

LabSolutions Insight™ LCMS CL

Quick Start Guide

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

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Introduction

Read this Quick Start Guide thoroughly before using the product.

Thank you for purchasing this product.

This manual describes the operation 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.

Keep this manual for future reference.

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Precaution symbols are indicated using the following conventions:

Indication	Meaning
 NOTE	Emphasizes additional information that is provided to ensure the proper use of this product.

The following symbols are used in this manual:

Indication	Meaning
 Hint	Indicates information provided to improve product performance.

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1.1 Overview

LabSolutions Insight LCMS CL is a software program for analyzing data of multiple samples acquired using LC-MS/MS. Using this software, users can check and analyze measurement data of multiple samples in an integrated manner.

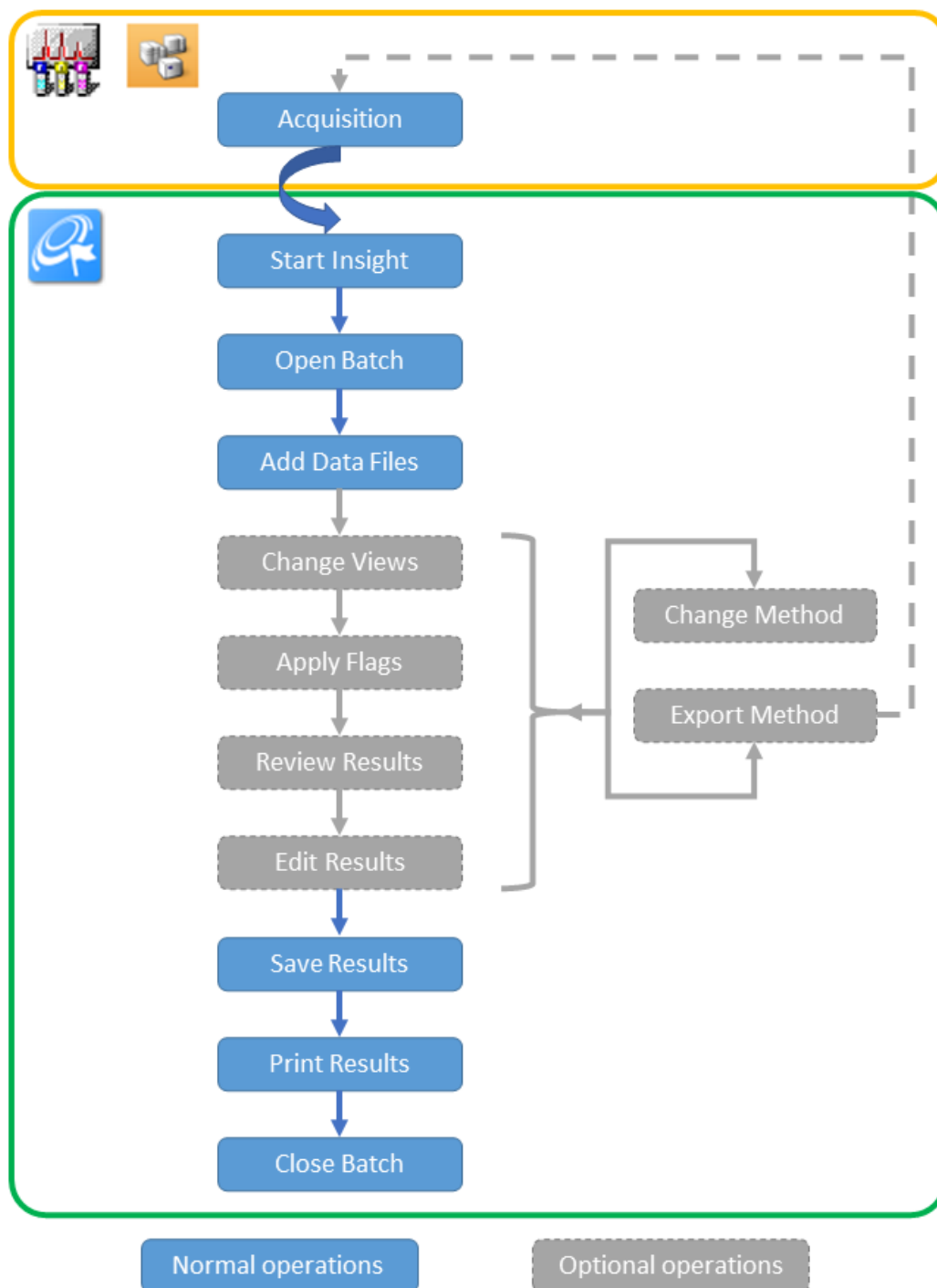
In addition, a flag can be set (flagging) based on specified criteria for information acquired from LC-MS/MS measurement such as concentration, retention time, and ion ratio of the target compounds. This can significantly reduce the time spent on data analysis. Furthermore, there is an option to only include flagged target compounds from multi-sample data in a printed report.

 **NOTE** This manual has been created on the assumption that the reader already has basic knowledge on the operation of Shimadzu's LC-MS/MS and LabSolutions CL. Accordingly, names and terms specific to LabSolutions CL is used throughout this manual. It is recommended that first-time users and those unsure of any points refer to the instruction manual for LC-MS/MS, LC-MS/MS Operation Guide, and LabSolutions CL Help.

2 Getting Started

2.1 Data Analysis Workflow

Analyze data using the following workflow.



2.2 Which Mode Shall I Use?

LabSolutions Insight LCMS CL operates in two modes.

- Data mode
- Processing mode

Please refer to the User Manual for detailed descriptions of each mode and how to switch between the modes.

The following table can be used to determine which mode best suits your needs. Once you have decided on the mode to use, please consult your LabSolutions Insight administrator in order to achieve the desired configuration.

Data mode	Processing Mode
It is necessary to use features only available in LabSolutions CL.	All processing can be completed using Insight features.
It is necessary to review data in LabSolutions CL.	Data review will only take place in Insight.
Only one set of processing parameters is required per dataset.	Several sets of processing parameters are required per dataset so that results can be compared.
Original data should be updated to show processing results.	Processed results should be managed per dataset without altering the original data files.

Data mode	Processing mode
Go to sections	Go to sections
"3.1 Start Insight"	"3.1 Start Insight"
"3.2 Open Batch (Data Mode)"	"3.3 Open Batch (Processing Mode)"
"3.4 Add Data Files"	"3.4 Add Data Files"
"3.5 Change Views"	"3.5 Change Views"
"3.6 Apply Flags"	"3.6 Apply Flags"
"3.7 Review Results"	"3.7 Review Results"
"3.8 Edit Results"	"3.8 Edit Results"
"3.9 Change Method (Data Mode)"	"3.10 Change Method (Processing Mode)"
	"3.11 Export Methods (Processing Mode)"
"3.12 Save Results (Data Mode)"	"3.13 Save Results (Processing Mode)"
"3.14 Print Results"	"3.14 Print Results"
"3.15 Close Batch"	"3.15 Close Batch"

3

LabSolutions Insight LCMS CL Operations

3.1 Start Insight

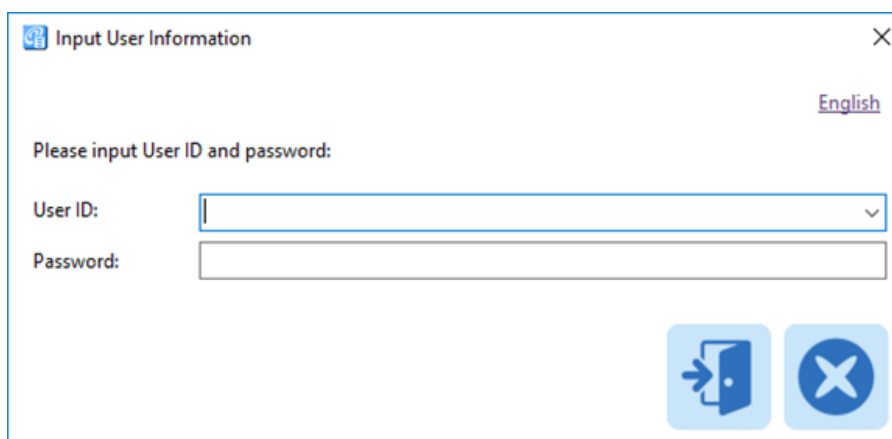
1

Run the [LabSolutions Insight LCMS CL] program by clicking on the  icon on the desktop.

2

Input the user name in [User ID] and password in [Password] and click on the  button. The following user name and password are available by default.

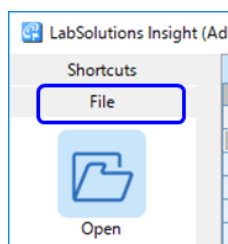
	When LabSolutions CL is installed.	When LabSolutions CL is not installed
User ID	admin	admin
Password	(blank)	admin



3.2 Open Batch (Data Mode)

1

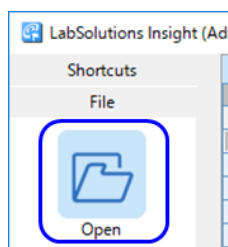
From the menu bar, click on the [File] menu band.



3

2

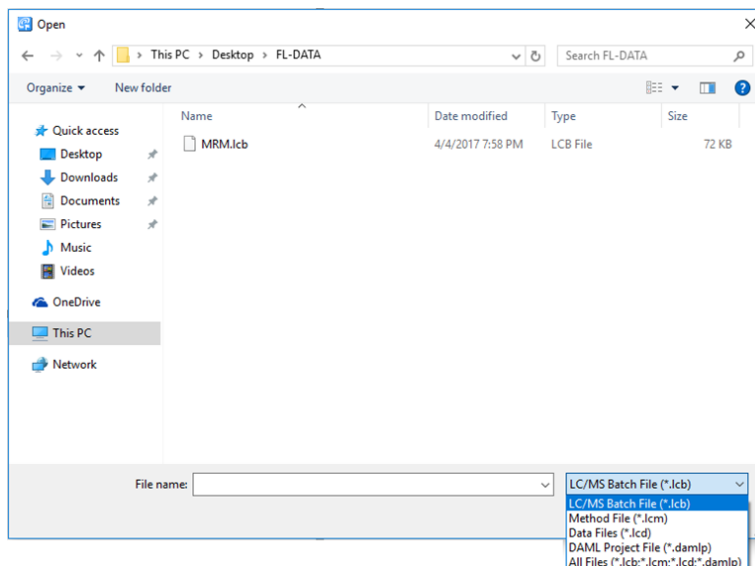
Click on the [Open] icon.



3

Open a batch.

Select a batch file acquired using the Shimadzu real time analysis program ([LabSolutions CL Real Time Analysis]) or a LabSolutions Insight LCMS CL project file (DAML file). Click [Open].



Open a Batch (LCMS)

4

Results of the data files registered to the batch file are displayed.

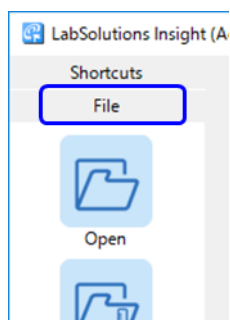
NOTE If the acquisition was performed using multiple method files within one batch, the data set acquired using the method file in the first row is displayed. When batch processing builds calibration curves, data set acquired using the method file that contains the calibration curves is displayed.

NOTE If the method file specified in the batch is not found, data is not displayed. In such a case, load the method first then add data files. Please see ["3.9 Change Method \(Data Mode\)"](#) and ["3.4 Add Data Files"](#) for operation details.

3.3 Open Batch (Processing Mode)

1

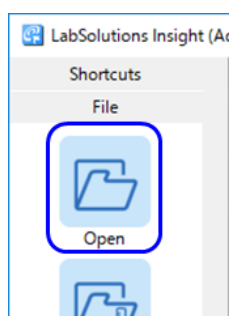
From the menu bar, click on the [File] menu band.



3

2

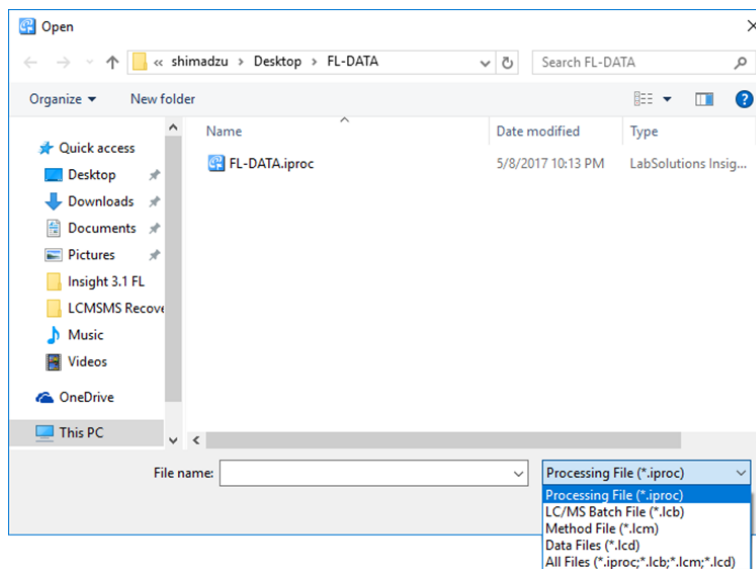
Click on the [Open] icon.



3

Open a batch.

Select a LabSolutions Insight LCMS CL processing file (iproc file) or a batch file acquired using the [LabSolutions CL Real Time Analysis] program. Click [Open].



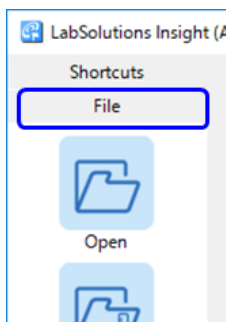
Open a Processing File

3.4 Add Data Files

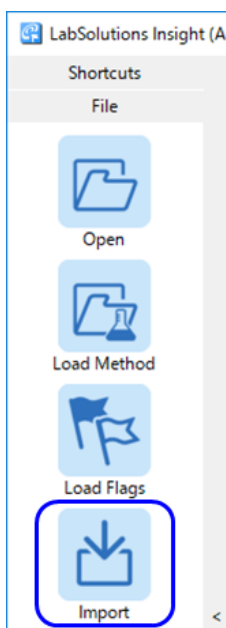
To show results of some more data files, perform the following procedures.

1

From the menu bar, click on the **[File]** menu band.

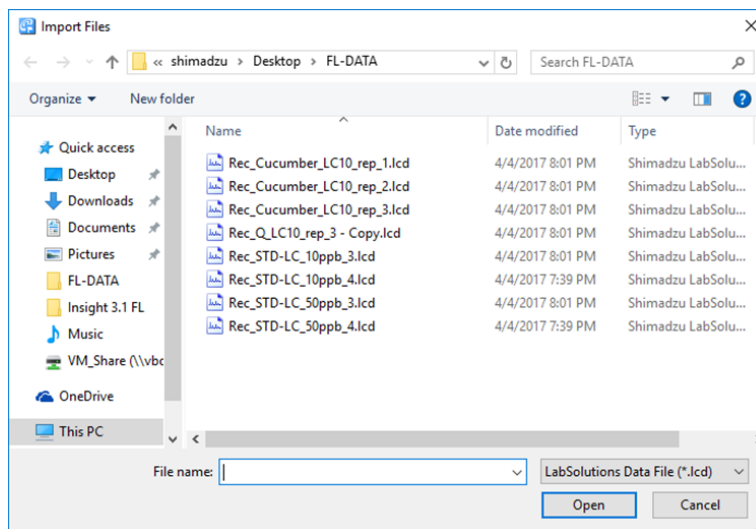
**2**

Click on the **[Import]** icon.

**3**

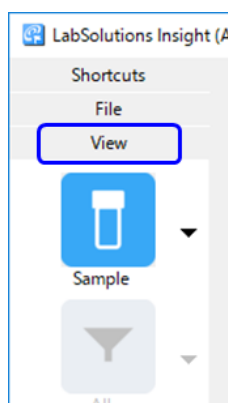
3

Select data file(s) and click [Open]. For LCMS data, select a file with the extension “.lcd”.



3.5 Change Views

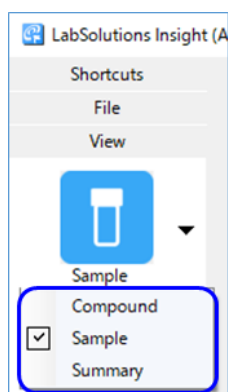
Select how the analysis results are to be displayed.
From the menu bar, click on the [View] menu band.



3

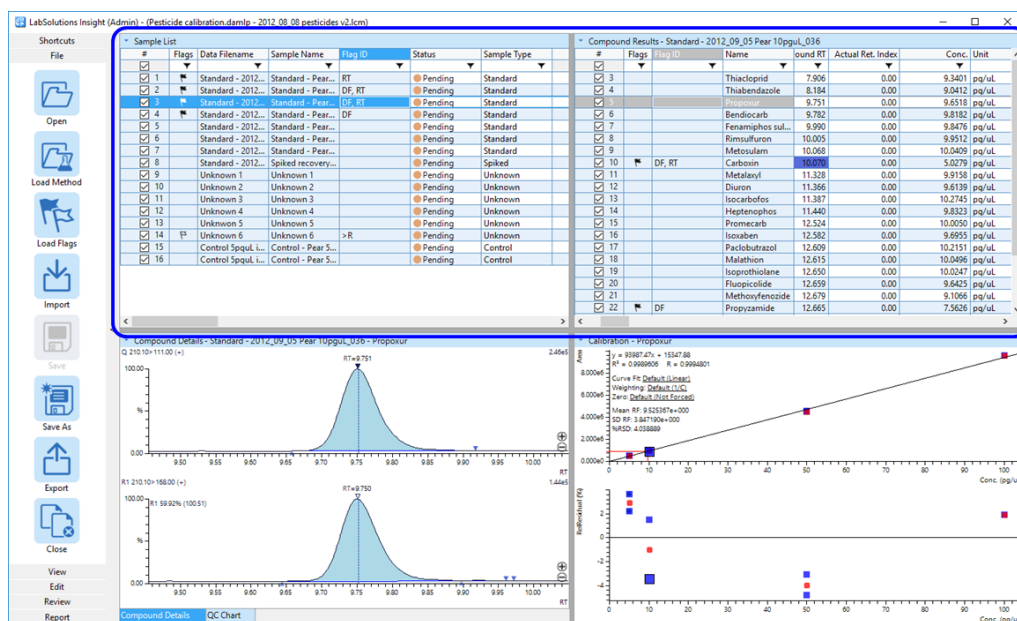
3.5.1 Layout the table area

Tables can be displayed in three different ways. Select a layout to suit your needs.
Click on the top button and select a layout from the three options in the drop down list.



■ [Compound] View

View results of each compound by selecting a data file.



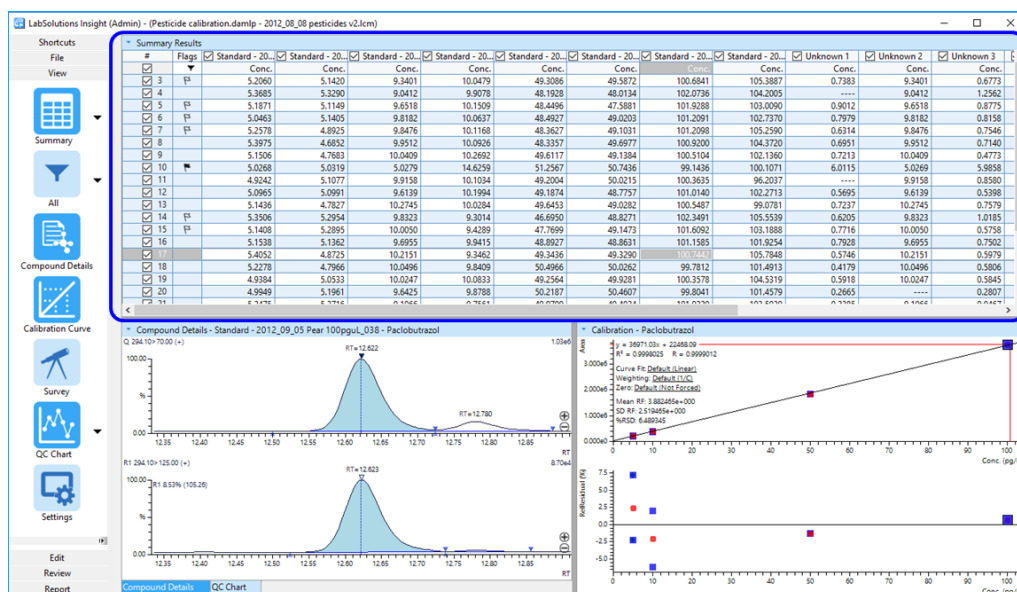
■ [Sample] View

View results of each data file by selecting a compound.



■ [Summary] View

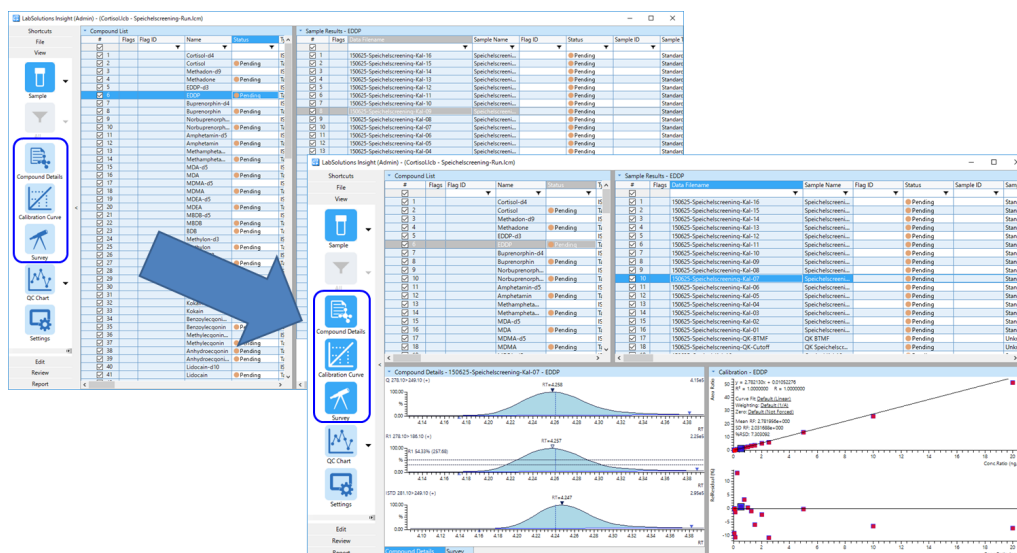
View results for all compounds for all data files in a single table.



3

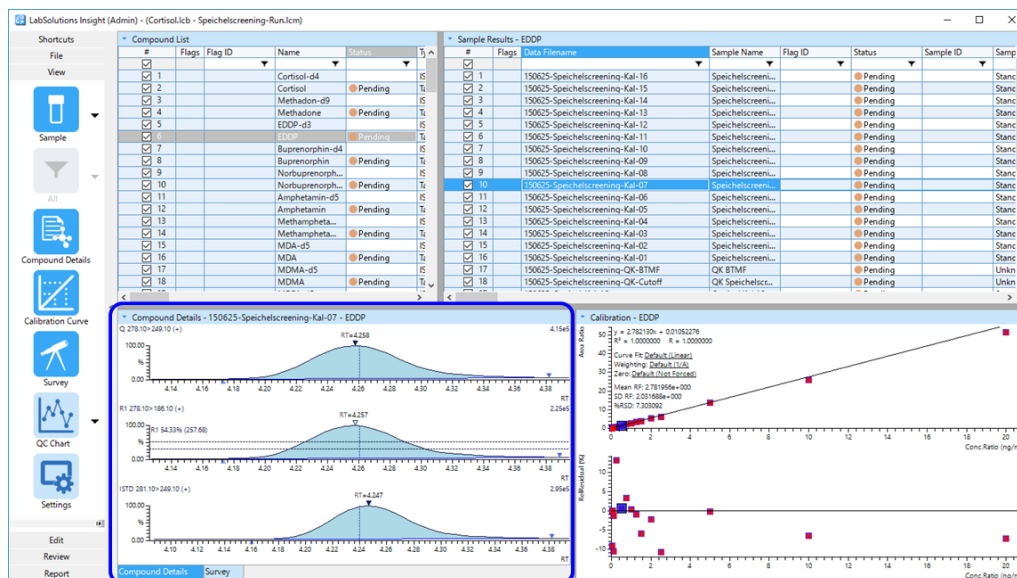
3.5.2 Layout the graph area

There are three common graphs that can be displayed. Enable the necessary graphs using the menu bar.

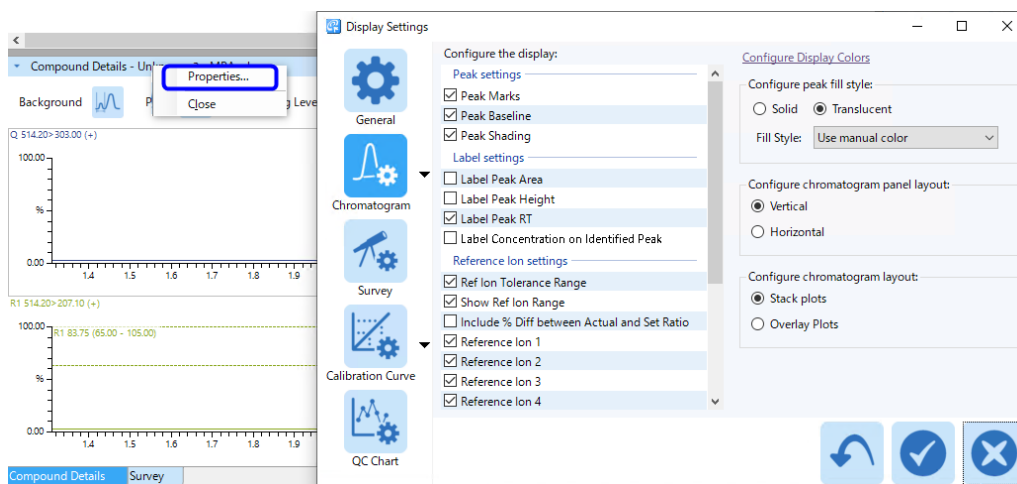


■ [Compound Details]

When [Compound Details] is enabled, the chromatogram for the selected compound is displayed.

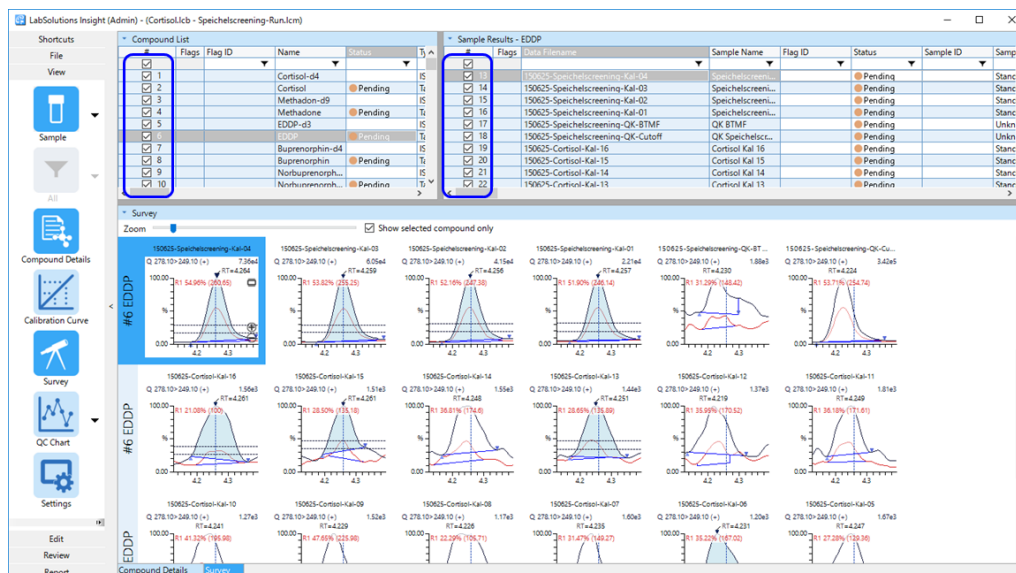


When displaying the reference ion chromatograms, options are available to either overlay them on the target chromatograms or to show them stacked. Right-click on the [Compound Details] title bar and select [Properties] to configure the graph display settings.

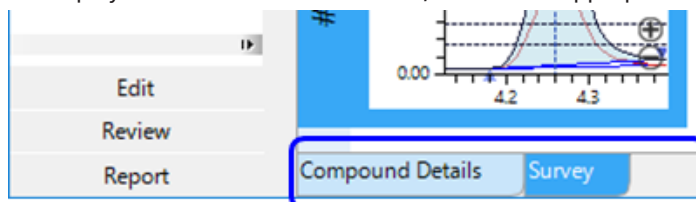


■ [Survey]

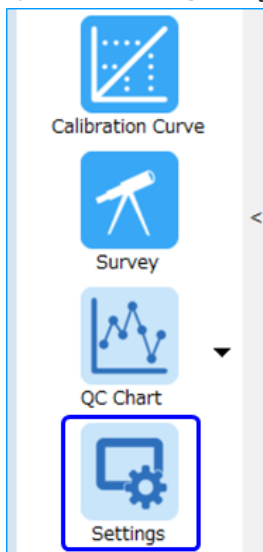
When [Survey] is enabled, chromatograms of all registered compounds in the selected data file(s) are displayed as a table. To display chromatograms in the [Survey] area, tick the checkbox for the applicable data files and compounds.



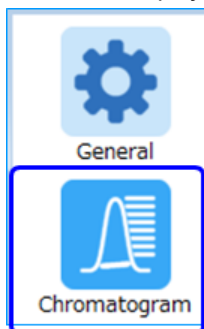
Hint Both [Compound Details] and [Survey] can be enabled at the same time. To display one in front of the other, select the appropriate tab sheet.



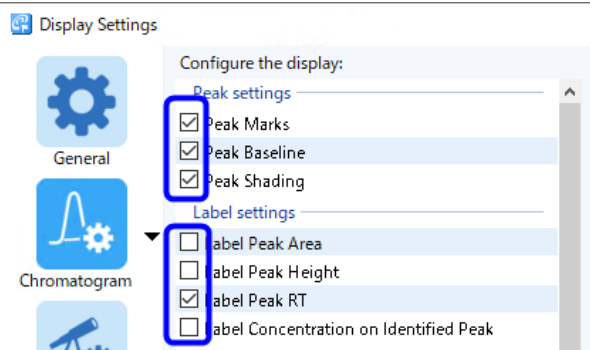
- Hint** Annotations for the chromatogram peaks can be customized.
- 1) Click on the [Settings] button.



- 2) In the [Display Settings] window, click on [Chromatogram].



- 3) At [Peak settings] or [Label settings], tick the checkbox(es) for item(s) to display.



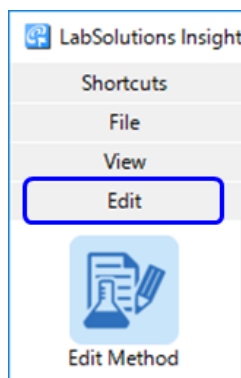
- 4) Click on the  button.

3.6 Apply Flags

Specify the conditions to set flags on the analysis results. Flags can be used to determine if acquired quantitative results exceed threshold values, or for quality control.

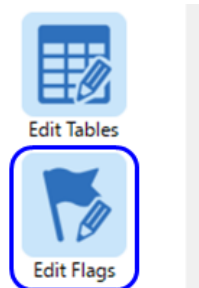
1

From the menu bar, click on the [Edit] menu band.

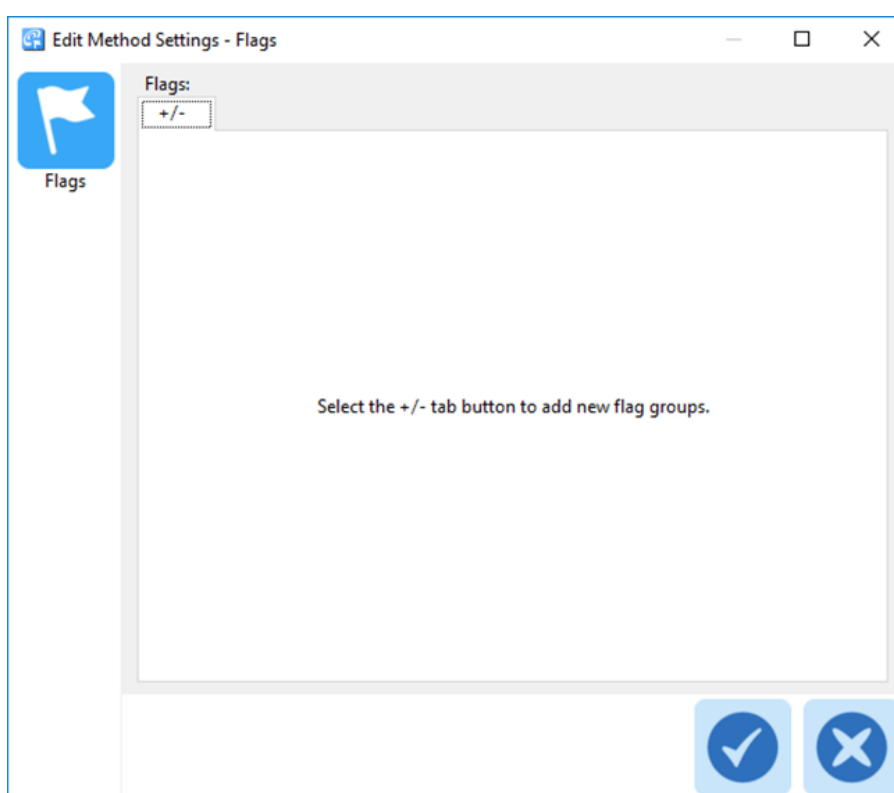
**3**

2

On the menu bar, click the [Edit Flags] icon.

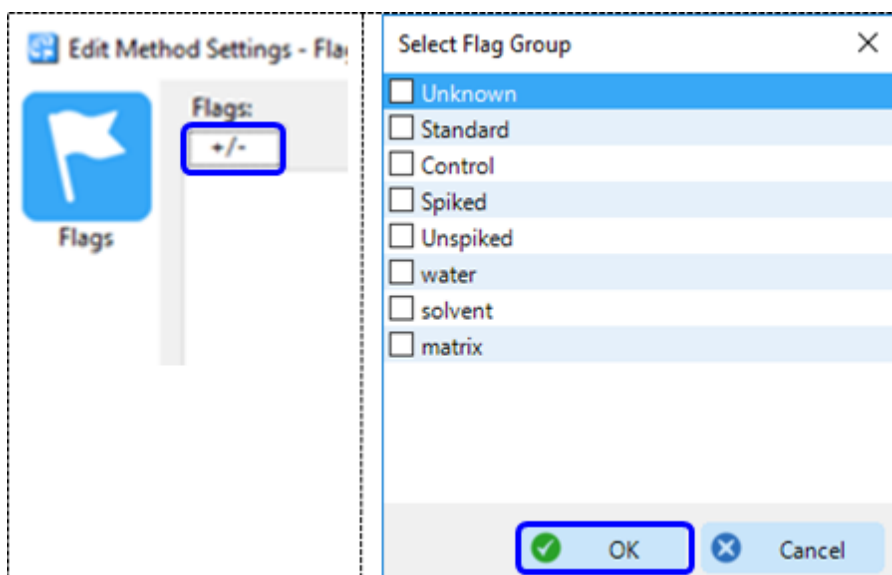


The [Edit Method Settings - Flags] sub-window is displayed.



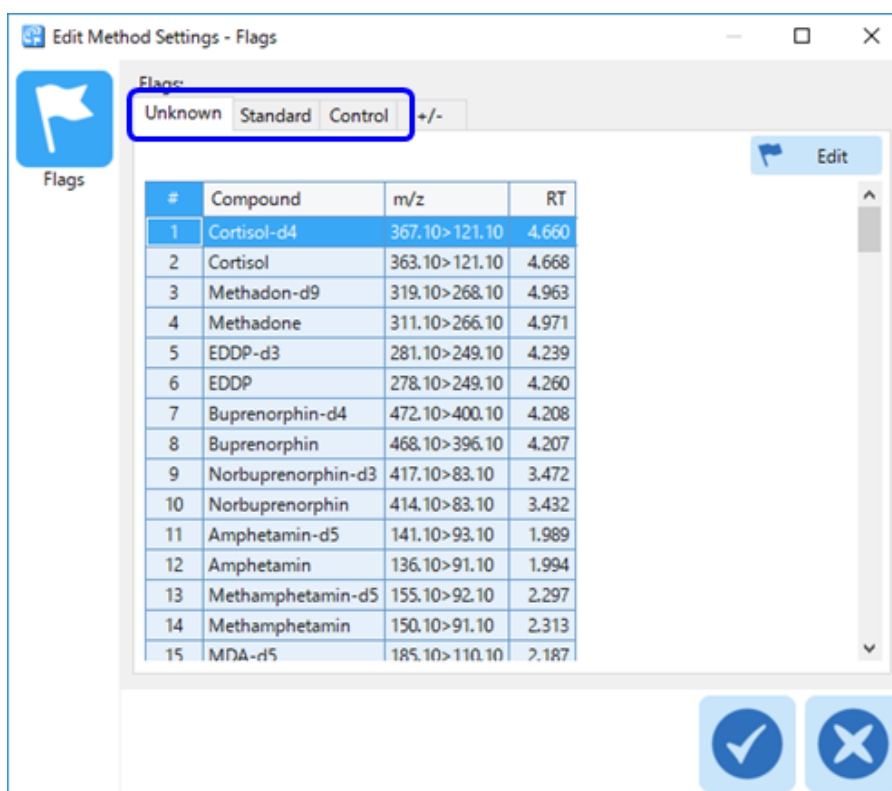
3

Click on the [+/-] tab, tick the checkbox(es) for flag group(s), and click [OK]. For available flag groups, please see ["4.1 Configurable Flag Types"](#).



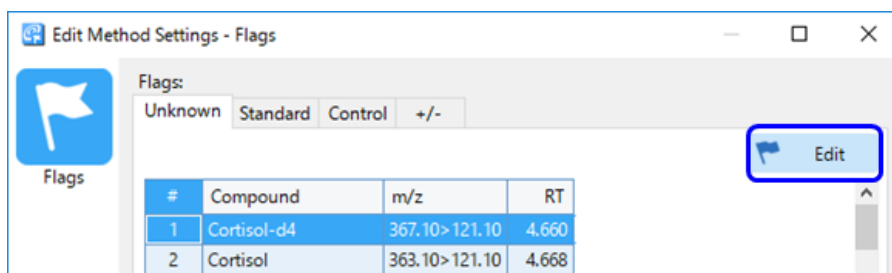
4

Click on the tab to select a flag group to configure.



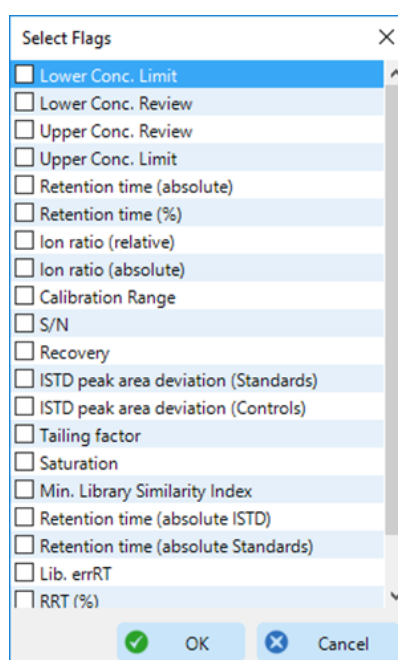
5

Click on the [Edit] button to select the items to configure.



6

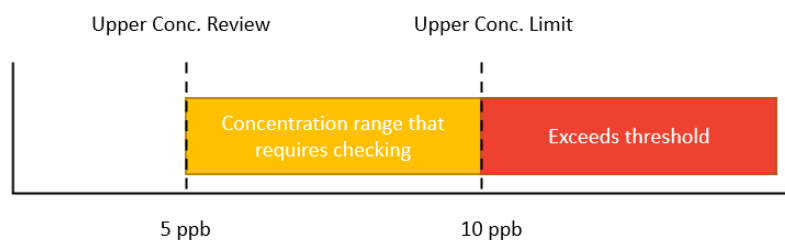
The [Select Flags] sub-window is displayed. Tick the checkbox(es) for item(s) to set thresholds for and click [OK].



7

Enter the threshold values for flagging.

Example: Set the concentration thresholds as shown in the figure below.



Edit Method Settings - Flags

Flags: Unknown Standard Control +/-

Edit Result

#	Compound	m/z	RT	Upper Conc. Review	Upper Conc. Limit
1	Dichlorvos	237.95>109.00	1.156	5	10
2	Mevinphos, mixture of cis and trans isomers	225.10>127.10	1.183	5	10
3	Prohydrojasmon	255.10>135.20	1.373	5	10
4	Flufenacet	364.15>152.20	1.518	5	10
5	Dicrotophos	237.80>112.20	1.555	5	10
6	Phosphamidon	300.00>174.00	1.579	5	10
7	Cycloate	216.25>83.10	1.803	5	10
8	Isoxaflutole	360.15>251.15	1.813	5	10
9	Diallate	270.15>86.25	1.830	5	10
10	Fluazinam_neg	462.80>416.10	1.912	5	10
11	Phoxim	299.00>96.90	2.050	5	10
12	Tridemorph	298.50>43.10	2.051	5	10
13	Spiroxamine	297.90>144.10	2.061	5	10
14	Pirimicarb	239.25>72.10	2.097	5	10
15	Isouron	212.20>72.00	2.106	5	10
16	Thiofanox sulfone	267.90>251.30	2.110	5	10
17	Aldicarb	208.20>116.10	2.194	5	10
18	Cyflufenamid	413.20>295.15	2.229	5	10
19	Triadimefon	294.00>69.00	2.236	5	10
20	Lactofen	479.20>344.05	2.306	5	10

Flags icon Score Weights icon

Confirm Cancel

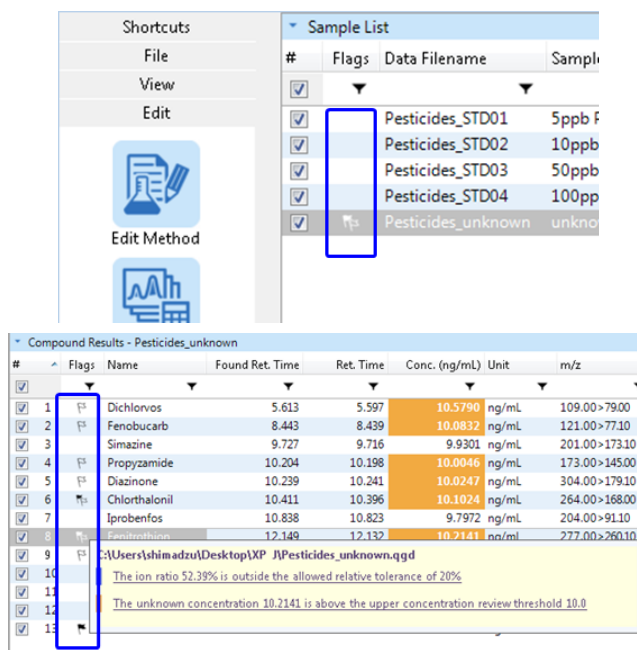
8

Click the  button to confirm the settings.

3

3.7 Review Results

After flagging, the  mark is displayed for data that meet the flagging conditions. In addition, items that meet the flagging conditions are colored depending on the flags that have been set. Click the flag icon to view the flagging details.



The screenshot shows the LabSolutions Insight LCMS CL interface. On the left is a menu bar with options: Shortcuts, File, View, Edit, and Edit Method. The main window is divided into two panes. The top pane, titled 'Sample List', contains a table with columns: #, Flags, Data Filename, and Sample. The bottom pane, titled 'Compound Results - Pesticides_unknown', contains a table with columns: #, Flags, Name, Found Ret. Time, Ret. Time, Conc. (ng/mL), Unit, and m/z. A blue box highlights the flag icon in the Flags column of the Compound Results table.

#	Flags	Name	Found Ret. Time	Ret. Time	Conc. (ng/mL)	Unit	m/z
1		Dichlorvos	5.613	5.597	10.5790	ng/mL	109.00>79.00
2		Fenobucarb	8.443	8.439	10.0832	ng/mL	121.00>77.10
3		Simazine	9.727	9.716	9.9301	ng/mL	201.00>173.10
4		Propyzamide	10.204	10.198	10.0046	ng/mL	173.00>145.00
5		Diazinone	10.239	10.241	10.0247	ng/mL	304.00>179.10
6		Chlorthalonil	10.411	10.396	10.1024	ng/mL	264.00>168.00
7		Iprobenfos	10.838	10.823	9.7972	ng/mL	204.00>91.10
8		Unknown	12.149	12.132	10.2141	ng/mL	277.00>260.10

3.7.1 Show flagged compounds only

Only the results that need to be reviewed can be displayed by filtering on the flags.

1

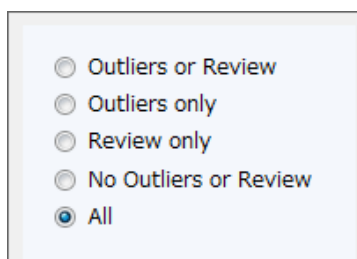
On the menu bar, click the [Flags filter] icon.



2

The setting sub-window shown below is displayed.

For concentration only, a flag can be set in two levels (Outliers and Review). Items other than concentration are flagged for Outliers only.



The screenshot shows a sub-window for flagging settings. It contains five radio button options:

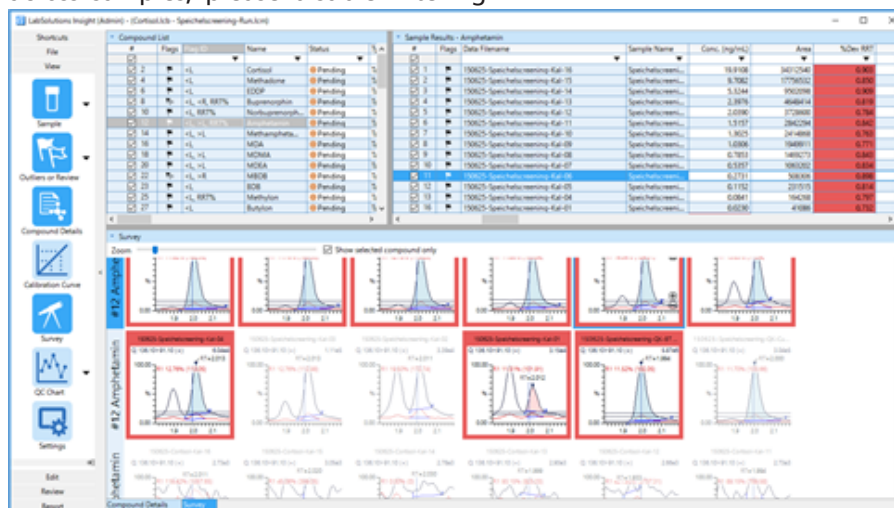
- ☐ Outliers or Review
- ☐ Outliers only
- ☐ Review only
- ☐ No Outliers or Review
- ☒ All

3

Only items that meet the filtering conditions are displayed.

Sample Results - Amphetamine						
#	Flags	Data Filename	Sample Name	Conc. (ng/mL)	Area	%Dev RRT
1		150625-Speichelscreening-Kal-16	Speichelscreen...	19.9108	34312540	0.903
2		150625-Speichelscreening-Kal-13	Speichelscreen...	9.7082	17756332	0.890
3		150625-Speichelscreening-Kal-14	Speichelscreen...	5.1744	9500098	0.909
4		150625-Speichelscreening-Kal-12	Speichelscreen...	2.3975	4648414	0.879
5		150625-Speichelscreening-Kal-12	Speichelscreen...	2.0590	3728900	0.784
6		150625-Speichelscreening-Kal-11	Speichelscreen...	1.5157	2842294	0.842
7		150625-Speichelscreening-Kal-10	Speichelscreen...	1.3025	2414868	0.763
8		150625-Speichelscreening-Kal-09	Speichelscreen...	1.0305	1949911	0.771
9		150625-Speichelscreening-Kal-08	Speichelscreen...	0.7853	1460273	0.848
10		150625-Speichelscreening-Kal-07	Speichelscreen...	0.5357	1063202	0.834
11		150625-Speichelscreening-Kal-05	Speichelscreen...	0.2731	508306	0.898
12		150625-Speichelscreening-Kal-05	Speichelscreen...	0.1152	231515	0.614
13		150625-Speichelscreening-Kal-04	Speichelscreen...	0.0841	164268	0.797
16		150625-Speichelscreening-Kal-01	Speichelscreen...	0.0790	41886	0.732
17		150625-Speichelscreening-QK-BTME	QK BTME	11.8531	21830822	0.857
25		150625-Cortisol-QK-L2	QK Cortisol L2	-----	-----	-----
36		150625-Cortisol-QK-L1	QK Cortisol L1	-----	-----	-----

- NOTE** • When filtering is applied [Survey] “hides” the chromatograms that have been filtered out. If chromatograms for flagged compounds need to be examined across samples, please disable filtering.



- When filtering is applied, Reports also exhibits the same behavior as Survey. Please see Section "3.14 Print Results" for details on Reports.

3

3.8 Edit Results

Identified peaks can be edited by manual identification and manual peak integration. The calibration curve type can also be changed and data files can be replaced with different files.

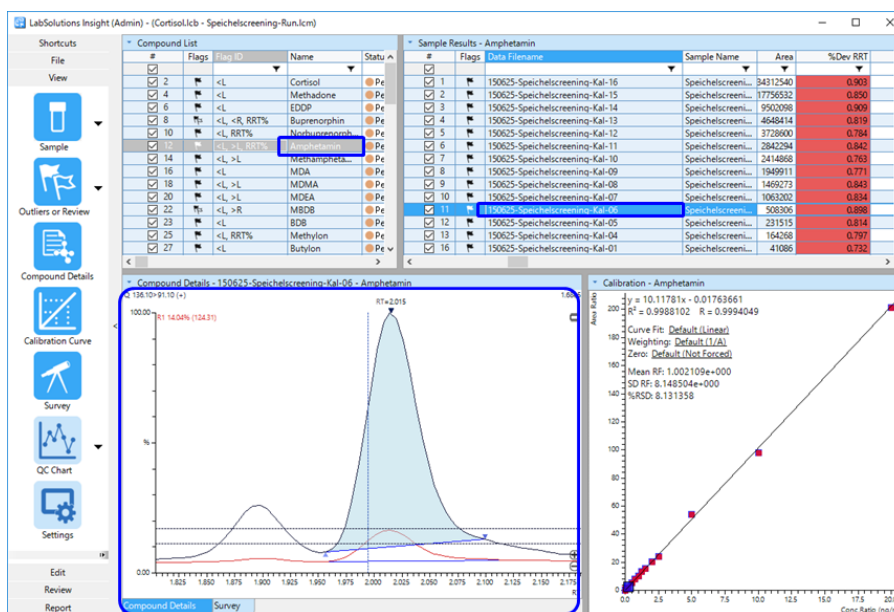
Results can be edited in [Compound Details] or [Survey] (See Section "3.5.2 Layout the graph area").

3.8.1 Edit identification results

Follow the procedures described below to edit automatically integrated and identified peaks. The examples show the procedure in [Compound Details] for clarity, although the same operations can be performed in [Survey].

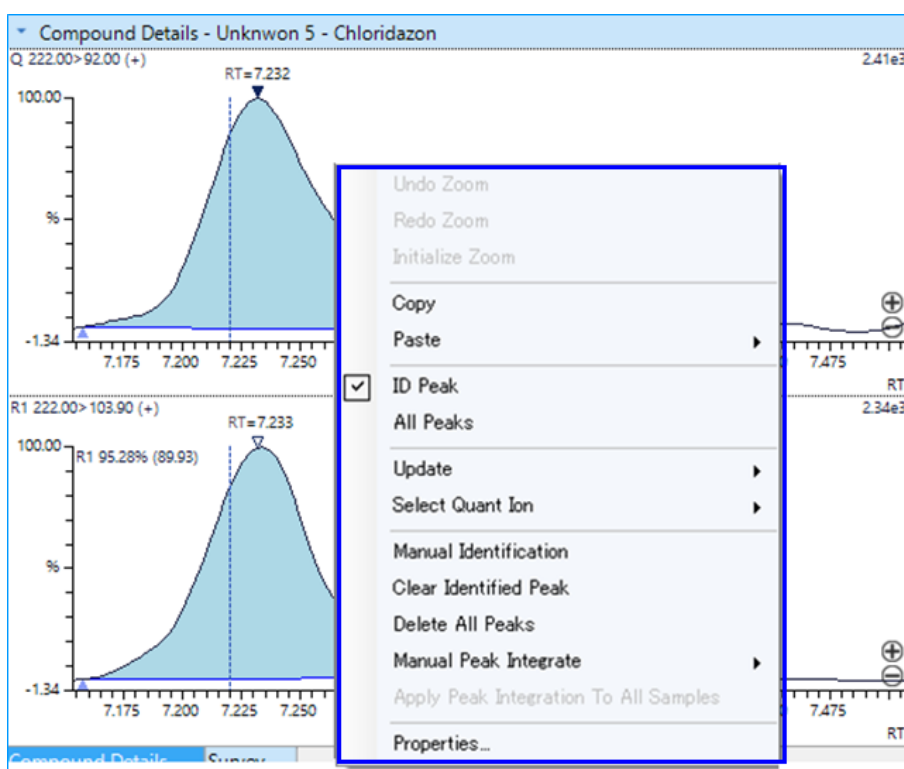
1

Select the compound to edit from the chromatogram or table. In the case of using Survey, directly select the chromatogram to be edited.



2

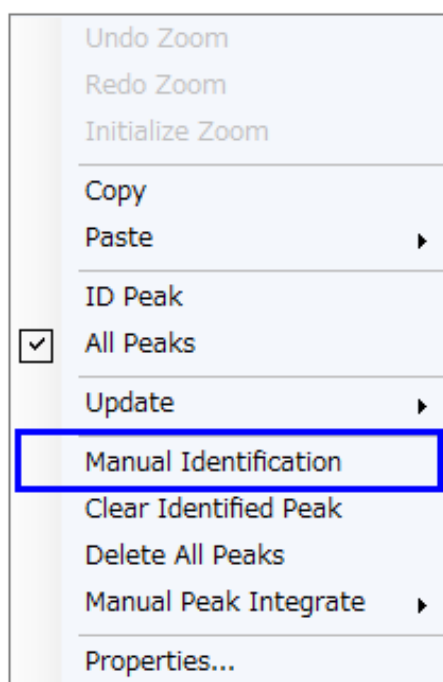
Perform manual identification or manual peak integration.
Right-click in the chromatogram view.

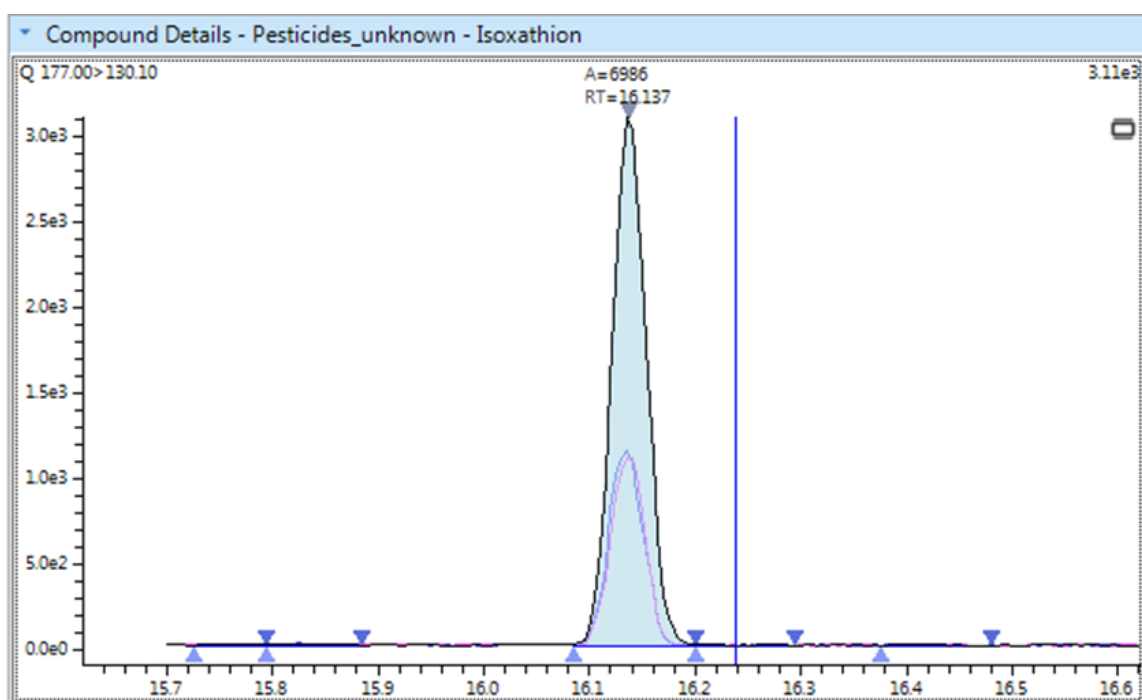


3

■ Manual identification procedures

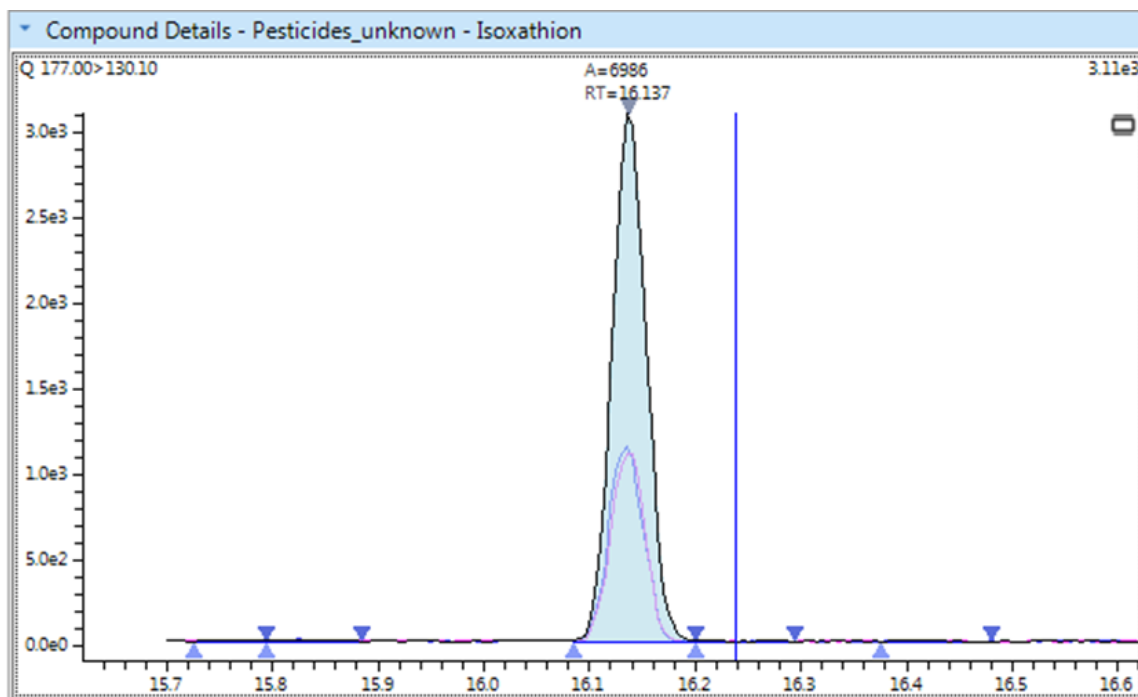
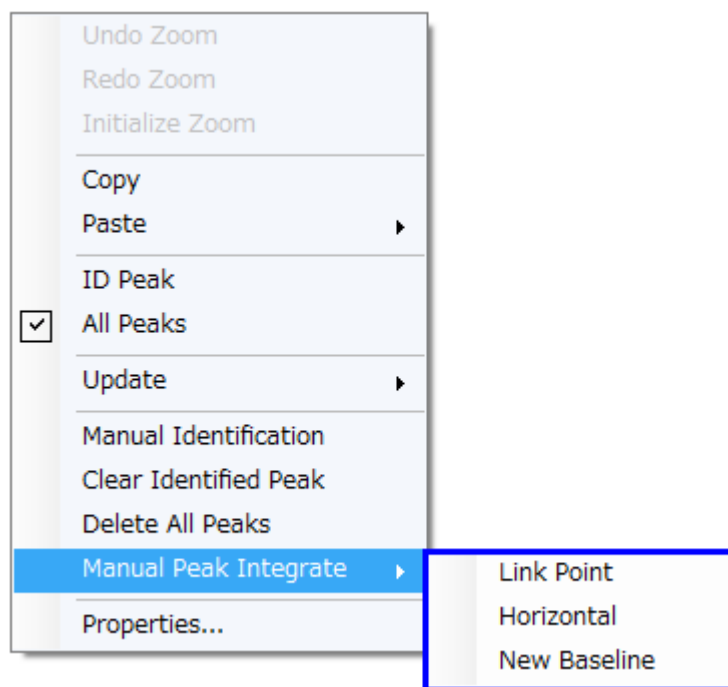
Click on the [Manual Identification] menu item. Position the blue line onto the peak to be identified.





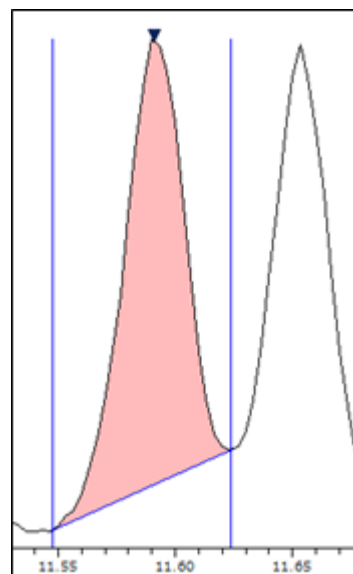
■ Manual peak integration procedures

Click on the [Manual Peak Integrate] menu item. Move the blue line with the left mouse button pressed. The retention time at which the button is pressed is the starting point of the peak. The retention time at which the button is released is the end point of the peak.

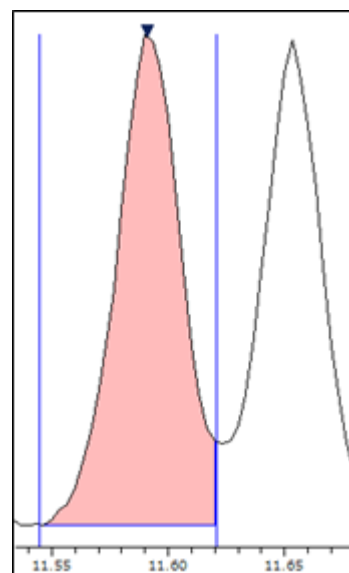


[Link Point] :

A baseline connecting two points on the peak can be drawn. Click on the [Link Point] menu item. Select two points on the peak using two blue lines.

**[Horizontal]:**

A baseline parallel to the horizontal axis connecting two points can be drawn. Click on the [Horizontal] menu item. Select two points on the peak using two blue lines in the same way as [Link Point].

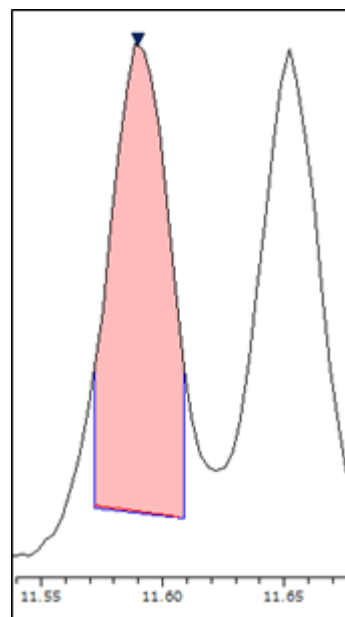


[New Baseline]:

A baseline connecting two arbitrary points. Click on the [New Baseline] menu item. Select two arbitrary points on the peak.

 **Hint** Manual integration is possible using the shortcuts below.

Link Point	Shift key + Right mouse button drag
Horizontal	Ctrl key + Right mouse button drag
Manual Identification	Shift key + Ctrl key + Right click
Clear Identified Peak	Shift key + Ctrl key + Right double click



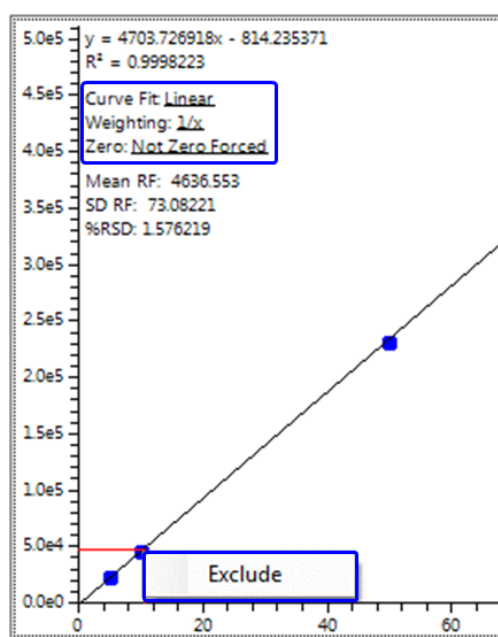
3

3.8.2 Edit calibration curve information

Follow the procedures described below to edit the calibration curve information.

1

The calibration curve information that can be changed is underlined. Click on the underlined items to change them. Right-click on a calibration point to exclude it from the calibration curve.



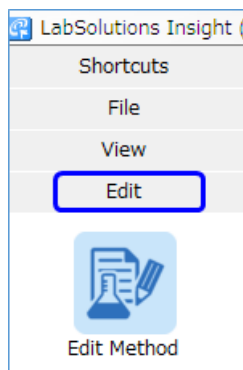
 **Hint** It is possible to edit the Curve Fit type, Weighting, Zero through and whether to enable or disable calibration points.

3.8.3 Edit tables

Follow the procedures below to change the sample types and calibration levels. This function can be used in conjunction with the Import function to swap calibration data in and out of a data set. Please see Section "[3.3 Open Batch \(Processing Mode\)](#)" for details on adding data files to the current set.

1

From the menu bar, click on the [Edit] menu band.

**2**

Click on the [Edit Tables] button to enter the edit tables mode. The [Edit Tables] button turns dark blue to indicate the mode is activated.



3

In either [Sample List] or [Sample Results], select a sample to edit. Right click in the Sample Type column to show a context menu. Select [Edit] to reveal a list of sample types to select from. The drop down list can be displayed by double clicking in the [Sample Type] field as well. Select the appropriate sample type.

Sample List							Compound	
#	Flags	Data Filename	Sample Name	Flag ID	Status	Sample Type	Cal Poir	Flags
1		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
2		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
3		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
4		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
5		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
6		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
7		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
8		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
9		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
10		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
11		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
12		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
13		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
14		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
15		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
16		150625-Speiche...	Speichelscreeni...	RRT%	Pending	Standard		
17		150625-Speiche...	QK BTMF	<L, >L, >R	Pending	Unknow		
18		150625-Speiche...	QK Speichelscr...	<L, <R	Pending	Unknow		
31		150625-Cortisol...	Cortisol Kal 4	RRT%	Pending	Standard		
35		150625-Cortisol...	QK Cortisol L2	<L, <R	Pending	Unknow		
36		150625-Cortisol...	QK Cortisol L1	<L, <R	Pending	Unknow		

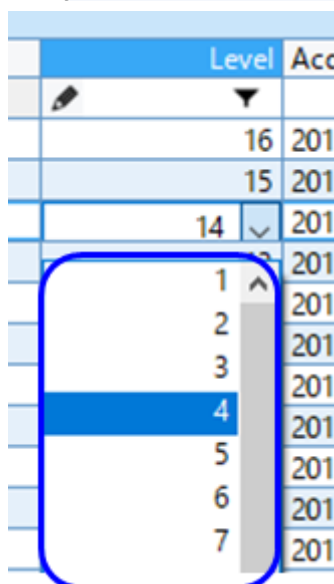
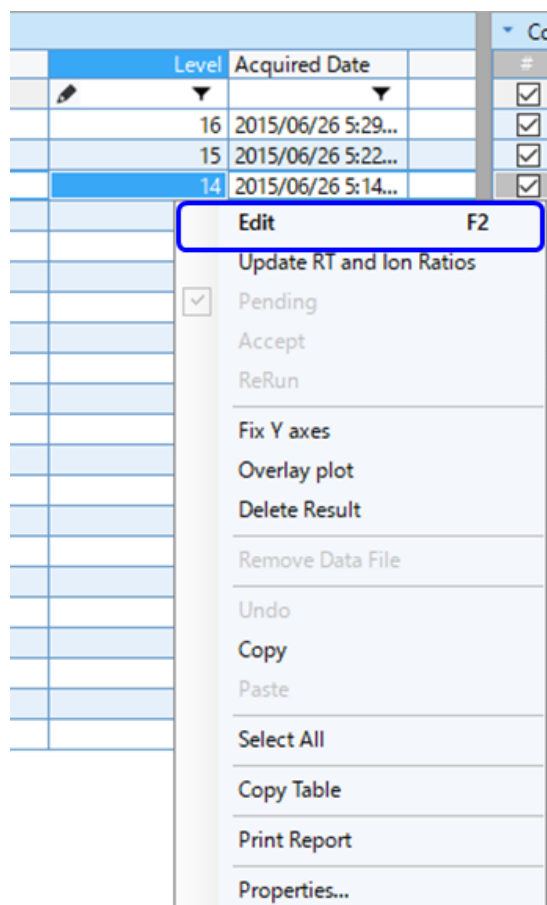
Edit F2
Update RT and Ion Ratios
Pending
Accept
ReRun
Fix Y axes
Overlay plot
Delete Result
Remove Data File
Undo
Copy
Paste
Select All
Copy Table
Print Report
Properties...

Data Filename	Sample Name	Sample ID	Sample Type
2012_09_05...	2012_09_05...		Standard
2012_09_05...	2012_09_05...		Standard
2012_09_05...	2012_09_05...		Standard
2012_09_05...	2012_09_05...		Standard
2012_09_05...	2012_09_05...		Unknown
2012_09_05...	2012_09_05...		Standard
2012_09_05...	2012_09_05...		Control
2012_09_05...	2012_09_05...		Unspiked
2012_09_05...	2012_09_05...		Spiked
2012_09_05...	2012_09_05...		water
2012_09_05...	2012_09_05...		solvent
2012_09_05...	2012_09_05...		matrix

3

4

Similarly, right click in the [Level] column to show a context menu. Select [Edit] to reveal a list of levels to select from. The drop down list can be displayed by double clicking in the [Level] field as well. Select the appropriate sample level.



5

Once all editing is finished, click on the [Edit Tables] button again to exit the edit tables mode. This will prompt a recalculation of the calibration curves and quantitation results.

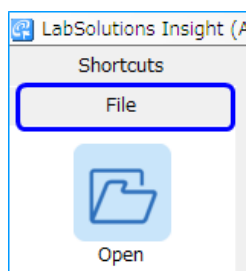
3.9 Change Method (Data Mode)

3.9.1 Apply a method file

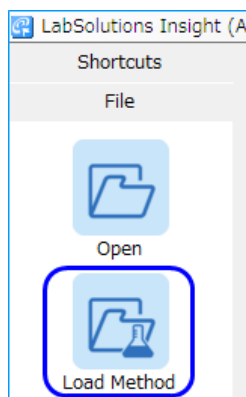
Target compounds and calibration curves can be changed by applying a method file. All open data files and the current method file will be closed. Standard samples referenced in the new method file will be shown. Other samples will need to be added manually using the Import function (see Section "3.4 Add Data Files").

1

From the menu bar, click on the [File] menu band.

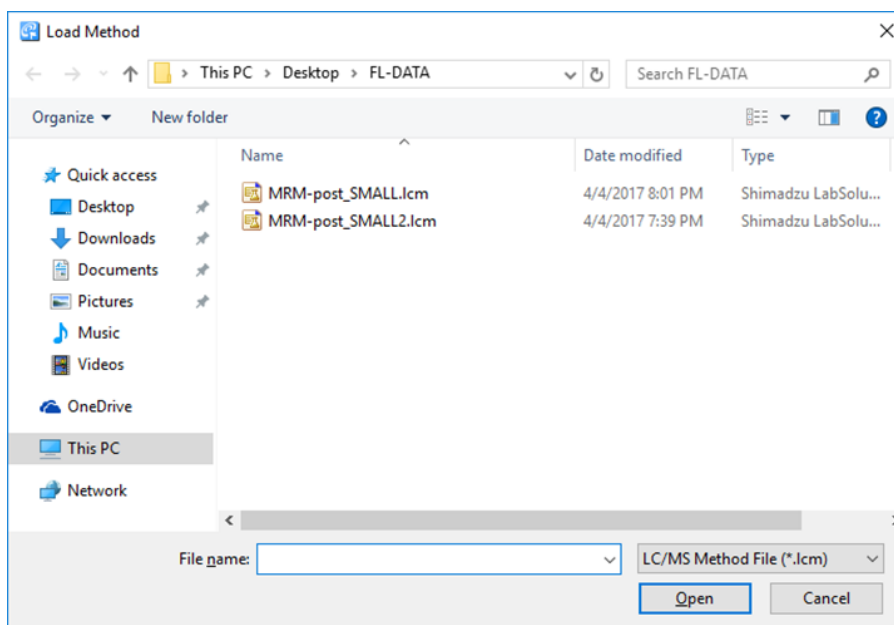
**2**

Click on the [Load Method] icon.

**3**

3

Select a method to load.
A method can be an lcm file (LabSolutions CL method file).

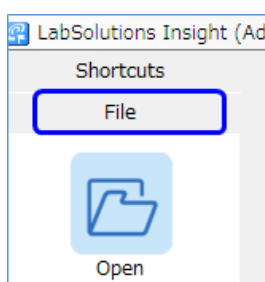


3.9.2 Apply flagging thresholds

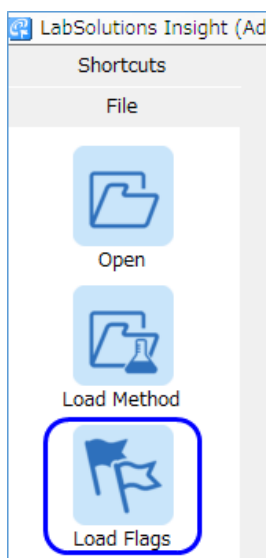
It is possible to apply flagging to the current batch by opening a DAMLP file containing flagging thresholds.

1

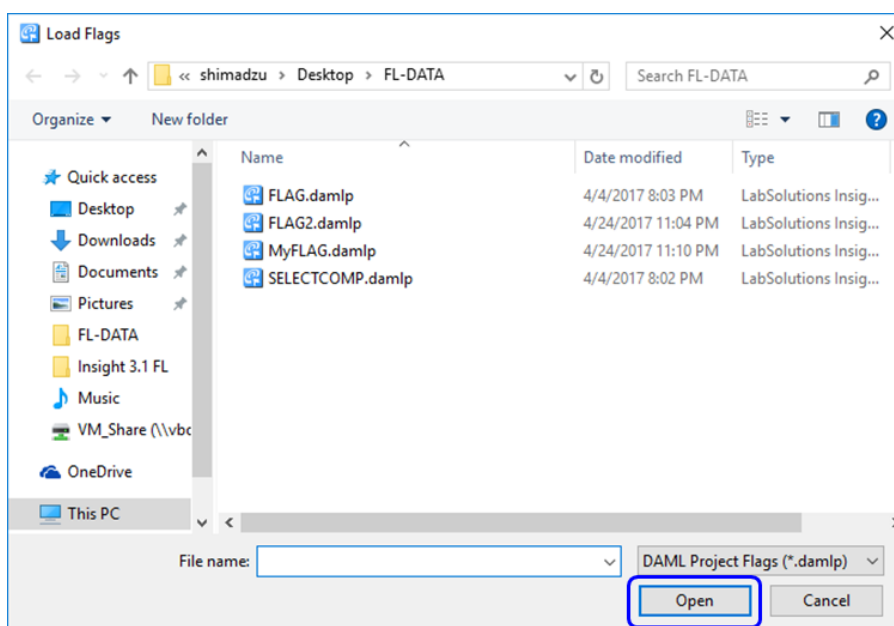
From the menu bar, click on the [File] menu band.



2 Click on the [Load Flags] icon.



3 Select a DAMLP file containing flagging thresholds and click on the [Open] button.



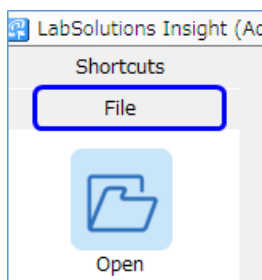
3.10 Change Method (Processing Mode)

3.10.1 Apply a method file

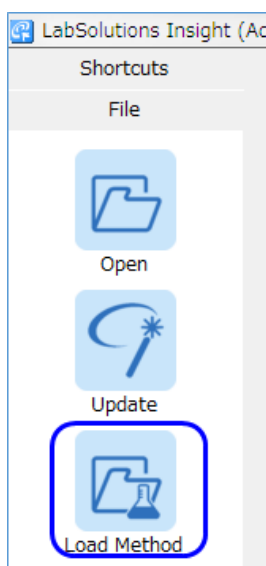
Target compounds and calibration curves can be changed by applying a method file. Note that all other method parameters including flagging thresholds and selected compounds will be replaced as well.

1

From the menu bar, click on the [File] menu band.

**2**

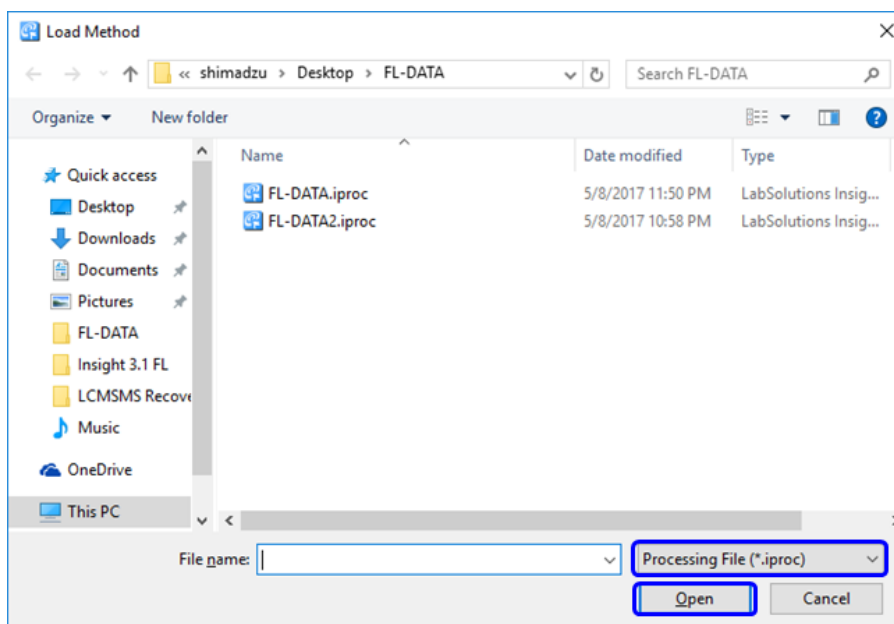
Click on the [Load Method] icon.



3

Select a method to load.

A method can be a processing file or LabSolutions CL method file (lcm file). Use the drop down list to change the type of method file to load, as necessary.



Click on [Open] to load the method.

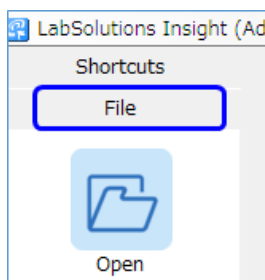
3

3.10.2 Apply flagging thresholds

It is possible to apply flagging to the current batch by opening a DAMLP file containing flagging thresholds.

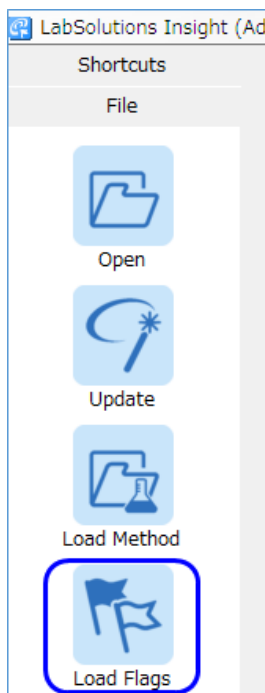
1

From the menu bar, click on the [File] menu band.



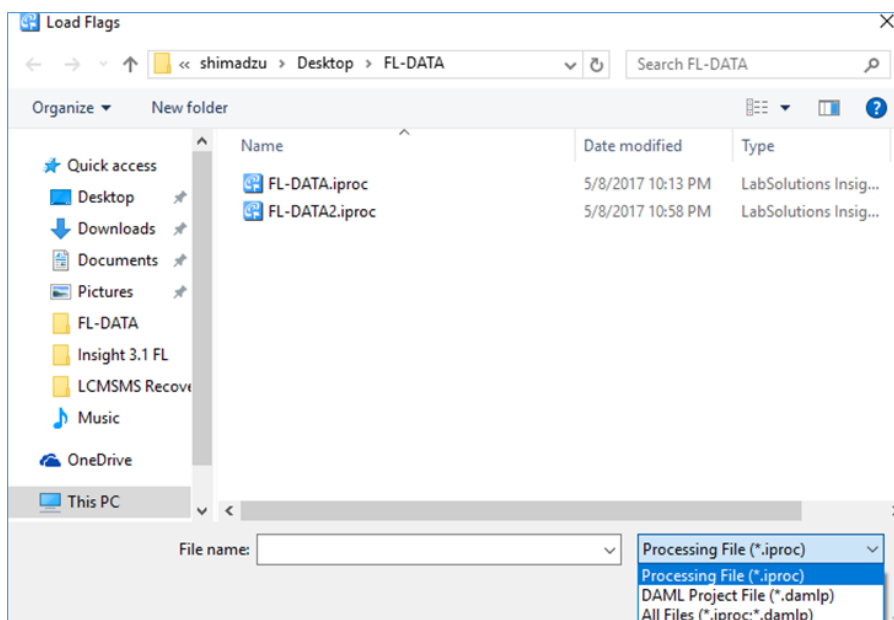
2

Click on the [Load Flags] icon.



3

Select a processing file (iproc file) or DAMLP file containing flagging thresholds and click on the [Open] button.

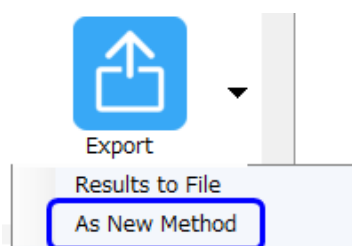


3.11 Export Methods (Processing Mode)

The current method can be exported to a LabSolutions CL method file so that edits made in Insight can be applied to the next round of acquisitions.

1

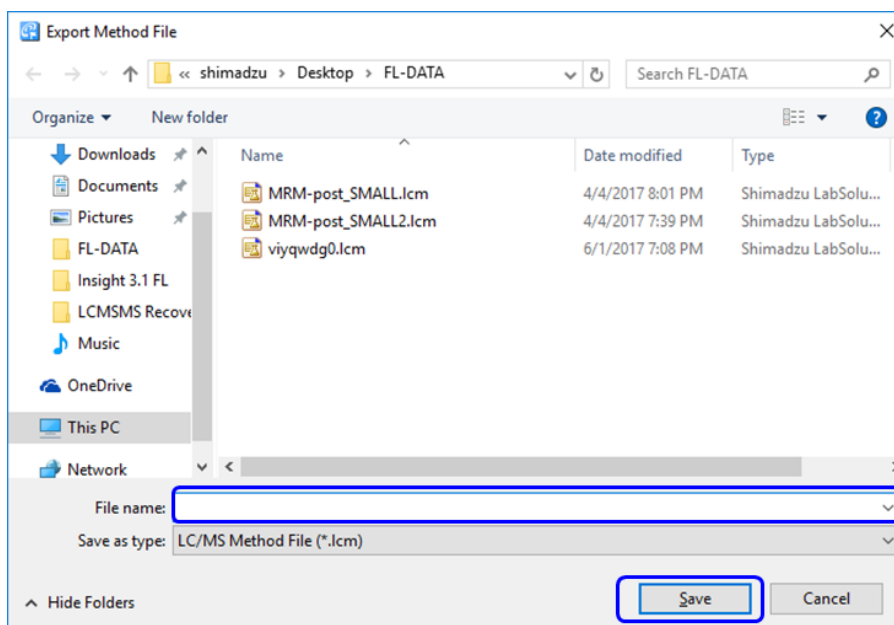
Click on the [Export] button to show a drop down menu. An additional option to export a method file is shown. Select [As New Method].



2

Enter a name for the new method and click on [Save].

Make sure to change the file type to lcm for LabSolutions CL. (The default type is iProm.)

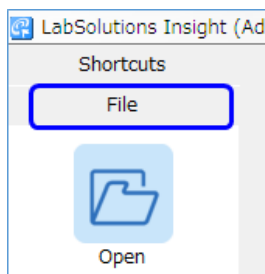


3.12 Save Results (Data Mode)

Follow the procedures described below to save analysis data.

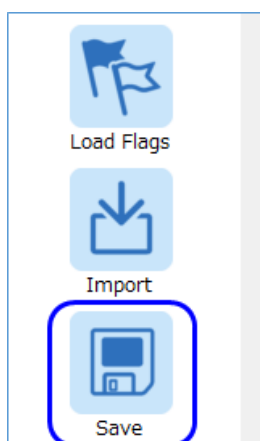
1

From the menu bar, click on the [File] menu band.



2

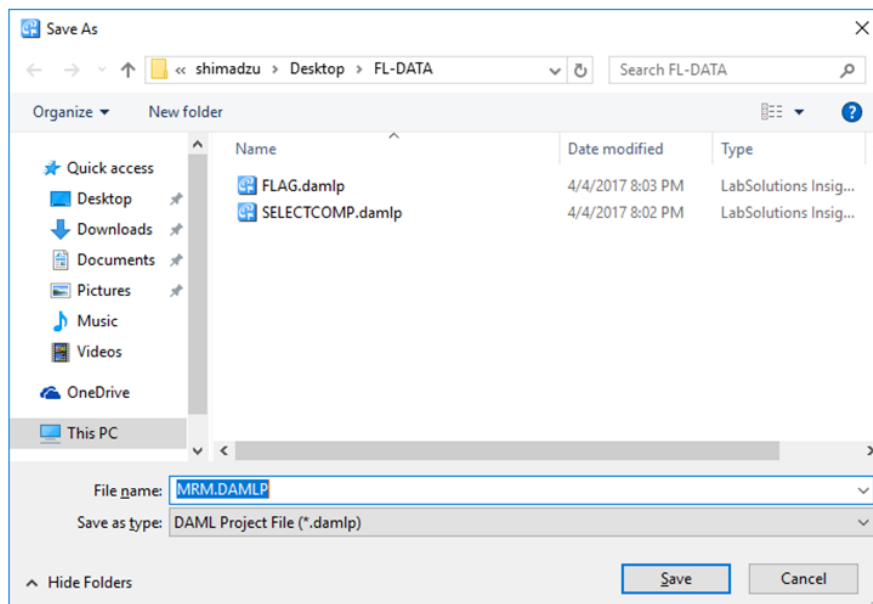
Click on the [Save] icon.



3

If the current batch was opened using a DAMLP file, the file is simply overwritten.

- NOTE**
- 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. Click on [Save] to save with the default name for the DAMLP file, or enter a new file name then click [Save].



- If the data has 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.

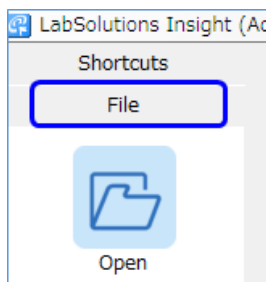
3

3.13 Save Results (Processing Mode)

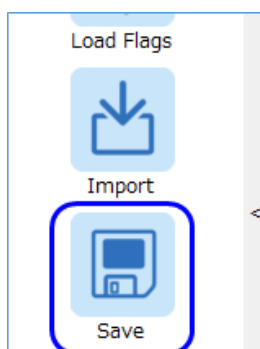
Follow the procedures described below to save analysis data.

1

From the menu bar, click on the [File] menu band.

**2**

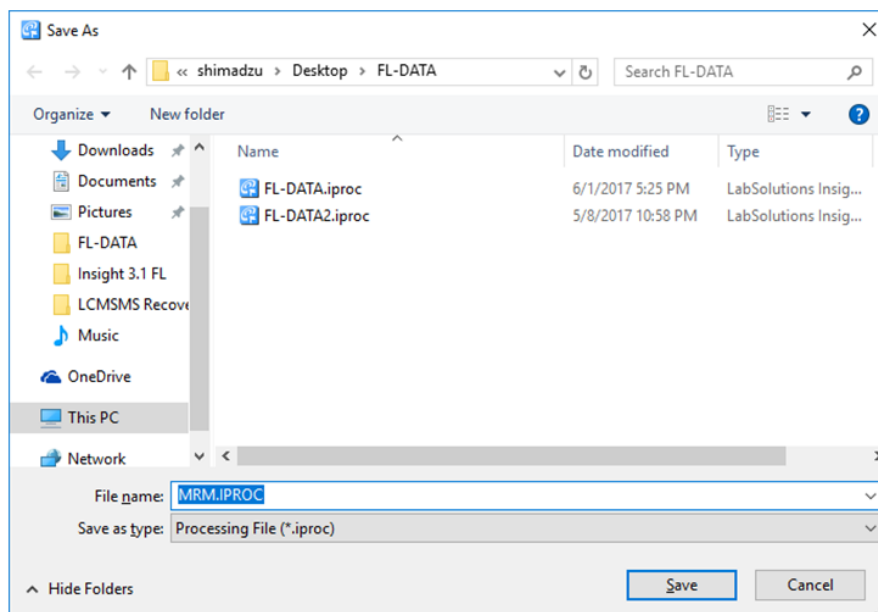
Click on the [Save] icon.



3

If the current batch was opened using a processing file, the current processing file is simply overwritten.

- NOTE**
- 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. Click on [Save] to save with the default name for the processing file, or enter a new file name then click [Save].



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

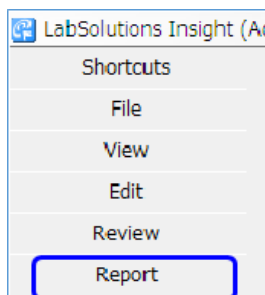
3

3.14 Print Results

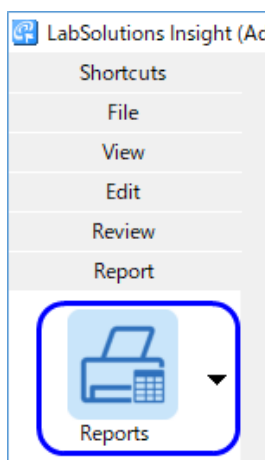
3.14.1 Print results for all samples

Follow the procedures described below to output data analysis results.

- 1 From the menu bar, click on the [Report] menu band.



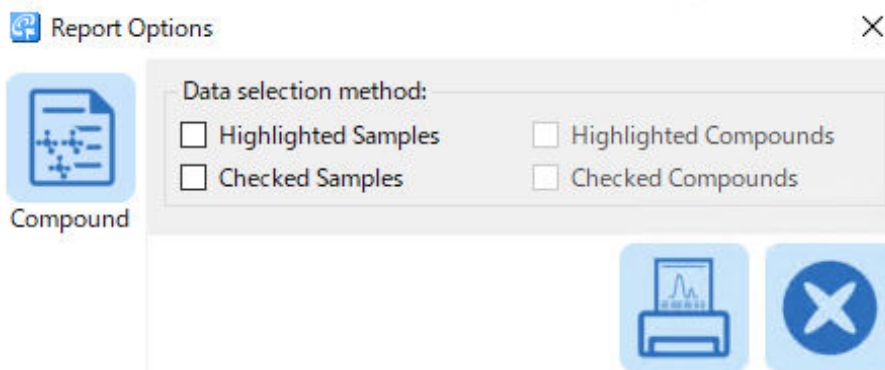
- 2 Click the [Reports] icon. The report templates set in [Report Configuration] are shown in the drop-down list. Select the report template.



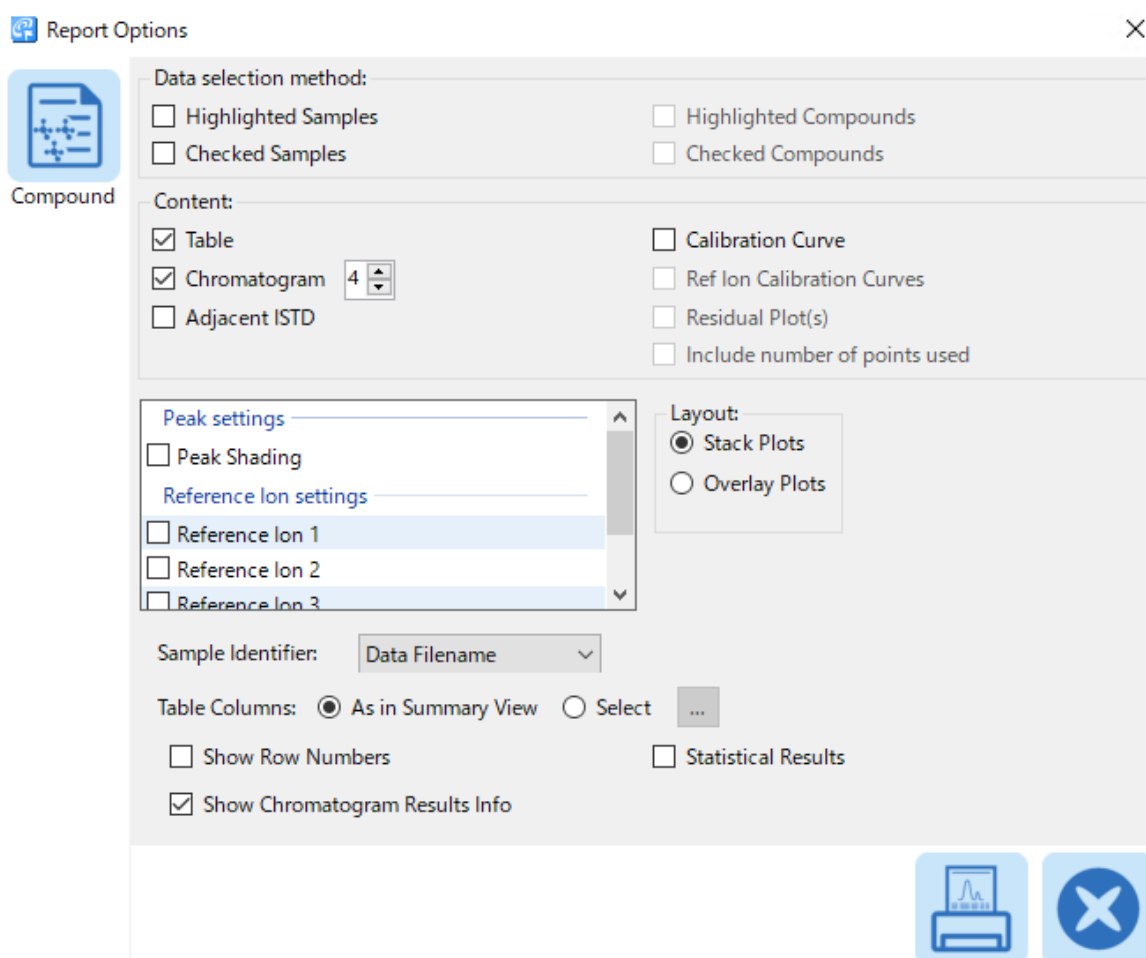
3

Configure reporting options.

When the status of the selected template is "Locked", only the sample and compound to be printed will be selected. When it is not "Locked", the detail of the report can be set in the [Report Options] dialog.



When Locked



When not Locked

The tables below list some of the items that can be configured in various templates. Further details are explained in the Report Configuration Guide.

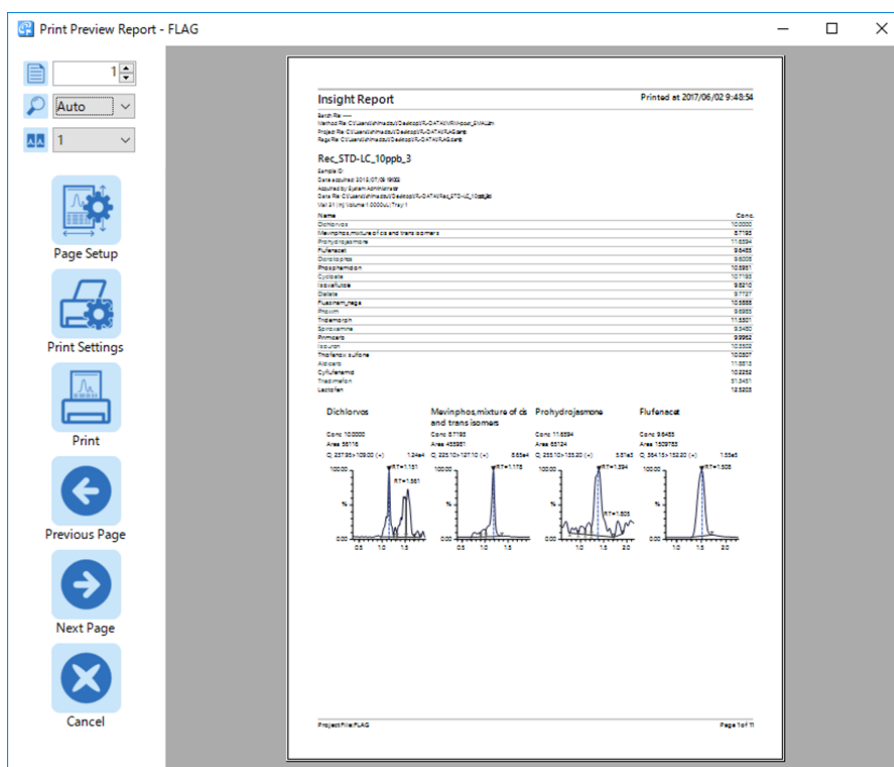
Data selection method	Print the checked samples and compounds. When no item is checked, all the samples and compounds are reported. [Highlighted] : Prints the items selected in the list. [Checked] : Prints the items checked in the list.
Content	[Table]: Print the summary table. [Chromatogram]: Print chromatograms. [Adjacent ISTD] : The chromatogram of the corresponding ISTD compound is also shown. [Calibration Curve]: Print the calibration curve. [Ref Ion Calibration Curves]: Print calibration curves for reference ions. Only available if target calibration curve is printed. [Residual Plot(s)]: Print residual plots for calibration curve(s). [Include number of points used]: Print the number of standards and controls used to build the calibration curve(s).
	Set the upper limit of the number of chromatograms or calibration curves displayed in one row. For calibration curves, this could be the hypothetical number of curves to be printed in one row in order to determine the size of the graph.
Audit Trail Logs (Processing mode only) (Batch and Comparison reports only)	Includes the audit trail log at the end of the report. All audit trail entries are printed even if filtering or data selection are applied.
Reference Ion Settings	Select reference ion(s) to use.
Sample Identifier	Select the sample title.
Layout	[Stack Plots]: Target ion(s) and reference ion(s) are displayed stacked. [Overlay Plots]: Target ion(s) and reference ion(s) are displayed overlaid.
Table options	[Same columns as summary view]: Uses the same columns as Summary View. [Select from table style]: Selecting this option pops up the table style configuration window.
Orientation	[By Compound]: Reports summary results for each reported compound. [By Sample]: Reports summary results for each reported sample. This option is only available for Batch and Comparison reports.
Individual report on each Compound	The report is printed individually on each sample or compound. This option is only available for Batch and Comparison reports.
Page Break on new compound	A new page is used for each compound or sample. This option is only available for Batch and Comparison reports.

Show Sample Details	Select this option and choose the sample details to print from a list.
Show Chromatogram Results Info	Show peak integration and quantitation results information for each chromatogram.

Click on the  button.



The report print preview is displayed. Click on the  (Print) button to start printing.



3.14.2 Print result for selected sample (Data Mode)

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

In order to use this function, LabSolutions CL must be installed.

Folder: C:\GCMsolution\SampleData

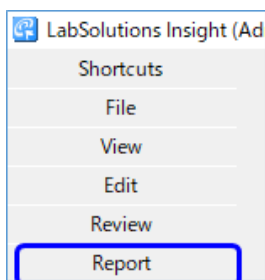
	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Report Output	Report File
1	5ppb Pesticides	STD-0001	1:Standard	n Curve.qgm	Pesticides STD001.qgd	1	☐ Print	
2	10ppb Pesticides	STD-0002	1:Standard	n Curve.qgm	Pesticides STD002.qgd	2	☐ Print	
3	50ppb Pesticides	STD-0003	1:Standard	n Curve.qgm	Pesticides STD003.qgd	3	☐ Print	
4	100ppb Pesticides	STD-0004	1:Standard	n Curve.qgm	Pesticides STD004.qgd	4	☐ Print	
5	unknown Pesticides	UNK-0005	0:Unknown	n Curve.qgm	Pesticides_unknown.qgd	1	☐ Print	pest0GR

1

Save results. (See Section "3.12 Save Results (Data Mode)".)

2

From the menu bar, click on the [Report] menu band.



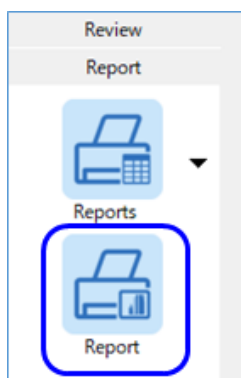
3

Select a data file to be printed.

Sample List			
#	Flags	Data Filename	Sample Name
☒			
☒ 1		150625-Speiche...	Speichelscreeni...
☒ 2		150625-Speiche...	Speichelscreeni...
☒ 3		150625-Speiche...	Speichelscreeni...
☒ 4		150625-Speiche	Speichelscreeni

4

Click on the [Report] icon to start printing based on the report format specified in the batch file at the time of sample acquisition.



NOTE The [Report] icon cannot be used if a report format file is not specified in the batch table at the time of sample acquisition.

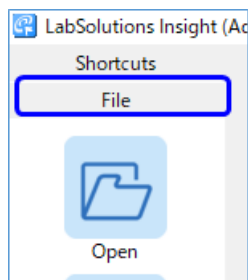
3

3.15 Close Batch

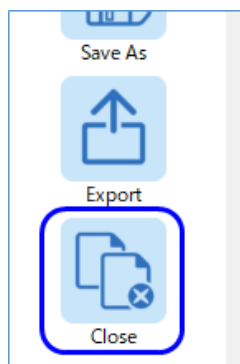
The current batch can be closed at any time.

1

From the menu bar, click on the [File] menu band.

**2**

Click on the [Close] button. If there are any edited data or method files, you will be prompted to save them.



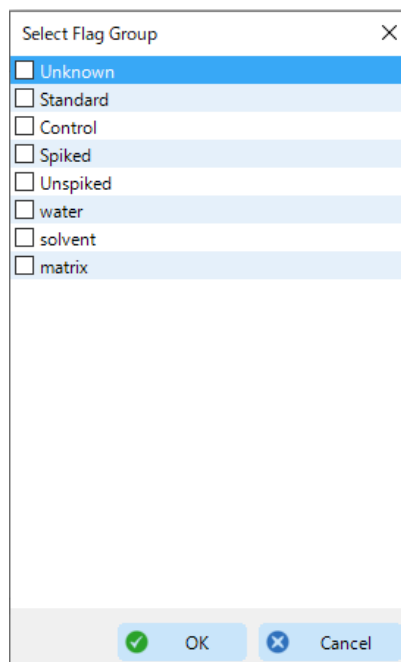
In Data mode, if the batch was not opened as a DAMLP file, you will be prompted on whether to save it as a DAMLP file.

Similarly, in Processing mode, if the batch was not opened using a processing file, you will be prompted on whether to save it as a processing file.

4 Appendix

4.1 Configurable Flag Types

In LabSolutions Insight LCMS CL, the eight flag groups listed below can be used by default.



Flag Group	Description
Unknown	Setting for unknown samples
Standard	Setting for standard samples
Control	Setting for control samples
Spiked	Setting for spiked samples
Unspiked	Setting for unspiked samples
water	Flag for preset blank
solvent	Flag for preset blank
matrix	Flag for preset blank

Tick the checkbox(es) for the flag group(s) to use. Click on [Edit] to add or delete flags. Flags that can be set vary according to the flag group as shown in the table below. Flags with "✓" mark are available for each flag group.

Flags	Unknown	Standard	Control	Spiked	Unspiked	Blank
Lower Conc. Limit	✓					
Lower Conc. Review	✓					
Upper Conc. Review	✓					
Upper Conc. Limit	✓					
RT Diff (absolute)	✓	✓	✓	✓	✓	✓
RT Diff (%)	✓	✓	✓	✓	✓	✓
Retention time (absolute)	✓	✓	✓	✓	✓	✓
Retention time (%)	✓	✓	✓	✓	✓	✓
Ion ratio (relative)	✓	✓	✓	✓	✓	
Ion ratio (absolute)	✓	✓	✓	✓	✓	
Calibration Range	✓					
R ²		✓				
%Difference		✓	✓	✓		
Accuracy		✓	✓	✓		
%RSD conc.		✓	✓			
%RSD area		✓	✓			
Blank concentration						✓
S/N	✓	✓	✓	✓	✓	✓
Recovery	✓	✓	✓	✓	✓	✓
ISTD peak area deviation (Standards)	✓		✓	✓	✓	✓
ISTD peak area deviation (Control)	✓	✓		✓	✓	✓
Tailing factor	✓	✓	✓	✓	✓	✓
Saturation	✓	✓	✓	✓	✓	✓
Retention time (absolute ISTD)	✓	✓	✓	✓	✓	✓
Retention time (absolute Standards)	✓	✓	✓	✓	✓	✓
RRT (%)	✓	✓	✓	✓	✓	✓
RRT (absolute)	✓	✓	✓	✓	✓	✓
Min. Similarity Index	✓					
RF Deviation		✓				
Asymmetry	✓	✓	✓	✓	✓	✓
Confidence	✓	✓	✓	✓	✓	✓
Mass Error (mDa)	✓	✓	✓	✓	✓	✓

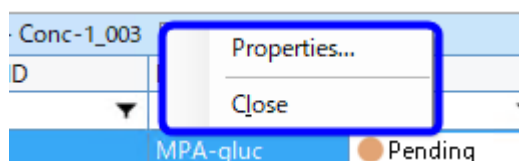
Flags	Unknown	Standard	Control	Spiked	Unspiked	Blank
Mass Error (ppm)	✓	✓	✓	✓	✓	✓
Mass Error Criteria	✓	✓	✓	✓	✓	✓

4.2 Table Column Settings

In LabSolutions Insight LCMS CL, table columns can be added, deleted, and re-ordered.

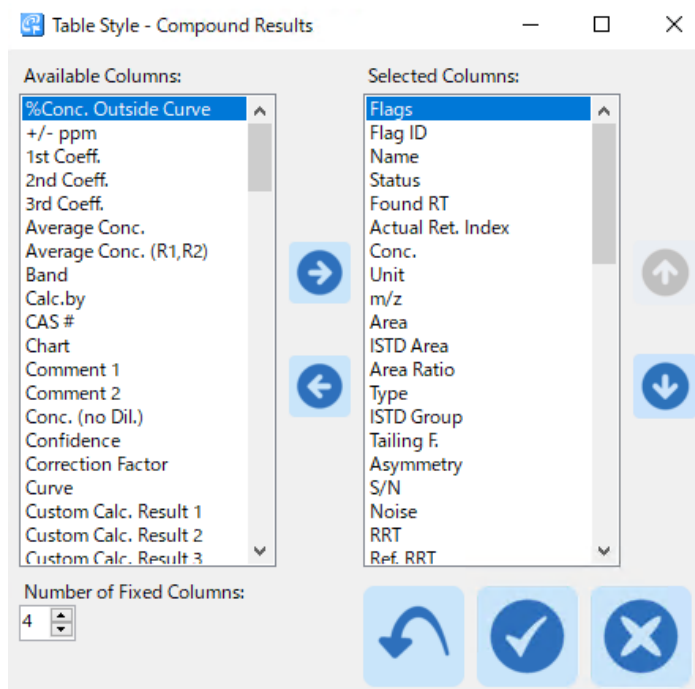
1

Right-click on the title bar of a table or click on the  button at the far left of the title bar. Then, click on [Properties].



The [Table Style] sub-window is displayed.

Items listed in [Selected Columns] are displayed on the table in the listed order.



2

Use the left and right arrow  buttons to add or delete items and use the

up and down arrow 
 buttons to re-order them.

3

Click on the  button to finish the operation. To undo the process and revert to default, click on the  button.

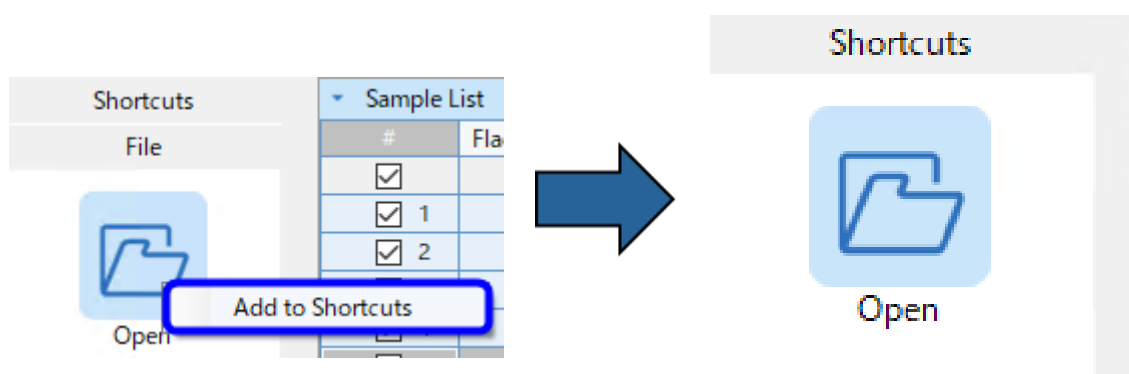
4

4.3 Shortcut Function

In LabSolutions Insight LCMS CL, buttons on the menu bar can be registered as shortcuts. The buttons registered as shortcuts can also be re-ordered or deleted at will. Users can add items used frequently to [Shortcuts] menu band. [Shortcuts] can be customized for each user.

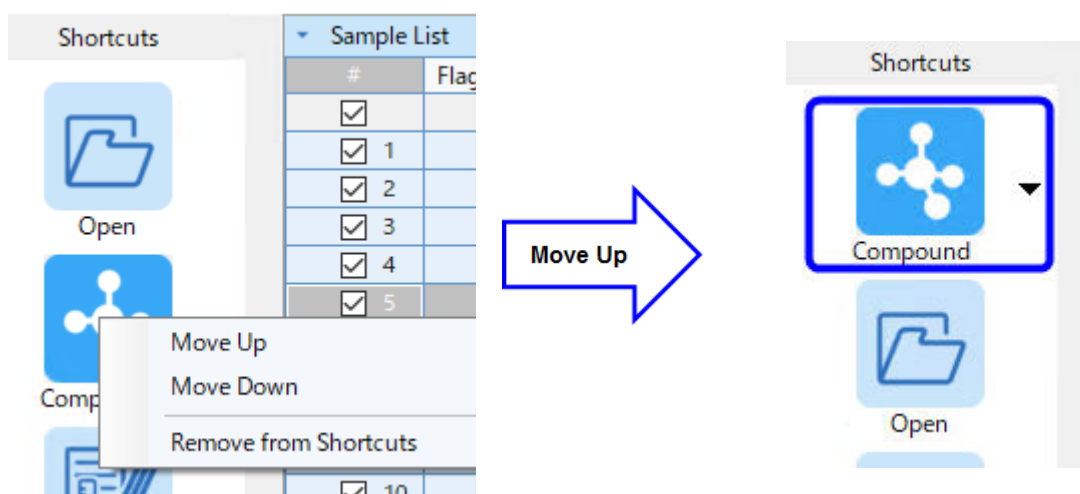
1

Right-click on the button to register.
Click on [Add to Shortcuts]. The button is added to [Shortcuts].



2

Right-click on the button registered in [Shortcuts].
Click on [Move Up] or [Move Down]. The order of the buttons changes.
To delete a button, click on [Remove from Shortcuts].

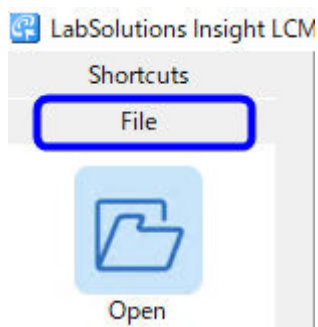


4.4 Exporting Analysis Results

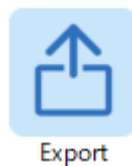
In LabSolutions Insight LCMS CL, the analysis result table can be exported as a "tab-delimited text (.txt)," "tab-separated value (.tsv)," or "comma-separated value (.csv)" format file.

1

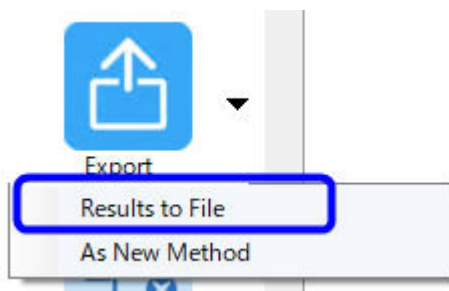
From the menu bar, click on the [File] menu band.

**4**

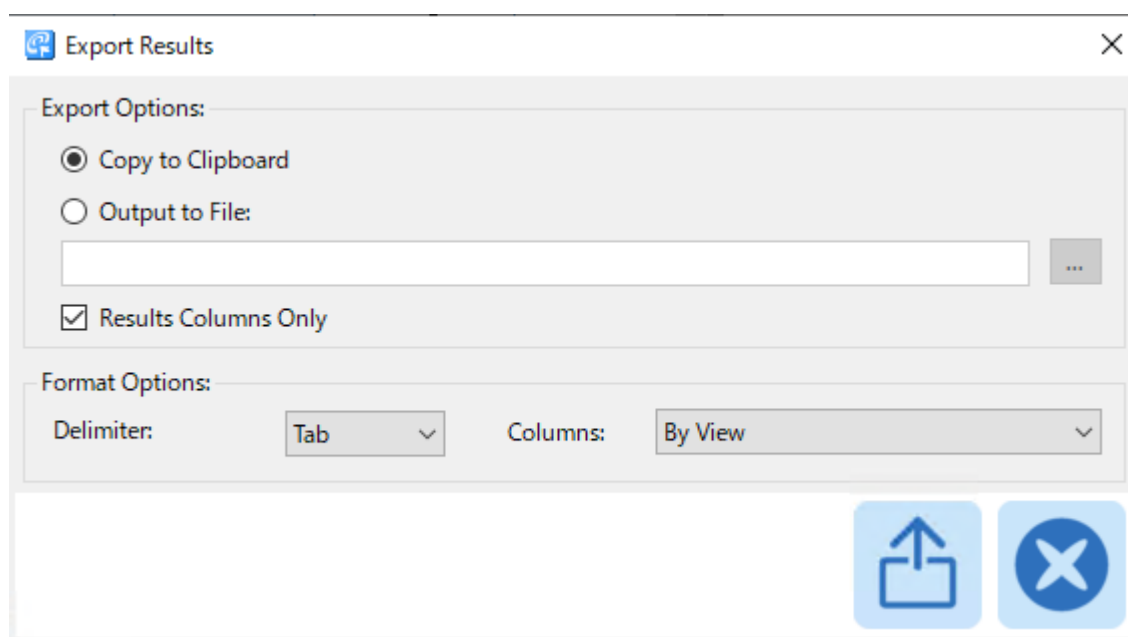
- Click on the [Export] icon (Data mode).



For Processing mode, the [Export] icon presents a drop down list. Select [Results to File].



The [Export Results] sub-window is displayed.



- Configure settings in the [Export Options] and [Format Options] area and click on the  button.