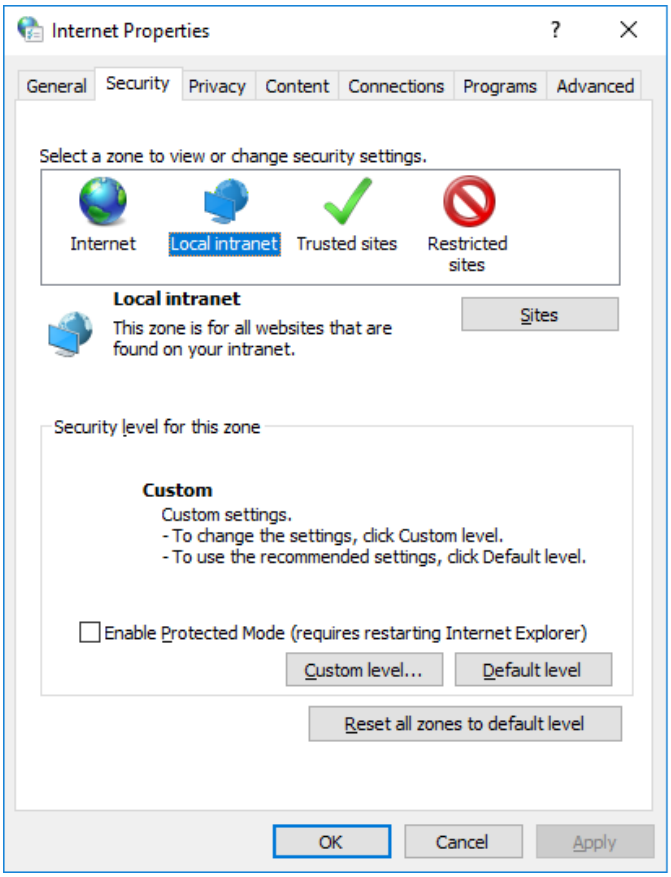
NOTE

Make sure to make arrangements to allow the Client to access the Server through its firewall. Please consult your site IT manager for details as security policies differ from site to site.

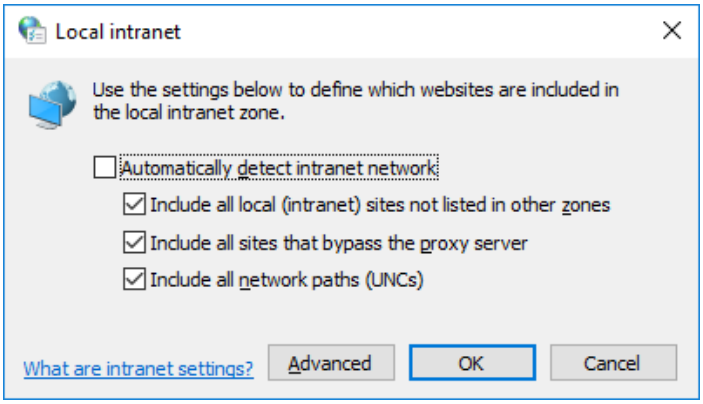
NOTE

When allowing more users to access Insight set up for handling GCMS data, additional users must be added to the GCMSsolution user management database using the PC on which GCMSsolution can be activated (e.g. the Server PC). Once new users are added, the user management database must be copied to all Client PCs again.

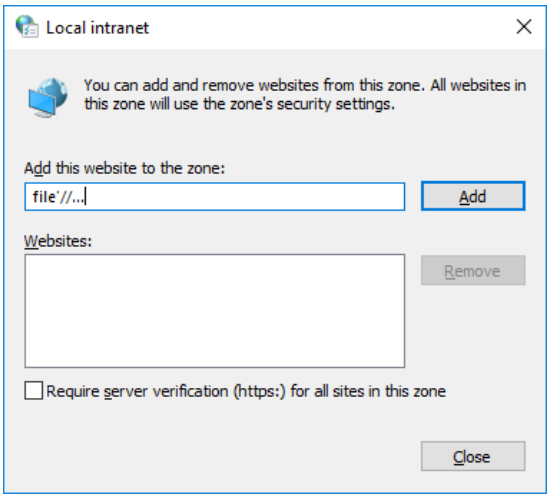
Set the Internet Option in the Client so that the Server is recognized as a secure site on the local intranet to avoid Insight invoking security warnings when it starts up. Go to [Control Panel] - [Internet Options] then click on [Local Intranet]



Click on Sites.



Click on Advanced.

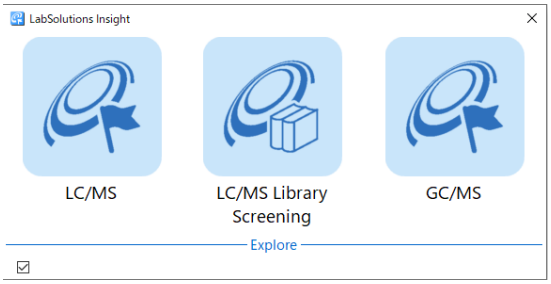


Add the location of the Server in the form file://<server location>. For example, file://test32. test32 is name of server pc.

4.3.2 Using Shared Insight

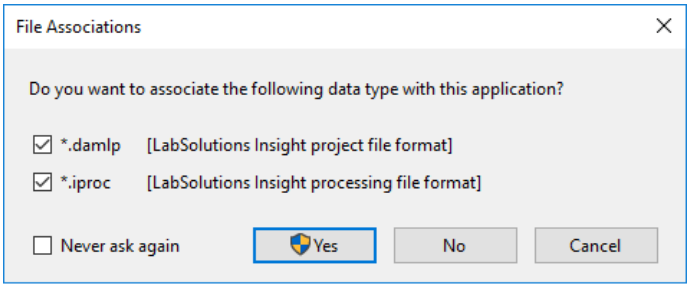
Double click on the LabSolutions Insight icon created following the steps in Section "4.3.1 Setting up Shared Insight" to start Insight. Select OK for any security messages that appear.

The Insight Launcher is displayed.



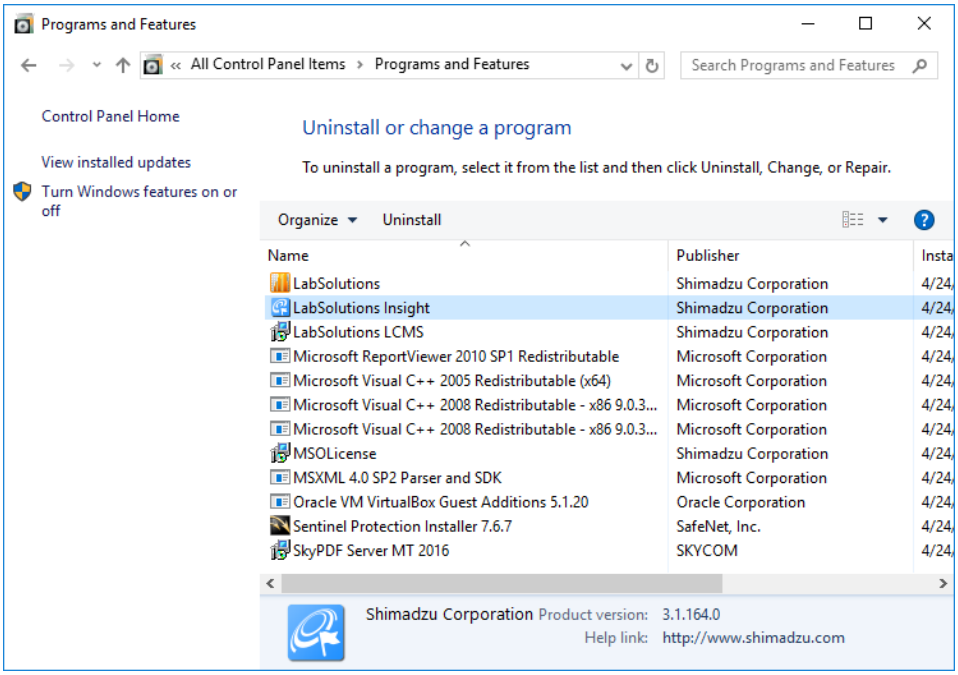
Select the required version of Insight to proceed. If a version of Insight is not available for use, e.g. because some software components are not installed, then the icon comes up greyed in the launcher.

On starting up, Insight will ask whether to associate the DAMLP file type with Insight. Select Yes to associate DAMLP files with Insight. Otherwise, select No or Cancel. Check the Never ask again check box to not show this message on starting Insight.



4.4 Uninstallation

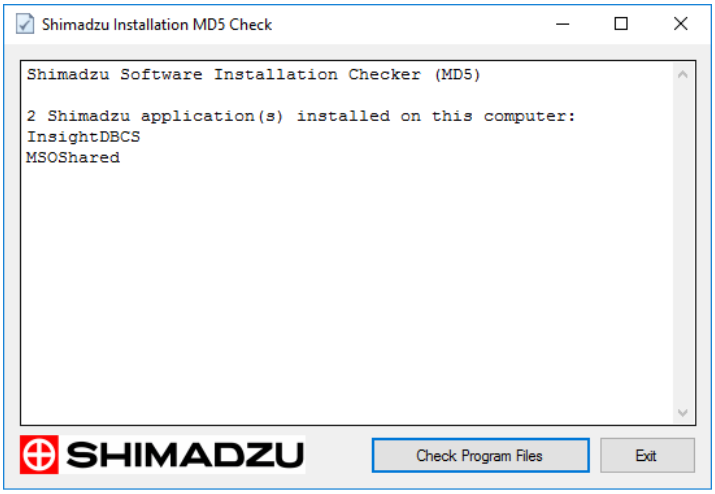
To uninstall LabSolutions Insight Software, select **Start Menu** > **Control Panel** > **Uninstall a Program.**



4.5 Program Alteration Check

LabSolutions Insight Software incorporates a function to check that the program is installed correctly and the program is not altered after the installation.

To open this program select **Start Menu** > **All programs** > **LabSolutions Insight** > **Installation MD5 Check**



Selecting **Check Program Files** initiates the program check and the result is displayed.

Appendix A: Export formats

Output item list (Format: By View (Compound))

This format is used when [By View] is selected for the format option and [Compound View] is selected for the current display setting. The format for numbers is determined according to the Application Configuration settings.

Item	Content	Format
Header (Items displayed as the header of tables)		
ID #	Compound ID	Numeric
Name	Compound name	String
Fixed (items always displayed regardless of display settings)		
ID	Row Number	Numeric
Flag	Flag status	String Outliers Review
Flag ID	Flag ID	String
Data Filename	Data file name	String
Variable (items selected according to the table style settings)		
＋items added to [Selected Columns] in options for Compound View		

Output item list (Format: By View(Summary))

This format is used when [By View] is selected for the format option and Summary View is selected for the current display setting. The format for numbers is determined according to the Application Configuration settings.

When the summary is displayed by samples vs compounds

Item	Content	Format
Fixed (items always displayed regardless of display settings)		
Data Filename	Data file name	String
Flags	Flag status	String Outliers Review
Sample Name	Sample name	String
Sample ID	Sample ID	String
	(Compound name)	String
＋items added to [Selected Columns] in options for Summary View		

When the summary is displayed by samples vs compounds

Item	Content	Format
Fixed (items always displayed regardless of display settings)		

Name	Compound name	String
Flags	Flag status	String Outliers Review
	(Sample information)	String
＋items added to [Selected Columns] in options for Summary View		

Output item list (Format: Fixed format (Compound vs. Sample)

This format is used when [Fixed format (Compound vs Sample)] is selected for the format option. The format for numbers is determined according to the Application Configuration settings.

	A	B	C	D	E	F	G
1	#1						
2	Name	MPA-gluc					
3		Flags	Flag ID	Data Filename	Sample Name	Sample ID	Sample Type
4	1			Blank_system	Blank_system		Unknown
5	2			Blank-solvent	Blank_solvent		solvent
6	3			Conc-1_001	Conc-1		Standard
7	4			Conc-2_001	Conc-2		Standard
8	5			Conc-3_001	Conc-3		Standard
9	6			Conc-3_002	Conc-3		Standard
10	7			Conc-2_002	Conc-2		Standard
11	8			Conc-1_002	Conc-1		Standard

Output item list (Format: Fixed format (Sample vs. Compound)

This format is used when [Fixed format (Sample vs Compound)] is selected for the format option. The format for numbers is determined according to the Application Configuration settings.

	A	B	C	D	E
1	#1				
2	Data Filename	Blank_system	Sample Name	Blank_system	Sample ID
3		Name	Flags	Flag ID	Sample Type
4	1	MPA-gluc			Unknown
5	2	d3-MPA-gluc			Unknown
6	3	MPA			Unknown
7	4	d3-MPA			Unknown
8	#2				
9	Data Filename	Blank-solvent	Sample Name	Blank_solvent	Sample ID
10		Name	Flags	Flag ID	Sample Type
11	1	MPA-gluc			solvent
12	2	d3-MPA-gluc			solvent
13	3	MPA			solvent
14	4	d3-MPA			solvent

Appendix B: Definitions

LabSolutions Insight uses many data analysis parameters, and outputs many processing and evaluation results. Many of these values are common to LabSolutions and/or GCMSsolution but some are unique to LabSolutions Insight. The parameters and results and their definitions are listed below. For further information, please refer to the User Guides for LabSolutions LCMS and or GCMSsolution, or their online manuals.

Item	Content	
Compound Information		
ID#	Compound ID	
Name	Compound name	
Type	Displays the type of compound.	
	Reference	
	ISTD	
	Target	
	ISTD & Reference	
m/z	Mass per charge	
Group #	Displays the group number set in the compound table.	
Event	Individual MS condition at analysis is "event", event number is displayed.	
Sample Information		
Sample ID	Sample ID	
Data Filename	Data file name	
Sample Name	Sample name	
Sample Type	Sample type	
	Unknown	
	Standard	
	Control	
	Unspiked	
	Spiked	
	water	Note: "water", "solvent" and "matrix" are user-defined blanks that can be set in Application Configuration.
	solvent	
	matrix	
Vial	Vial number	
Tray	Tray number	
Inj Vol	Injection amount[µl]	

Aqcuired Date	Analysis date yyyy/mm/dd hh:mm:ss
Aqcuired By	Name of analyst
Integration parameters	
Mode ID	Data processing mode IDs. IDs and their meanings are as follows.

DISPLAYED ID	MEANING
Auto	Auto Integration/Identification
M	Manual Integration
MI	Manual Identification
MI R1	Manual intengration applied to Ref 1
	Same for Ref 2 to 5
NI	No Identified peak
IR	Outisde of reference ion ratio range.
ND(W/B)	Outisde of Window/Band range.
BMSI	Under minimum similarity index
NP	No peak
+(S)	Peak saturated
+<>R1	Switched with Ref 1
	Same for Ref 2 to 5.
	Note: + indicates ID can appear on its own or in conjunction with other IDs, e.g. Auto (S)

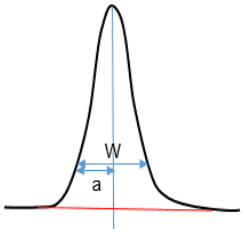
Mode	Data processing modes corresponding to Mode ID above.
Band	Identification parameter. See User Guide 3.21 Edit Method for details.
Slope	Peak integration parameter. Method value is used when set to "Default". Can be set individually for GCMS.
Width	Peak integration parameter. Method value is used when set to "Default". Can be set individually for GCMS.
Drift	Peak integration parameter. Method value is used when set to "Default". Can be set individually for GCMS.
Window/Band	Identification method (Window or Band). Method value is used when set to "Default". Window or Band method is used when these values are set.

Default
Window

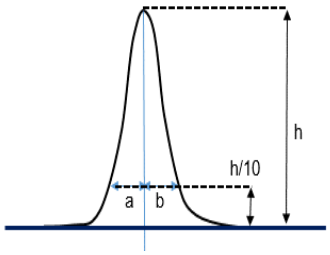
	Band	
Noise From	Start time for noise calculation (minutes).	
Noise To	End time for noise calculation (minutes).	
Noise Calc. Method	Noise calculation method.	
	(LCMS)	(GCMS)
	ASTM	ASTM
	RMS	RMS
	EP	Peak to Peak
	USP	
	JP	
Calibration Curve		
Cal Point	Select whether to include in the calibration curve.	
Level	Calibration curve level. Calibration curve is built using concentrations set for each level. Refer to "Std Conc" below.	
Std. Conc.	Concentration of standard or control sample for the specified level.	
Concentrations	Concentrations of all levels.	
Calc.by	Value by which to calculate concentrations (area or height). Method value is used when set to "Default".	
	Default	
	Area	
	Height	
Curve	Curve type to fit to calibration points to create calibration curves.	
	Default	
	Linear	
	Point to Point	
	Quadratic	
	Cubic	
	Mean RF	
Zero	Whether to force calibration curve through origin. Method value is used when set to "Default".	
	Default	
	Not Zero Forced	
	Zero Forced	
	Line to Level # 1	

Weight	Calibration curve weighting method. Method value is used when set to "Default". Default None 1/C^2 1/C 1/A^2 1/A
1st Coeff.	First coefficient of the calibration curve.
2nd Coeff.	Secondary coefficient of the calibration curve.
3rd Coeff.	Third coefficient of the calibration curve.
Intersection	Intersection of the calibration curve.
Group Type	Type of calibration when using Grouping. Default Group Calib. Conc. Sum.
RF	$\text{Response Factor(RF)} = \frac{\text{Measured response}}{\text{Concentration}}$ When internal standard method is used: $\text{Response Factor(RF)} = \frac{\frac{\text{Measured response (target)}}{\text{Measured response (ISTD)}}}{\frac{\text{Concentration (target)}}{\text{Concentration (ISTD)}}}$
RF Mean (level)	Mean RF Claculated when there are two or more "standard" type samples of the same level.
RF SD (level)	RF standard deviation. Calculated when there are two or more "Standard" type samples of the same level.
RF %RSD (level)	Relative standard deviation (%) of RF. Calculated when there are two or more "Standard" type samples of the same level.
RF Mean (curve)	Average RF across entire calibration curve. Calculated for “Standard” samples.
RF SD (curve)	Standard deviation of RF across entire calibration curve. Calculated for “Standard” samples.
RF %RSD (curve)	Relative standard deviation of RF across entire calibration curve given in %. Calculated for “Standard” samples.

RF RSE (curve)	Relative Standard Error of the calibration curve. Calculated for “Standard” samples. $$RSE = 100 \times \sqrt{\sum_{i=1}^{n} \frac{\left[\frac{x_i' - x_i}{x_i}\right]^2}{n-p}}$$ Note that RSE is not calculated for cubic or Manual RF curves.
RF Deviation	$$\text{RF Deviation} = \frac{\lvert\ \text{RF Mean(level)} - \text{RF Mean(curve)}\ \rvert}{\text{RF Mean(curve)}}$$
R	Correlation coefficient of calibration curve
R2	The contribution rate of the calibration curve, the determination coefficient (which is the square of the correlation coefficient, used as an index of the effective figure of the concentration).
Analysis Result	
Flags	Two discrete types of flags. See User Guide 2.6.2 Flag types for details. Outliers Review
Flag ID	Flag identifiers. See User Guide2.6.3 Flag ID for details.
Conc. (*)	Conc. (unit) Concentration calculated from calibration curve.
Unit	Unit of concentration
RT	Set retention time. Please refer to user guide 3.15.2 Update RT/ Ion Ratio on how to update.
Found RT	Retention time (minutes) of the identified peak. If peaks are not identified, please check retention time and method identification parameters (Identification method, identification peak selection, spectrum Confirmation etc).
RT Diff	Difference (msec) between retention time of identified peak and set retention time.
RT %Diff	$$\text{RT Diff(\%)} = \frac{\text{RT Diff}}{\text{RT}} \times 100$$ * Refer to RT and RT Diff for further information.
Area	Area of identified peak
Height	Height of identified peak
Peak Start	Start time (minutes) of identified peak
Peak End	End time (minutes) of identified peak
Accuracy(%)	The ratio (%) of the concentration calculated from the calibration curve to the concentration set in the standard sample Accuracy (%) = 100 - %Diff

%Diff	Diff(%) between set concentration and concentration calculated from calibration curve %Diff = 100 - Accuracy (%)
%RSD (Conc)	Percentage representation of concentration RSD (relative standard deviation). Calculated for each level when the sample type is standard or control and there are two or more samples of the same level.
%RSD (Area)	Percentage representation of concentration RSD (relative standard deviation). Calculated for each level when the sample type is standard or control and there are two or more samples of the same level.
Noise	Noise value calculated based on setting.
S/N	Ratio of identified peak intensity to noise value.
Std RT Diff	The difference between the average retention time of all the standard samples and the retention time of the identified peak.
%Conc. Outside Curve	When the calculated concentration is larger than the maximum calibration point (set maximum concentration) or smaller than the minimum calibration point (set minimum concentration), the value is calculated as follows. $\%\text{Conc. Outside Curve} = \frac{\text{Concentration - maximum or minimum point}}{\text{maximum or minimum point}} \times 100$ Note: It is not calculated for standard sample.
Dil. Factor	Coefficient to multiply set concentration by.
Analysis Result(LCMS only)	
Width(50%)	Full width at half maximum of the identified peak.
Tailing F.	5% Tailing factor (Symmetry Factor). In the figure below, "W" is the peak width at 5% height, and "a" is the width of the first half of the peak (starting point to apex) at the 5% peak height. Tailing factor is calculated as W/2a. 
Tailing F(10%)	10% Tailing factor. In the "Tailing F.", "W" is the peak width at 10% height, and "a" is the width of the first half of the peak (starting point to apex) at the 10% peak height. 10% Tailing factor is calculated as W / 2a.

Asymmetry	Indicator for peak symmetry. In the figure below, it is calculated as b/a.



Analysis Result(GCMS only)	
SI	Similarity with standard spectrum
Ret. Index	Set retention index. Retention index is an indicator of retention time of components using the retention time of the reference compound (n-alkane) peak.
Actual Ret. Index	The actually measured retention index.
Sample Amt.	Coefficient to multiply set concentration by.
Data Comment	Supplementary information can be added as required.
Reference Ion	
Ref. Mode	Referece ion mode used for identification. Method values are used when set to "Default".

(LCMS)	(GCMS)
Default	Default
Absolute	Relative
Relative	Absolute
Absolute or Relative	
Simply Calculate	

Ref 1~5 *m/z*	Mass to charge ratio of reference ions 1 to 5
Ref 1~5 Set Ratio	Displays the set reference ion ratio (intensity ratio of reference ions 1 to 5 to target ion intensity). For details, refer to the following contents of the user guide. 3.15.2. Update RT / Ion Rations 3.26.1. Update RT and Ion Ratios For more detailed setting method, refer to LabSolutions LCMS, GCMSsolution instruction manual or help.
Ref 1~5 Range	Range of ion ratio (%) in which target ions are identified. Edit by chancing the Default Ion Allowance value in [Edit Method] [Identification] tab.
Ref 1~5 Measured	Measured reference ion (1-5) intensities.

Ref 1~5 Actual Ratio	Reference ion ration calculated from measured intensities (reference ion intensity / target ion intensity).
Ref 1~5 Std Ratio %Diff	Difference ratio of ion ratio of each sample to the averaged standard sample ion ratios for each reference ion (Ref-n).* Averaged Std Ref-n = Average of Ref-n Actual Ratio of all standard samples $\text{Ref 1~5 Std Ratio \%Diff} = \frac{\lvert \text{Averaged Std Ref-n-Ref-n Actual Ratio} \rvert}{\text{Averaged Std Ref-n}} \times 100$
Ref 1~5 Noise	Noise value of reference ion 1 to 5
Ref 1~5 S/N	S/N of reference ion 1 to 5
Ref 1~5 Conc.	Reference ion concentrations
Average Conc.	Average of quantifier ion and reference ions (1-5). When reference ion concentrations are not calculated, quantitation ion concentration is given.
Average Conc.(R1,R2)	Average of quantifier ion and reference ions 1 and 2. When reference ion concentrations are not calculated, quantitation ion concentration is given.
ISTD(Internal Standard Method)	
ISTD Name	Compound name of ITSD
ISTD Amount	ISTD amount set in method
ISTD Group	ISTD group number set in method
ISTD Area	Area of internal standard compound
ISTD Height	Height of internal standard compound
Area Ratio	The ratio of identified peak's area to internal standard compound's area.
Height Ratio	The ratio of identified peak's height to internal standard compound's height.
ISTD RT	Retention time (actual measurement) of the identified ISTD compound peak
ISTD RT Diff	The difference between the retention time (actual measurement) of the ISTD compound and the retention time of the identified peak
ISTD %Diff (Stds) Area	Area ratio of ISTD to average of standard sample ISTDs.
ISTD %Diff (Controls) Area	Area ratio of ISTD to average of control sample ISTDs.
Ref. RRT	Reference relative retention time. $\text{Ref. RRT} = \frac{\text{set RT}}{\text{set ISTD RT}}$ * Refer to RT for information on "set RT".

RRT	Relative retention time. $$RRT = \frac{\text{Found RT}}{\text{ISTD RT}}$$ * Refer to Found RT and ISTD RT for further information.
%Dev RRT	Difference ratio between Ref. RRT and RRT. $$\%\text{Dev RRT} = \frac{\text{RRT-Ref. RRT}}{\text{Ref. RRT}} \times 100$$
Recovery Test	
spiked	Spiked amount
Recovery	Recovery rate obtained as a result of recovery test. In order to perform the recovery calculation, it is necessary to set the sample type to "Unspiked" or "Spiked" and set the spiked amount.
Others	
Status	Display the review status. See User Guide 3.29 Review for details.
Custum Calc. Result 1~5	Display custom calculation results.
Comment 1, 2	Supplementary information such as the compound characteristics can be entered as required.