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Compound Discoverer

User Guide for LC Studies

Software Version 3.3 SP2

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ThermoFisher SCIENTIFIC

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For Research Use Only. Not for use in diagnostic procedures.

Contents

Preface

This guide describes how to use the Compound Discoverer™ application to qualitatively process RAW data files with a targeted or untargeted workflow. A targeted workflow evaluates the mass spectral data for the presence of specific compounds. An untargeted workflow evaluates the mass spectral data, predicts the elemental composition of unknown compounds, and searches mass spectral databases to identify these compounds.

To familiarize yourself with the Compound Discoverer application, follow the tutorials that are available from the application Help menu.

Contents

Access the documentation

The Compound Discoverer application includes these manuals as PDF files:

- *Compound Discoverer User Guide for LC Studies*
- *Compound Discoverer User Guide for GC Studies*
- *Compound Discoverer Tutorial for GC CI Workflows*
- *Compound Discoverer Tutorial for GC EI Workflows*
- *Compound Discoverer Tutorial for E & L Studies*
- *Compound Discoverer Metabolism Tutorial*
- *Compound Discoverer Metabolomics Tutorial*

- *Compound Discoverer Stable Isotope Labeling Tutorial*
- *Compound Discoverer BioCyc Tutorial*
- *Compound Discoverer Reporting Quick Start Guide*

The Compound Discoverer application also includes a context-sensitive Help system, which means that you can access content-specific Help for each page or dialog box in the user interface by pressing the F1 key (or equivalent keys) on your computer keyboard. You can also open the Help system to the Welcome page by choosing Help > Compound Discoverer Help from the application menu bar.

For information about accessing the manuals, see these topics:

- View the user guides and tutorials
- Download the user documentation for any Thermo Scientific product

View the user guides and tutorials

❖ **To view the Compound Discoverer manuals**

- From the application window, choose **Help > Manuals**.

–or–

a. Do one of the following:
   - From the Microsoft Windows™ 10 taskbar, click the **Start** button, .
   - From the Microsoft™ Windows™ 11 taskbar, click the **Start** button, , and click **All Apps**.

b. Choose **Thermo Compound Discoverer 3.3**

c. Select a manual (PDF file).

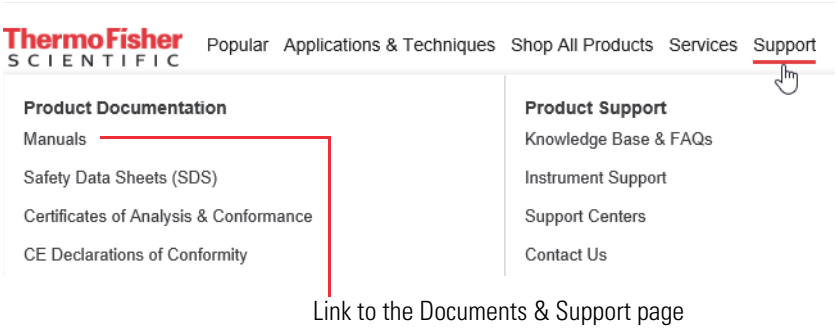
The list of manuals includes two user guides (one for each study type), two tutorials for GC studies, five tutorials for LC studies by field of study (vertical market), and one quick start for reporting.

Download the user documentation for any Thermo Scientific product

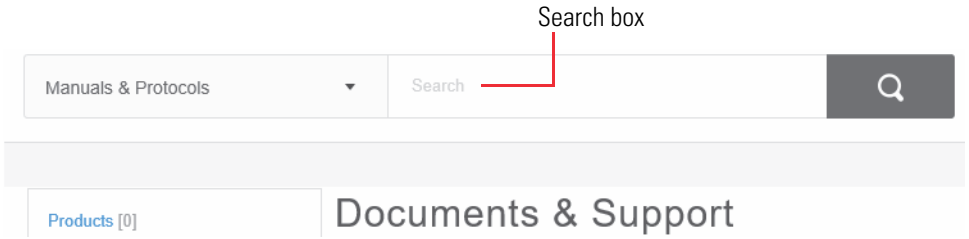
You can find user documentation for Thermo Scientific products on the Thermo Scientific website.

❖ **To download user documentation from the Thermo Scientific website**

1. Go to thermofisher.com.
2. Point to **Support**, and then click **Manuals** under Product Documentation on the left.



3. On the Documents & Support page, type the product name in the search box, and then click the **Search** icon.



4. In the results list, click the title to open the document in your web browser, save it, or print it.

System requirements

The Compound Discoverer 3.3 application can process data files produced by high-resolution accurate-mass (HRAM) Thermo Scientific™ mass spectrometers, such as the Orbitrap Fusion™, Q Exactive™, and Exactive™.

Table 1 lists the hardware and software requirements for the processing computer.

Table 1. Hardware and software requirements for the processing computer

System	Minimum requirements
Hardware	• 3.4 GHz dual-core processor • 16 GB RAM • 500 GB hard drive • USB port • Display monitor resolution of 1920 × 1080
Software	• Microsoft Windows 10 64-bit operating system or Microsoft Windows 11 64-bit operating system • Microsoft .NET Framework 4.8 • Microsoft Office 2013 • PDF reader
System settings	• To run processing workflows with online mass spectral database searches, the computer must have unblocked access to the mass spectral databases on the Internet. • The computer must have the correct time and date settings and be synchronized with Internet time. • The Region and Language setting for the operating system must be set to English (United States).

Table 2 lists the recommended hardware configurations for enhanced performance using the Compound Discoverer application.

Table 2. Recommended hardware configurations for enhanced performance

System	Recommended configurations
Hardware	• Dual 8-core processor (for example, 2x Intel™ Xeon™ Gold 6134 CPU @ 3.20 GHz) • 64 GB RAM • 1 TB SSD (solid-state disk) hard drive for OS • 2nd 3 TB (conventional disk) hard drive for data storage • USB port • Two 27 in. UHD monitors: Display monitor resolution of 3840 × 2160 pixels

To check the access to the mass spectral databases, the time and date settings, and the Internet time, see Chapter 17, "Test communication to the online databases."

To verify that the system meets the minimum requirements, see these topics:

- Check the computer specifications
- Check the format setting for region and language

Check the computer specifications

❖ To check the computer specifications

1. From the Windows Explorer directory, right-click **OSDisk (*Drive*:)** (the directory for the hard drive where the operating system is installed) and choose **Properties**.

   The OSDisk (Drive:) Properties dialog box opens. This dialog box lists the file system (NTFS or FAT) and the free disk drive space.

2. In the Windows search box, type **System**. Then, click **System Information**.

   The System Information page opens. This page lists the operating system; the processor type, speed, and number of cores; the installed RAM; and the system type (32-bit or 64-bit).

Check the format setting for region and language

Table 3 provides instructions for checking the operating system's region and language setting.

Table 3. Instructions for checking the format setting for region and language

Operating system	Steps
Windows 10 or 11	1. In the search box, type **Region Settings** and press ENTER. 2. On the Region page, under Regional Format, select **Recommended [English (United States)]**

Installation instructions

Thermo Compound Discoverer is a licensed application. After you install the application, you can use it for up to 60 days without activating the software license.

After you order the Compound Discoverer 3.3 application, you will receive a software media kit that includes a key-shaped USB flash drive with the installation executable. In addition, you will receive an email from Thermo MS Licensing providing you with the information that you need to activate the software license.

When you are upgrading the software from a previous version of the application, you can find the software installer and a license on the LSMS Software Download and Licensing Portal.

IMPORTANT Read the following:

- The installation requires the Windows 10 64-bit operating system. For the recommended hardware requirements and system settings, see "System requirements."
- The Compound Discoverer 3.3 SP2 licensing process requires an Internet connection to validate the software license. You can install the application on a computer without Internet access and complete the activation process on a computer with Internet access.
- The Compound Discoverer application is supported for US-English Only locale.

Note The following versions of the Compound Discoverer application can coexist on the same computer: 1.0, 2.0, 2.1, 3.0, 3.1, 3.2, and 3.3 SP2.

The installation executable includes three installers. The Thermo Compound Discoverer 3.3 installer installs the Compound Discoverer application. The Thermo mzCloud Offline Library installer installs four mzVault libraries that are July 2021 snapshots of the online mzCloud mass spectral database, and the Thermo mzVault installer installs the mzVault application.

To install the applications and the libraries, see these topics:

- Install the Compound Discoverer application
- Install the mzCloud offline libraries
- Install the mzVault 2.3 SP1 application
- NIST libraries for GC EI Orbitrap data

Install the Compound Discoverer application

❖ **To install the Compound Discoverer application**

1. Do one of the following:
   a. Insert the Compound Discoverer USB flash drive into a USB port on your computer.
   b. Open Windows Explorer and select the USB drive to view its contents.
   c. Locate the executable: XStart_Compound Discoverer.exe.

   –or–

   a. Go to the following website address:

      https://thermo.flexnetoperations.com

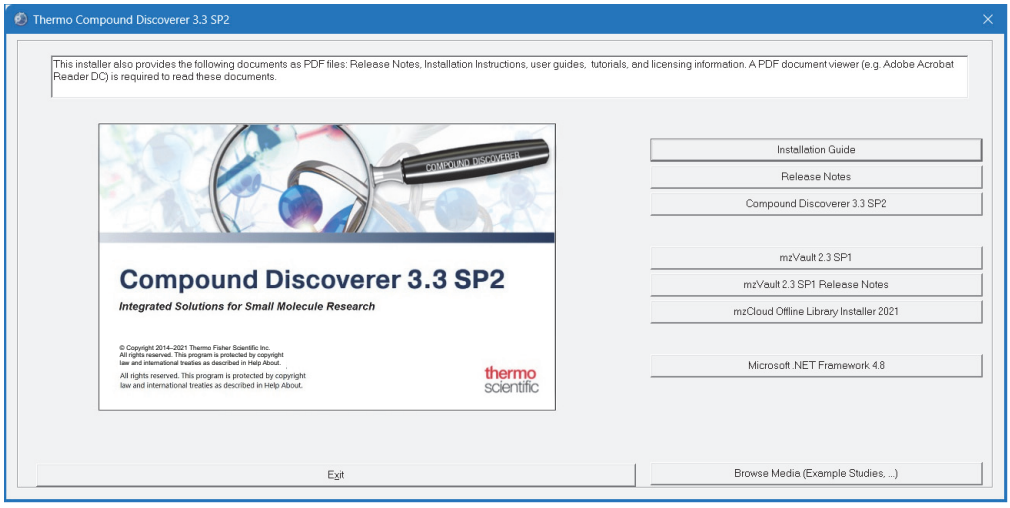
   b. Log in to your account. If you do not have an account, click **Register** and create one.
   c. On the left side of the Life Sciences Mass Spectrometry Software Download and Licensing Portal, click **Product List** under Software and Services.
   d. On the Product List page, click the **Demo** link.
   e. On the Product Information page, click the **Compound Discoverer 3.3 SP2** link.
   f. On the Product Download page, in the File Name column, click the down arrow to the left of Compound Discoverer 3.3 SP2.zip, click **Save As**, and then save the compressed zipped folder to your computer.
   g. Extract the contents of the zipped folder, and locate the executable: XStart_Compound Discoverer.exe.

   Note If you are upgrading from the Compound Discoverer 3.0, 3.1, or 3.2 software, which is a free upgrade, you can also find your software license on the Product Download web page.

2. Double-click **XStart_Compound Discoverer.exe**.

   The installation wizard starts.

Figure 1. Compound Discoverer installation wizard



3. Click **Compound Discoverer 3.3 SP2**.

   The installation wizard opens to the License Agreement page.

4. Select the **I Agree to the License and Trial License Terms and Conditions** check box.
5. (Optional) Open the System Requirements page and check whether your system meets the minimum requirements.
6. Click **Install**.
7. At the Prompt, click **Yes**.

   The installation starts.

8. (Optional) When the Successfully Installed page appears, click **IQ Report** to view the Installation Qualification report.
9. Click **Close** to close the installation wizard.

Install the mzCloud offline libraries

After you install the mzCloud offline libraries, they appear in the Spectral Libraries view of the Compound Discoverer application.

❖ To install the mzVault libraries

1. If the installer restarted your computer, double-click **XStart_Compound Discoverer.exe** to restart the installer.
2. Click **mzCloud Offline Library Installer** to install the mzVault libraries.

Install the mzVault 2.3 SP1 application

To create mass spectral libraries from your own data acquired with a high-resolution accurate-mass (HRAM) Thermo Scientific mass spectrometer, install the mzVault 2.3 SP1 application. The Compound Discover installer includes an installer for the mzVault application.

❖ To install the mzVault application

1. If the Compound Discoverer installer is not open, open it as follows:
   a. Locate the XStart_Compound Discoverer executable.

      You can find the executable on the USB drive provided in the Compound Discoverer application media or in the zip folder that you downloaded from the product download web site.

   b. Double-click **XStart_Compound Discoverer.exe**.
2. Click **mzVault 2.3 SPI**.

   The Thermo mzVault Installshield Wizard opens.

   Note If you have an earlier version of the application, follow the instructions to remove it, and then restart the mzVault 2.3 SP1 installer.

   If your computer meets the minimum requirements, the Next button becomes available.
3. Click **Next** to continue.
4. When the installation is complete, click **Finish**.

NIST libraries for GC EI Orbitrap data

To process GC EI Orbitrap data with the Compound Discoverer application, Thermo Fisher Scientific recommends that you install at least one NIST MS Search formatted EI-MS library on the processing computer. The Compound Discoverer installer does not include any NIST formatted libraries. You can purchase them from third-party vendors and install them separately within the NIST MS Search folder.

Customers who purchased an LC/MS system from Thermo Fisher Scientific on or after January 1, 2018 are eligible for a free copy of the NIST 2020 MSMS library. You can obtain a compatible version (that has been converted to the mzVault format) for use in the Compound Discoverer application by sending an email message to Licensing at ThermoMSLicensing@thermofisher.com. Include the Sales Order number or the Purchase Order number for the instrument in the email.

Customers who purchased the NIST 2020 library elsewhere can obtain the converted version for use in the Compound Discoverer application by sending a proof of purchase for the library to Licensing at ThermoMSLicensing@thermofisher.com.

NIST 2020 MSMS library for LC/MS/MS data

Customers who purchased an LC/MS system from Thermo Fisher Scientific on or after January 1, 2018 are eligible for a free copy of the NIST 2020 MSMS library. You can obtain a compatible version (that has been converted to the mzVault format) for use in the Compound Discoverer application by sending an email message to Licensing at ThermoMSLicensing@thermofisher.com. Include the Sales Order number or the Purchase Order number for the instrument in the email.

Customers who purchased the NIST 2020 library elsewhere can obtain the converted version for use in the Compound Discoverer application by sending a proof of purchase for the library to Licensing at ThermoMSLicensing@thermofisher.com.

Special notices

Make sure that you follow the precautionary statements presented in this guide. The special notices appear in boxes.

Special notices include the following: Important, Note, and Tip.

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

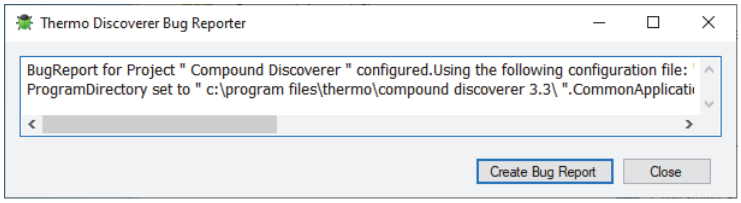
Create and submit a bug report

If you discover a software error in the Compound Discoverer application, report the error to the Compound Discoverer support team.

❖ To report an error in the application

1. From the Compound Discoverer menu bar (on the processing computer where the error occurred), choose **Help > Create Bug Report**.

   The Thermo Discoverer Bug Reporter dialog box opens.



2. Click **Create Bug Report**.

   The application creates a report of your computer configuration and stores it as a Compound Discoverer Bug Report (*timestamp*).zip on your computer desktop.

3. Send a detailed error description with screenshots and the bug report as an attachment to the following email address:

   CD.support@thermofisher.com

Contact us

Contact	Email	Telephone	QR Code
U.S. Technical Support	us.techsupport.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
U.S. Customer Service and Sales	us.customer-support.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
Global support	❖ **To find global contact information or customize your request** 1. Go to thermofisher.com. 2. Click **Contact Us**, select the country, and then select the type of support you need. 3. At the prompt, type the product name. 4. Use the phone number or complete the online form. ❖ **To find product support, knowledge bases, and resources** Go to thermofisher.com/us/en/home/technical-resources. ❖ **To find product information** Go to thermofisher.com/us/en/home/brands/thermo-scientific.		
	❖ **For Compound Discoverer customer support questions** Send an email message to CD.support@thermofisher.com.		

1

Introduction to Compound Discoverer

Compound Discoverer is a qualitative data-processing application that uses accurate mass data, isotope pattern matching, fragment matching, and mass spectral library searches for the structural identification of small molecules. It can process the accurate-mass spectra from the entire product line of Thermo Scientific high-resolution mass spectrometers. It can also display the graphical data acquired from a variety of LC detectors: UV-visible and photodiode array (PDA) detectors that are controlled by a Thermo Scientific data system and third-party analog detectors that are connected to the analog input channels of a Thermo Scientific mass spectrometer (MS).

The Compound Discoverer application is a study-based application—that is, all data processing takes place from within the study environment. When data processing is complete, the application automatically stores the result file or files in the study folder. See "Directory structure for Compound Discoverer studies."

This introduction describes the features and enhancements in this release and how to set up the application window, choose the size of the toolbar icons, and manage the recently used file lists on the Start Page. In addition, the overview topic summarizes the application workflow from starting the application to reporting the results of an analysis.

For details, see these topics:

New features and enhancements

The Compound Discoverer application uses a study format to define the experimental variables for a set of samples. It uses a customizable node-based processing workflow to process Xcalibur™ RAW files and create either a single result file with statistical analyses for the input file set or one result file per input file without any statistical analyses.

Some of the workflow nodes in the processing workflows require input from the customizable lists and libraries for the application. For LC studies, these lists and libraries include the structures of known compounds, mass lists, adduct ions, chemical transformations, ion definitions, neutral losses, Metabolika pathways, compound classes (fragment lists), and mass spectral libraries.

The result file from data processing includes a set of result tables and graphical views that are based on the processing workflow. The application provides graphical views for displaying chromatograms and spectra and statistical views for comparing the detected compounds by sample file or sample group.

The application comes with defined templates for the processing workflows and reports.

These topics describe the new features and enhancements in the Compound Discoverer 3.3 application and the enhancements in the two service packs (3.3 SP1 and 3.3 SP2):

- Enhancements in the Compound Discoverer 3.3 SP2 release
- Enhancements in the Compound Discoverer 3.3 SP1 release
- New features in Compound Discoverer 3.3 for LC studies
- Enhancements in Compound Discoverer 3.3

Enhancements in the Compound Discoverer 3.3 SP2 release

For LC studies, the Compound Discoverer 3.3 service pack 2 (SP2) application includes the following enhancements:

- Additional spectral libraries in the Spectral Libraries library

  See "Spectral Libraries view."

- Additional mass lists in the Mass Lists library, including new mass lists for the identification of compounds in the PFAS family

  See "Mass Lists view."

- New PFAS compound class file in the Compound Classes library

  See "Compound Classes view."

- New processing workflow template for identifying the per- and polyfluoroalkyl substances (PFAS) family of compounds

  See "Defined processing workflow templates," and "PFAS identification."

  For more information about using the Compound Discoverer application to identify compounds in the PFAS family, refer to the following document:

  http://assets.thermofisher.com/TFS-Assets/CMD/Application-Notes/an-001826-lsms-pfas-analysis-workflow-compound-discoverer-an001826-na-en.pdf

- Additional transformation reaction, PFAS Chain Shortening, for the PFAS family of compounds in the Transformations list

  See "Transformations view."

- Increased limit for the number of compounds that you can export to the molecular networks viewer

  The limit is now 3.000 compounds. See "Send compounds to the molecular networks viewer."

Enhancements in the Compound Discoverer 3.3 SP1 release

For information about the enhancements in the Compound Discoverer 3.3 SP1 release, see these topics:

- Enhancements common to both study types in the Compound Discoverer SP1 release
- Enhancements for LC studies only in the Compound Discoverer SP1 release

Enhancements common to both study types in the Compound Discoverer SP1 release

The Compound Discoverer 3.3 SP1 application includes the following enhancements for both study types (LC and GC):

- The Mass List Editor can now open compound lists with a file size of up to 600 MB.
- The Natural Product Atlas database in the mass lists available from the Lists & Libraries menu has been updated to version 2021_08. See "Mass Lists view."
- The performance of the Map to BioCyc Pathways node has been improved to reduce the run time of the mapping process.

Enhancements for LC studies only in the Compound Discoverer SP1 release

The Compound Discoverer 3.3 SP1 application includes the following enhancements for LC studies only:

- The Fill Gaps node includes a new parameter that lets you specify a less restrictive retention time tolerance for filling the gaps for compounds across the input files. For the Gap Filling node, gaps are missing chromatographic peaks for putative compounds in one or more of the input files for an analysis. See "Fill Gaps node."
- Peak ratings are now available for chromatographic peaks that the Fill Gaps node gap-filled by using a matching ion or a re-detected peak for the missing peak.

New features in Compound Discoverer 3.3 for LC studies

The Compound Discoverer 3.3 application includes the following new features for LC studies:

- Improved chromatographic peak detection and integration

  The Detect Compounds and Find Expected Compounds nodes

  – Are significantly faster and more sensitive than the original Detect Compounds (Legacy) and Find Expected Compounds (Legacy) nodes.

  – Provide improved peak integration.

  – Include an option to base the mass trace and chromatographic peak area for each compound on the most intense isotope in the isotopic pattern or all the detected isotopes. Both options use the specified minimum number of isotopes to validate the mass traces.

    See the Use Most Intense Isotope Only parameter in the Detect Compounds node and the Find Expected Compounds node.

  – Include a baseline integration option.

    See the Remove Baseline parameter in the Detect Compounds node and the Find Expected Compounds node.

  – Report the quality of the chromatographic peaks in the result tables.

    See Peak quality factor (PQF) columns in the result tables.

  Note The Detect Compounds (Legacy) node and the Find Expected Compound (Legacy) node, with some performance improvements, are still available for comparisons with existing analysis results.

- Improved chromatographic peak area determination for relative quantitation

  The Group Compounds and Group Expected Compounds nodes

– Find the most common adduct ion for each compound across all samples for relative quantitation. Provide the option to base the chromatographic peak area for each compound on the most common adduct ion or the summed area of all the detected ions.

  See the Area Integration parameter in the Group Compounds node and the Group Expected Compounds node.

  Note By default, the Area Integration parameter is set to Most Common Ion.

– Display the *m/z* value of the most common adduct ion in the m/z column and its ion definition in the Reference Ion column of the Compounds and Expected Compounds tables.

- New peak rating filter in the Group Compounds, Group Expected Compounds, and Differential Analysis nodes provides peak thresholding based on the quality of the chromatographic peaks.

  This peak rating filter lets you filter out low-quality chromatographic peaks without setting an overly restrictive minimum peak intensity threshold. To pass the filter, chromatographic peaks must have a peak rating equal to or greater than the user-specified threshold and be detected or found in at least the user-specified minimum number of input files submitted for analysis. See Chromatographic peak rating filter.

  Peaks that do not pass the peak rating thresholds in the Detect Compounds and Find Expected Compounds nodes are removed early in the processing workflow. This data reduction speeds up processing for the downstream nodes (gap, peak area refinement, identification, mapping, and scoring) and increases overall performance.

  The Differential Analysis node recalculates the peak ratings to capture changes in the peak areas from the Fill Gaps node and the peak area refinement nodes.

  The peak rating values of the chromatographic peaks are based on peak quality factors[1], relative peak area, and the coefficient of variance values (CVs).

- The Search mzCloud and Search mzVault nodes can perform MS^n searches against the library spectra in the mzCloud mass spectral database. The mzCloud search can retrieve KEGG IDs and compound class information from the online mzCloud mass spectral database and display these results in the Compounds table of the result file (analysis result).

  Tip The Search MSn parameter in the Search mzCloud and Search mzVault nodes is set to True in the processing workflow templates provided with the Compound Discoverer application. When you create your own custom processing workflow templates, you must set this parameter to True to perform MSn searches. See the Search MSn parameter in the Search mzCloud node and the Search mzVault node.

[1] Chetnik et al, MetaClean: a machine learning-based classifier for reduced false positive peak detection in untargeted LC-MS metabolomics data, http://www.ncbi.nlm.nih.gov/pmc/articles/pmc7895495/

- The new chromatographic peak alignment node—Align Retention Times (ChromAlign)[2] node— is faster and more sensitive than the original alignment node. In addition, you have the option to align the chromatographic peaks on the compound level in the Group Compounds and Group Expected Compounds nodes by setting the Align Peaks parameter to True.

Enhancements in Compound Discoverer 3.3

The Compound Discoverer 3.3 application includes the following enhancements for LC studies:

- Improvements to the molecular networking feature let you do the following:
  - Display chemical structures in the nodes.
  - Control the maximum cluster size.
  - Show only the backbone of each cluster.

  See Panes at the left of the molecular networks viewer.
- Support for data acquisition using multiple mass ranges. See the MS1 Mass Range parameter in the Select Spectra node.
- Support for data acquisition using multiple FAIMS compensation voltage (CV) values. See the FAIMS CV parameter in the Select Spectra node.
- Custom Tags Editor for creating, importing, and exporting tag definitions. See Custom color-coded tags for result table entries.
- Result Exporter processing workflow node (Post-Processing section) for automatically exporting result tables or specific columns in each result table to spreadsheet or text files. See Result Exporter node.
- New reporting options for displaying the mzCloud mirror plot, the study name, and the result file name in a report. The report templates provided with the Compound Discoverer application display the study name and the file name of the result file in the page header. The Customize Report dialog box automatically adds the study name and file name to the page header of new report templates.

  For information about adding an mzCloud mirror plot to a report template, see Add mzCloud mirror plots to a report template.
- An additional compound database—LipidMaps[3] Structure Database in the Mass Lists library. See Mass Lists view.

[2] ChromAlign: A two-step algorithmic procedure for time alignment of three-dimensional LC-MS chromatographic surfaces, RG Sadygov et al. Analytical Chemistry, 2006

[3] Sud et al, LMSD: LIPID MAPS structure database, http://www.ncbi.nlm.nih.gov/pubmed/17098933

- A new version of the mzCloud Offline Spectral Library (2021B) and two in-silico spectral libraries for lipids—LipidBlast[4] in the Spectral Libraries list. See Spectral Libraries view.
- The Grouping & Ratios page of an analysis shows information on the statistical test that the analysis will apply by using the selected groups and ratios.
- New Statistical Methods result table that provides detailed information on transformations (performed by the Differential Analysis node), statistical tests, scaling methods, gap filling, and QC methods that the analysis performed.

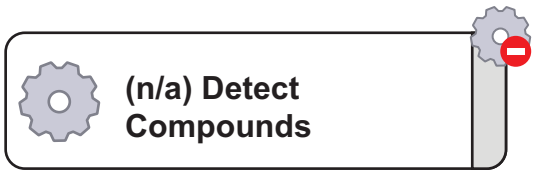
The Compound Discoverer 3.3 SP1 application includes the following enhancements:

- The Fill Gaps node includes a new parameter that lets the user specify a less restrictive retention time tolerance for filling the gaps for compounds across the input files for the analysis. For the Gap Filling node, gaps are missing chromatographic peaks for putative compounds in one or more of the input files for an analysis. See "Fill Gaps node."
- The Mass List Editor can now open compound lists with a file size of up to 600 MB.
- The Natural Product Atlas database in the mass lists available from the Lists & Libraries menu has been updated to version 2021_08.
- Peak ratings are now available for chromatographic peaks that the Fill Gaps node gap-filled by using a matching ion for the missing peak.
- The performance of the Map to BioCyc Pathways node has been improved, reducing the run time of the mapping process.

Obsolete (n/a) Detect Compounds node in legacy processing workflows

The Compound Discoverer 3.3 application includes new chromatographic peak detection and alignment algorithms. These new algorithms have obsoleted the original peak detection and alignment algorithms in previous versions of the application.

When you reprocess analysis results (result files) for untargeted analyses from previous versions of the Compound Discoverer application, a not available (n/a) warning appears on the Detect Compounds node. The current workflow issues table below the Workflow Tree area on the Workflows page of the Analysis view states that the node is not recognized by the application.



[4] Kind et al., LipidBlast in silico tandem mass spectrometry database for lipid identification, http://dx.doi.org/10.1038/nmeth.2551

You cannot partially reprocess legacy analysis results from untargeted analyses. To reprocess these results, you must replace the (n/a) Detect Compounds node with the Detect Compounds node or the Detect Compounds (legacy node) and fully reprocess the analysis. For details, see "Reprocess a legacy analysis result from an untargeted analysis."

Terminology used in the Compound Discoverer application

Table 4 describes the terminology that the Compound Discoverer application uses for its data-processing features.

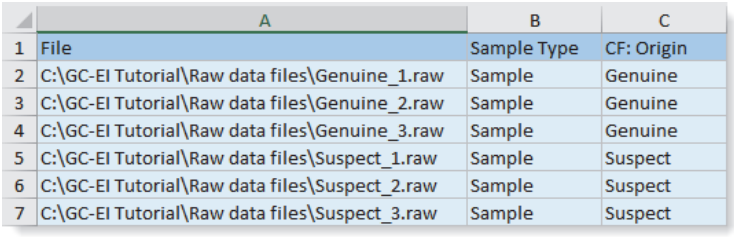
Table 4. Terminology used in the Compound Discoverer application (Sheet 1 of 3)

Term	Description
Analysis	An analysis consists of a processing workflow (which is a processing method consisting of multiple interconnected workflow nodes), a list of input files for processing, and the name of the result file that the analysis generates. In addition to the input files and the processing workflow, an analysis can also specify the sample groups and ratios for statistical analyses. You can select the processing workflow and the input files and set up the study factors and sample groups for an analysis by using the New Study and Analysis wizard. Or, you can set up an analysis from within a study.
Compounds	For LC studies, a compound (or component) is a chromatographic peak that the application detected for a specific molecular weight (within the specified mass tolerance) and retention time (within the specified tolerance). The Features table for a compound lists all the chromatographic peaks that make up the peak for the compound.
Expected compounds	For LC studies, an expected compound is a compound that the application generates by using the parent compounds and transformations that you specify. You specify the parent compounds and transformations in the Generate Expected Compounds node of a processing workflow. After the application generates a list of expected compounds, it searches for these compounds in the input files that you submit for analysis.
Features	Features are chromatographic peaks with specific *m/z* × RT dimensions that the Detect Unknown Compounds node detects. The Compound Discoverer application reports the chromatographic peak areas in counts × seconds.
Gap	In an extracted ion current (XIC) trace (chromatogram), gaps are missing data points—that is, the scan or scans acquired at specific time points in the chromatographic run do not include mass spectrum peaks for the compound's mass within the user-specified mass tolerance. For the gap filling nodes, gaps are missing chromatographic peaks for putative compounds in one or more of the input files for an analysis.
Input files	Input files are Xcalibur raw data files that you have added to a study. The study lists the relative location of the raw data files. If you move the raw data files to a different directory after you add them to a study, you must resolve their location before you start an analysis.

Table 4. Terminology used in the Compound Discoverer application (Sheet 2 of 3)

Term	Description
Study factors	Study factors are the experimental variables that you are testing for statistically significant effects on the sample population being studied. There are three types of study factors: • Categorical factors include non-quantifiable categories such as organism, matrix, tissue, gender, and so on. • Numerical factors include quantifiable variables such as time, amount, concentration, and so on. You can assign a unit to a numeric study factor; however, the unit is only a label and is not used in any calculations. • Biological replicate factors include non-quantifiable categories with samples from different entities of the same type under the same conditions and provide a measure of the variability associated with these conditions. Use the biological replicate factor for nested experiments. You can add only one biological replicate factor to a study.
Study files (studies)	Setting up an analysis to process raw data files takes place within the study environment. Studies include a list of input files with their location, the sample information for each file, and a list of the analyses run within the study. The sample information includes the file name, study factor values, and sample type for each sample. Study files also include the name and location of the folder where the Compound Discoverer application stores the result files that you generate by running analyses within the study. You can open result files from outside a study.
Study folders	Every study includes a folder for storing the results of the analyses run within the study. In addition, you can create multiple higher-level folders for storing the study-specific folders. See "Directory structure for Compound Discoverer studies."

Table 4. Terminology used in the Compound Discoverer application (Sheet 3 of 3)

Term	Description
Study templates	A study template file is any study file (.cdStudy) that includes defined study factors or a spreadsheet file (.xlsx) or tab-delimited text file (.txt) that includes all the study information. As shown in the following example, the required columns for a text or spreadsheet file are File (names and location of the raw data files), Sample Type, and CF:*study factor name* (one column for each study factor).  For information about creating study template files that include all the study information, see "Create a study template file that contains all the study information."
Result files	Result files contain the results of a specific processing workflow and input file set. Results files are also known as analysis results. See Chapter 8, "Review the analysis results."
Processing workflows	Processing workflows are node-based processing methods for processing raw data files. You can access the predefined processing workflow templates and your custom processing workflow templates only from within a study. See Chapter 6, "Create and edit processing workflows."
Parent compounds	For targeted analyses, a parent compound is an expected compound that you define in the Expected Compounds library and then select for analysis in a processing workflow. The result file from an expected compounds analysis includes an Expected Compounds table with a Parent Compound column. You can select multiple compounds for an expected compounds analysis. In the molecular network viewer, parent compounds are the starting compounds for the chemical transformations that you specify in the Generate Molecular Networks workflow node.

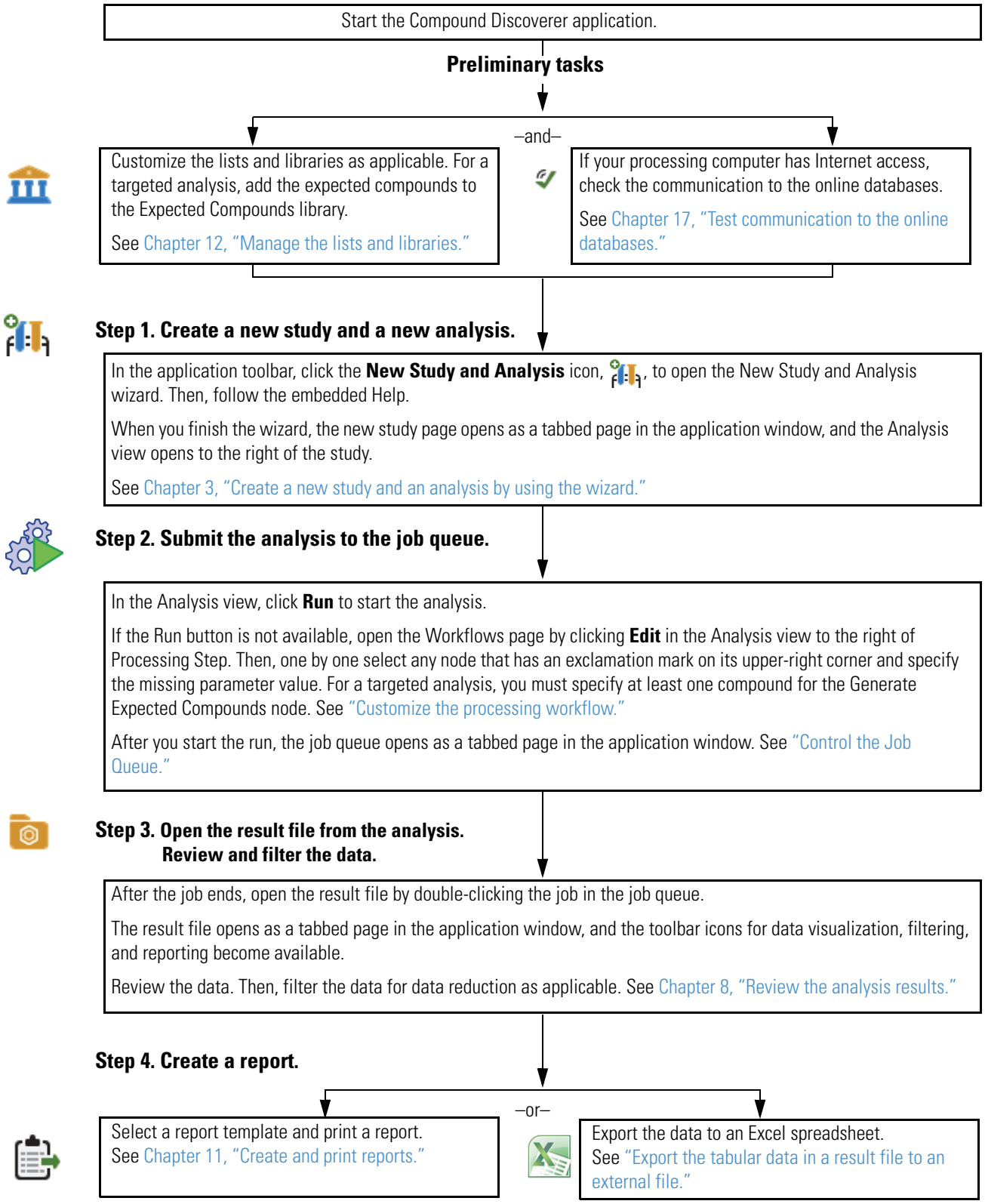
	A	B	C
1	File	Sample Type	CF: Origin
2	C:\GC-EI Tutorial\Raw data files\Genuine_1.raw	Sample	Genuine
3	C:\GC-EI Tutorial\Raw data files\Genuine_2.raw	Sample	Genuine
4	C:\GC-EI Tutorial\Raw data files\Genuine_3.raw	Sample	Genuine
5	C:\GC-EI Tutorial\Raw data files\Suspect_1.raw	Sample	Suspect
6	C:\GC-EI Tutorial\Raw data files\Suspect_2.raw	Sample	Suspect
7	C:\GC-EI Tutorial\Raw data files\Suspect_3.raw	Sample	Suspect

LC studies overview

Figure 2 summarizes the workflow for setting up a study and an analysis, submitting a set of input files for processing, and reviewing and reporting the results of the analysis.

For LC studies, there are two types of analyses—targeted and untargeted. In a targeted analysis, the application starts with a list of expected compounds. In an untargeted analysis, the application relies on matching the fragmentation spectra to compounds in a mass spectral database. You can create processing workflows (processing methods) that combine these two types of analyses.

Figure 2. Compound Discoverer workflow for LC studies



Start the Compound Discoverer application

You can start the application from the taskbar or the computer desktop.

❖ To start the Compound Discoverer application

Do one of the following:

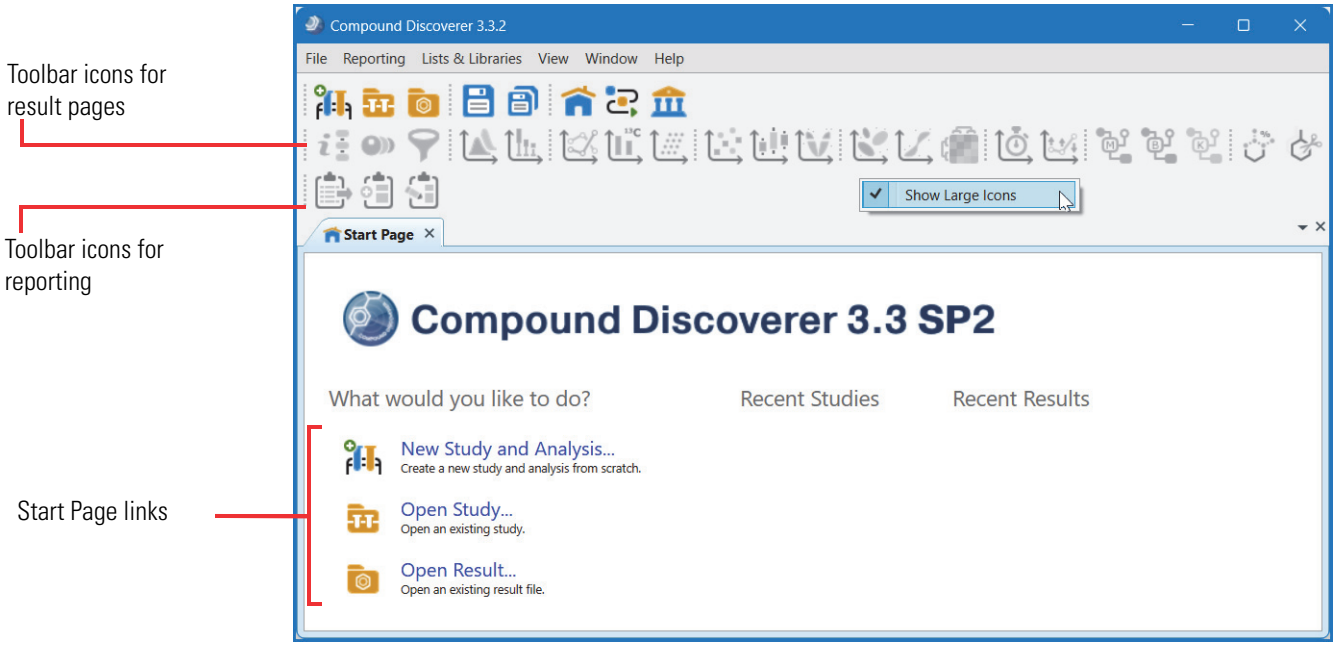
- From the taskbar, choose **Start > All Programs** (or **Programs**) **> Thermo Compound Discoverer**.
- From the computer desktop, double-click the **Compound Discoverer 3.3** icon, .

The Compound Discoverer window opens with the Start Page displayed as a tabbed document. As you create studies and process data, the application creates and populates the recent file lists to the right of the What Would You Like to Do? links.

Figure 3 shows the initial application window with large toolbar icons:

- The icons in the first row are always available.
- Most of the icons in the second and third rows become available when you open a result file.

Figure 3. Application window with the initial Start Page and large toolbar icons



For information about the toolbar icons and application menus, see "The Compound Discoverer window."

The Compound Discoverer window

The Compound Discoverer window contains a title bar, a menu bar, and a toolbar. From the application window, you can open all the other application views and pages by choosing a menu command or clicking a toolbar icon. The Start Page lists the recently opened study files and result files. See "Start the Compound Discoverer application."

These topics describe the menu bar, the toolbar, and the recently used files lists on the Start Page:

- Compound Discoverer menu bar
- Compound Discoverer toolbar
- Change the size of the toolbar icons
- Manage the recently used files lists on the Start Page

Note This user guide uses the following terms to describe the user interface:

- View—A dockable window that you can move to a second monitor.
- Page—A tabbed document. You can have many pages open simultaneously; however, only one of these pages is the active page.
- Dialog box (modal)— A graphical element that accepts user input. Only one modal dialog box can be open at a time. When it is open, a modal dialog box blocks you from working in other parts of the application.
- Pane—A defined area of an application view, page, or dialog box.
- Prompt—A pop-up message box that you must dismiss to continue.

Compound Discoverer menu bar

Table 5 describes the menu commands in the menu bar at the top of the Compound Discoverer window.

Table 5. Compound Discoverer menu bar (Sheet 1 of 6)

Menu command	Description
File menu	
These commands are always available.	
New Study and Analysis	Opens the New Study and Analysis Wizard, which takes you through the process of selecting the studies folder for your study subfolders, creating a new study, and starting a new analysis.

Table 5. Compound Discoverer menu bar (Sheet 2 of 6)

Menu command	Description
Open Study	Opens the Open Study dialog box for selecting an existing study file to open. The Compound Discoverer study file type has the .cdStudy file name extension.
Open Result	Opens the Open Result File dialog box for selecting an existing result file or result view file. You do not need an active software license to open result files. The file name extension for result files that contain the data processing results is .cdResult. The file name extension for files that contain the display layout for the results tables, graphical views, and filter settings is .cdResultView. To restore the default layout for a result file, delete its associated result view file. **Note** You do not need an active software license to open result files.
Save	Saves recent changes to the current active page (selected tab), for example, the active study page or result page.
Save All	Saves recent changes to all the open pages in the application window.
Recent Studies	Displays a list of recent studies that you can open.
Recent Studies > Clear	Clears the Recent Studies list.
Recent Results	Displays a list of recent results that you can open.
Recent Results > Clear	Clears the Recent Results list.
Exit	Closes the application.
Reporting menu These commands are available only when a result page is active.	
Create Report	Opens the Open Report Design Template dialog box for selecting a report template to resolve specific data in the result file.
Create Report Template	Opens the Customize Report dialog box for setting up the main properties of a report template.
Edit Report Template	Opens the Open Report Design Template dialog box for choosing an existing report template to edit.

Table 5. Compound Discoverer menu bar (Sheet 3 of 6)

Menu command	Description
List & Libraries menu	
These commands are always available.	
Expected Compounds	Opens the Expected Compounds view for modifying the list of expected compounds.
	Note The Generate Expected node and Create Pattern Trace node require compounds from the Expected Compounds library. The Create Pattern Trace and the Pattern Scoring nodes require user-specified elemental compositions.
Transformations	Opens the Transformations view for modifying the list of transformations.
Neutral Losses	Opens the Neutral Losses view for modifying the list of neutral losses.
Ion Definitions	Opens the Ion Definitions view for modifying the list of ion definitions.
Adducts	Opens the Adducts view for modifying the list of adducts.
Mass Lists	Opens the Mass Lists view for modifying the list of mass list files or editing mass list files.
Spectral Libraries	Opens the Spectral Libraries view for modifying the list of mzVault database files.
Metabolika Pathways	Opens the Metabolika Pathways view for modifying the list of Metabolika pathways or editing a Metabolika pathway.
Compound Classes	Opens the Compound Class view for viewing or modifying the list of compound class libraries.
View menu	
The Start Page and Job Queue commands from this menu are always available. The other View commands are available only when a result file is active.	
Start Page	Opens the Start Page, which lists the most recently opened result files and study files.
Job Queue	Opens the Job Queue page for viewing the progress of the current analysis or the processing events of previous analyses.
Result Summary	Opens the Summaries view.
Custom Tags Editor	Opens the Custom Tags Editor for selecting the number of custom tags that you want to use for tagging items in the result tables and the text that you want to display for each tag.

Table 5. Compound Discoverer menu bar (Sheet 4 of 6)

Menu command	Description
Result Filters	Opens the Result Filters view for reducing the number of rows displayed in selected result tables.
Chromatograms	Opens the Chromatograms view for viewing chromatogram plots.
Mass Spectrum	Opens the Mass Spectrum view for viewing a spectral tree and the spectrum scans.
Trend Chart	Opens the Trend Chart view for setting up a box-and-whisker (Box Whisker selection) chart or a trendline chart.
Isotopologues Distribution Chart	Opens the Isotopologues Chart view. Available only when the active result file includes results from the Analyze Labeled Compounds node.
Mass Defect Plot	Opens the Mass Defect Plot view for examining the relationship between the mass defects of the detected or expected compounds and their molecular weights.
Result Charts	Opens the Result Charts view for setting up data graphs, such as scatter plots, histogram charts, bar charts, and pie charts. Use these views to visualize the data.
Descriptive Statistics	Opens the Descriptive Statistics view for viewing a box-and-whisker plot of all the compounds in the Compounds or Expected Compounds tables for the selected sample groups.
Differential Analysis	Opens the Differential Analysis view for viewing volcano plots and running differential analyses.
Principal Component Analysis	Opens the Principal Component Analysis view for evaluating multivariate data.
Partial Least Squares Discriminant Analysis	Opens the Partial Least Squares Discriminant Analysis view.
Hierarchical Cluster Analysis	Opens the Hierarchical Cluster Analysis view.
Retention Time Corrections	Opens the Corrected Retention Times view. Available only when the active result file includes data from multiple input files. To view the retention time correction curves for one or more input files, select the input files of interest in the Input Files table.
Compound Area Corrections	Opens the Compound Area Corrections view. Available only when the active result file includes data from Quality Control samples.

Table 5. Compound Discoverer menu bar (Sheet 5 of 6)

Menu command	Description
Metabolika Pathways	Opens the Metabolika Pathways view for viewing the Metabolika pathways that are mapped to the compounds data.
BioCyc Pathways	Opens the BioCyc Pathways view for viewing the BioCyc pathways that are mapped to the compounds data. Available only when the active result file includes mapped BioCyc pathways.
KEGG Pathways	Opens the KEGG Pathways view for viewing the KEGG™ pathways that are mapped to the compounds data. Available only when the active result file includes mapped KEGG pathways.
mzLogic Analysis	Opens the mzLogic Analysis view.
FISh Scoring Queue	Opens the FISh Scoring Queue view.
Window menu Use these commands to apply, save, manage, or reset layouts.	
Apply Layout	Displays the layouts list for selecting a layout.
Save Layout	Opens the Save Layout dialog box for naming the current layout.
Manage Layouts	Opens the Manage Result File Layout dialog box for renaming or deleting layouts.
Reset Layout	Closes and reopens the active result file to reset its layout.
Help menu These commands are always available.	
Compound Discoverer Help	Opens the Compound Discoverer Help, which is a compiled Help file with Contents, Index, and Search tabs. The Help contains context-sensitive topics; that is, pressing F1 opens the Help topic that corresponds to the current area of the application.
How to Use the Help	Opens the Compound Discoverer Help to the Using This Help topic.
Glossary	Opens the Compound Discoverer Help to the table of contents for the glossary.
Compound Discoverer Support Manuals	Displays links to the Compound Discoverer User Guide, Compound Discoverer Reporting Quick Start, Compound Discoverer tutorials, and Release Notes.

Table 5. Compound Discoverer menu bar (Sheet 6 of 6)

Menu command	Description
License Manager	Opens the License Manager page where you can activate your Compound Discoverer license or scan for missing application features.
Communication Tests	Opens the Communication Tests dialog box where you can run tests to check whether your data processing computer can connect to the external BioCyc Pathways, KEGG Pathways, mzCloud, and ChemSpider databases.
Create Bug Report	Creates a report of your computer configuration and stores it as a Compound Discoverer Bug Report (*timestamp*).zip on your computer desktop. To report software errors to Thermo Fisher Scientific, send a detailed error description with screen shots and attach this bug report to the email.
Configuration	Opens the Configuration page for setting global options, such as the maximum number of parallel analyses, the study management setting for automatically saving studies, the color maps, the mzCloud search settings, and your user credentials for the BioCyc mapping feature.
About	Opens the Compound Discoverer dialog box for viewing lists of the installed components and processing workflow nodes.

Compound Discoverer toolbar

Figure 4 shows the Compound Discoverer toolbar (when a result page is active).

Figure 4. Compound Discoverer toolbar (with small icons)

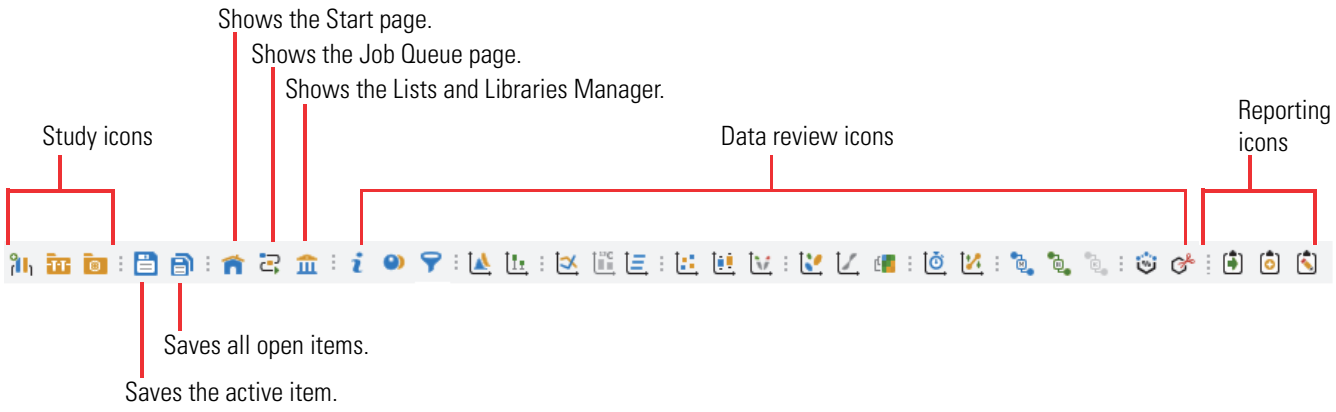


Table 6 describes the icons in the Compound Discoverer toolbar from left to right.

Table 6. Toolbar icons (Sheet 1 of 3)

Icon	Description
Study icons	
	Opens the New Study and Analysis Wizard that takes you through the process of specifying the studies folder for all your study subfolders, creating a new study, and starting a new analysis.
	Opens the Open Study dialog box for selecting the current version or a previous version of an existing study.
	Opens the Open Result File dialog box for selecting the current version or a previous version of a result file.
General icons	
	Saves the currently active item, such as a study or result file.
	Saves all the open pages, such as the study pages and the result pages.
	Opens the Start Page when it is not already open and makes it the active page.
	Opens the Job Queue page when it is not already open and makes it the active page.
	Opens the Lists and Libraries Manager where you can select to open one of the following editors: • Expected Compounds—For viewing or modifying a list of compounds • Transformations—For viewing or modifying a list of transformations • Neutral Losses—For viewing or modifying a list of neutral losses • Ion Definitions—For viewing or modifying a list of ion definitions • Adducts—For viewing or modifying a list of adducts • Mass Lists—For creating, editing, importing, exporting, or deleting mass lists • Spectral Libraries—For creating, editing, importing, exporting, or deleting mzVault database files • Metabolika Pathways—For adding, editing, importing, exporting, or deleting Metabolika pathways. • Compound Classes—For creating, editing, importing, exporting, or deleting compound class libraries of fragment structures

Table 6. Toolbar icons (Sheet 2 of 3)

Icon	Description
Data review icons	
Available when a result file is the current page in the application window. When the respective view is open, brings the view to the forefront or makes the view the active view.	
	Opens the Summaries view as a docked view. Available when the Summaries view is closed.
	Opens the Custom Tags Editor as a floating window.
	Opens the Result Filters view as a floating window.
	Opens the Chromatograms view as a docked view.
	Opens the Mass Spectrum view as a docked view.
	Opens the Trend Chart view as a docked view.
	Opens the Isotopologues Distribution Chart view as a docked view. Available when the opened result file includes an analysis of labeled compounds.
	Opens the Mass Defect Plot view as a docked view.
	Opens the Results Chart view as a floating window. The Results Chart view includes the following pages: Scatter Chart, Histogram Chart, Bar Chart, and Pie Chart.
	Opens the Descriptive Statistics view as a docked view.
	Opens the Differential Analysis view as a docked view.
	Opens the Principal Component Analysis view as a docked view.
	Opens the Partial Least Squares–Discriminant Analysis (PLS–DA) view as a docked view.
	Opens the Hierarchical Cluster Analysis view as a docked view.

Table 6. Toolbar icons (Sheet 3 of 3)

Icon	Description
	Opens the Retention Time Corrections view as a docked view. Available when the result file includes more than one input file.
	Opens the Compounds Area Correction view as a docked view.
	Opens the Metabolika Pathways view as a docked view. Available when the result file includes mapped BioCyc pathways.
	Opens the BioCyc Pathways view as a docked view. Available when the result file includes mapped BioCyc pathways.
	Opens the KEGG Pathways view as a docked view. Selecting an item in the KEGG Pathways result table opens the reference pathway for the item in the KEGG Pathway view. Available when the result file includes compounds mapped to KEGG pathways.
	Opens the mzLogic Analysis view as a docked view.
	Opens the FISh Annotations Queue view as a docked view.
Reporting icons Available when a result file (not necessarily the current page) is open in the application window.	
	Opens the Open Report Design Template dialog box for selecting a report template (.cdReportTemplate).
	Opens the Customize Report dialog box for setting up a custom report template.
	Opens the Open Report Design Template dialog box for selecting a report template (.cdReportTemplate).

Change the size of the toolbar icons

You can choose between large or small icons for the Compound Discoverer toolbar. By default, the toolbar displays large icons.

❖ **To change the size of the toolbar icons**

Do one of the following:

- To display small icons in the toolbar, right-click the application toolbar and choose ✔ **Show Large Icons**.
- To display large icons in the toolbar, right-click the application toolbar and choose **Show Large Icons**.

Note The check mark to the left of Show Large Icons indicates that the application is set to display large toolbar icons.

Figure 5 shows the toolbar set to display large icons.

Figure 5. Compound Discoverer toolbar with large icons

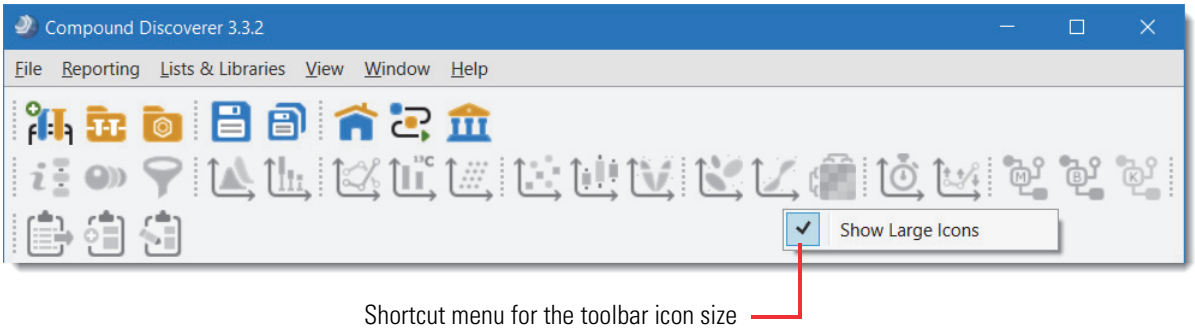
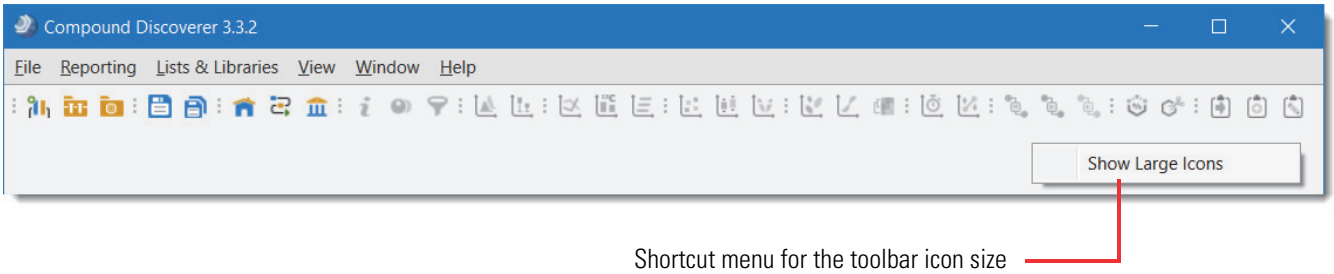


Figure 6 shows the toolbar set to display small icons.

Figure 6. Compound Discoverer toolbar with small icons



Manage the recently used files lists on the Start Page

The right side of the Start Page displays lists of the most recently opened study and result files. You can clear the recent file lists, remove files from these lists, keep one or more files at or near the top of each list, or open the folder where a specific study file or result file resides.

Table 7. Managing the recent files lists

Task	Procedure
Keep files at the top of a recent files list.	Click the pin icon to the left of the file name. The orientation of the pin changes from  to  . When you pin more than one file, the files appear at the top of the list in the order that you pin them.
Remove files from the recent files lists.	• To remove a single file, right-click the file and choose **Remove From List**. • To clear the entire list, right-click any file in the list and choose **Clear List**.
Explore the contents of a folder where a study file or a result file is stored.	Under the recent files list, right-click a study file or a result file and choose **Explore Path**. Windows Explorer opens to the folder for the selected study file or result file.

Auto-Hide the Start Page, the Chromatograms view, and the Mass Spectrum view

To make more space for other views, you can auto-hide the Start Page and the Chromatograms and Mass Spectrum views in the Compound Discoverer window. The auto-hide features collapses each of these items down to a small tab.

❖ To use the auto-hide feature

1. Right-click the page tab and choose **Dockable**.

   The Auto Hide command becomes available for the Start Page and the Chromatograms and Mass Spectrum views. This command remains unavailable for all other dockable pages.

2. Right-click the page tab and choose **Auto Hide**.

   The tab changes to a vertical tab on the left of the application window.

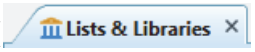
3. To view the hidden page, click its tab.

4. To hide the page, click anywhere in the application window outside the page borders.

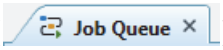
Show, hide, and rearrange the tabbed pages of the application

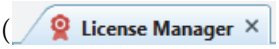
As you open top-level views, study files, and result files in the Compound Discoverer window, they open as tabbed pages (also known as documents) below the toolbar.

- Start Page (

)
- Lists and Libraries manager (

)
- Configuration (

)
- Job Queue (

)
- Report Templates ( *Report Template Name*)
- License Manager (

)
- Study files ( *Study Name* ×)
- Result files ( *Result File Name* ×)

Note Excluding the Start Page and Job Queue, views that open from the View menu or toolbar are not tabbed documents—that is, when they are open, they are not listed in the open files.

To display, dock, hide, or rearrange the tabbed pages (documents), see these topics:

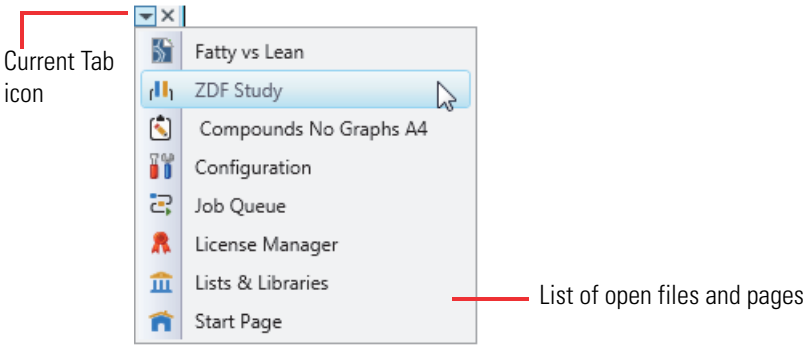
- Tabbed pages list
- Open a hidden tabbed page
- Tab groups
- Shortcut menu commands that control the layout of the tabbed pages
- Rearrange the tabbed pages and graphical views

Tabbed pages list

Although you can have all the tabbed pages (documents) open simultaneously (including multiple study files and result files) the number of tabs that the application can display is limited by the monitor size. As you open more files than the monitor can display, the tabs begin to disappear from view in the order that you opened the files. To indicate that one or more tabs are hidden, the Current Tabs icon changes from ▼ to ▼.

The following figure shows a list of open files and pages.

Figure 7. List of open files and pages



Open a hidden tabbed page

❖ **To display an open tabbed page (document) when its tab is hidden**

Click the **Current Tabs** icon, ▾, to display a list of open files. Then, select the appropriate tabbed page from the list.

The selected page becomes active.

Tab groups

In the Compound Discoverer window, when two or more tabbed pages (documents) are open in the same tab group, you can create more tab groups. Each tab group has its own Current Tabs icon, ▾. Figure 8 shows tab group examples.

Figure 8. Orientation of tab groups

Shortcut menu commands that control the layout of the tabbed pages

Table 8 describes the shortcut menu commands that control the properties of the tabbed pages (documents) in the Compound Discoverer window.

Table 8. Shortcut menu for tabbed documents (Sheet 1 of 2)

Command	Description
Dockable	Activates the Auto Hide command. Available for the Start Page and the result file views. This command is not available for the Job Queue page.
Tabbed Document	Makes the page a tabbed document. Available for the Start Page, Job Queue page, License Manager page, library pages, study pages, result file views, and report template pages.
Auto Hide	Hides the page while leaving the tab visible. Clicking the tab opens the page. Clicking outside the page closes the page if more than one tabbed document is open. The location of the tab depends on the position of the tabbed document in the application window. Available for the Start Page and the views in the View menu when these pages are dockable windows. This command is not available for the Job Queue page.
Hide	Closes the tabbed document.
Move to Previous Tab Group	Changes the position of the tabbed document. Available only when the application window contains two or more tabbed groups.
Move to Next Tab Group	Changes the position of the tabbed document. This command is available only when the application window contains two or more tabbed groups.
New Horizontal Tab Group	Moves the selected tabbed document to a new horizontal tab group. Available only when there are two or more tabbed documents that belong to the same tab group in the application window. Each tab group has its own Current Tab icon.

Table 8. Shortcut menu for tabbed documents (Sheet 2 of 2)

Command	Description
New Vertical Tab Group	Moves the selected tabbed document to a new vertical tab group. Available only when there are two or more tabbed documents that belong to the same tab group in the application window. Each tab group has its own Current Tab icon.

Rearrange the tabbed pages and graphical views

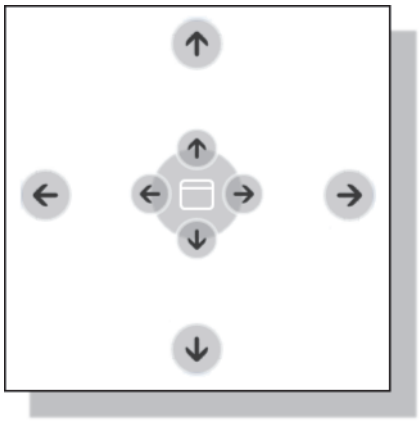
To make the best use of your screen space, rearrange the graphical views and tabbed pages (documents) as follows:

- Use the mouse pointer to move the graphical views that are available when you open a result file from one dock position to another dock position or to a second monitor.
- Use the mouse pointer or the shortcut menu commands to rearrange the tabbed pages within the application window. For information about using the shortcut menu commands, see "Shortcut menu commands that control the layout of the tabbed pages."

❖ To move a view or tabbed page to another position by using the mouse pointer

1. Drag the view by its title bar or the page by its tab. As you drag a view or a tabbed page by its title bar, a guide tool appears. The guide tool consists of four directional arrows (inner arrows) that are arranged in a diamond pattern around a central circle. In addition to the guide tool, a directional arrow (outer arrows) appears in the middle of each of the four window edges.

   Figure 9. Guide tool

2. After the guide tool appears, align the pointer with the appropriate directional arrow, and then release the mouse button.

Table 9. Rearranging views and tabbed pages by using the mouse pointer

Task	Procedure
Move a graphical view to another monitor.	Drag the pointer to the second monitor.
Move the selected view above the second view. Move the tabbed page to a horizontal group above the current group.	Drag the pointer to the inner up arrow,  .
Move the selected view below the second view. Move the tabbed page to a horizontal group below the current group.	Drag the pointer to the inner down arrow,  .
Move the selected view to the left of the second view. Move the tabbed page to a group on the left.	Drag the pointer to the inner left arrow,  .
Move the selected view to the right of the second view. Move the tabbed page to a group on the right.	Drag the pointer to inner right arrow,  .
Make both views tabbed.	Drag the title bar to the tabs icon.  The application displays the first view and creates a tab for the second view.
Move the selected view to the top or bottom of the window. Move the tabbed page to the top or bottom of the window.	Drag the pointer to the outer top arrow or the outer bottom arrow.
Move the first view to the left side or right side of the window. Move the tabbed page to the left side or right side of the window.	Drag the pointer to the outer arrow at the left of the window or the outer arrow at the right of the window.

Supported file formats

Table 10 describes the file types that the application can recognize or create.

Table 10. Supported file formats (Sheet 1 of 2)

File format	Description
Xcalibur RAW file	Contains unprocessed data acquired from a high-resolution, accurate mass (HRAM) Thermo Scientific mass spectrometer with a Thermo Scientific data system that is layered on the Thermo Foundation™ platform.
MOL format (.mol), compressed structure (.mcs), template (.tml)	Contains a two-dimensional compound structure. You can open structure files by using the Structure Editor or the Custom Explanations Editor.
SDF	Contains one or more two-dimensional compound structures. You can import compounds from an SDF file into the Expected Compounds library.
XLSX or tab-delimited text file	Contains the study information for a set of input files. See "Create a study template file that contains all the study information."
cdProcessingWF 	Contains the data processing instructions for the application. To create a processing workflow, you must start or open an analysis in a study.
cdAnalysis	Stores the processing workflow information.
cdStudy 	Stores the study information, which includes the names and locations of the input files, the sample information, and the relationship between the input files.
cdResult 	Contains the results produced by processing a set of raw data files and information about the analysis settings used to process the raw data.
cdResultView 	Contains the layout settings that the application uses to display the available tables and graphical views of a result file. These settings also include the applied result filters. Deleting this file erases all the custom layout settings and restores the display to the default layout settings.

Table 10. Supported file formats (Sheet 2 of 2)

File format	Description
cdReportTemplate	Contains the layout for reports that extract data from the following items in a result file: selected columns in one main table, selected columns in the related tables, and selected graphical views (MS1, MS2, and Chromatograms).
Inclusion set (.inclSet)	Contains all the parameter settings for generating an inclusion list with the Generate Xcalibur Inclusion List dialog box.
Filter Set (.filterset)	You can use filter set files for data reduction when reviewing and reporting the data in Compound Discoverer result files. The application comes with one predefined filter set file—Example Filter Set.filterset.
Mass list (.masslist)	Contains a mass list that is compatible with the Compound Discoverer mass list editor.
metabolika	Contains a metabolic pathway drawing that is compatible with the Compound Discoverer Metabolika Pathway editor.
mgf, mzML, mzDATA	Contains the mass spectral data that can be read by third-party mass spectrometry applications. To create any of these files types, use the Export Spectra Node in a processing workflow.
XML	You can export each library to an XML file, and you can import library entries from an XML file.
TAGS	Contains a set of user-defined custom tags.
text (.txt)	You can save the data points in the graphical views to a text file.
EMF, BMP, JPG, GIF, PNG, TIFF	You can save the images in the graphical views as image files of the following file types: enhanced metafile (.emf), bitmap (.bmp), Joint Photographic Group (.jpg), graphic interchange format (.gif), portable network graphics (.png), and tagged image file format (.tiff). You can open EMF files in a raster image editor or a vector image editor.
CSV	You can import the contents of a CSV file into a Mass List file.
CLIB	You can import the contents of a CLIB file as a Compound Class list. A compound class list contains the fragment structures that are common to the named compound class.
DB	You can import mzVault libraries into the Spectral Libraries list.
MSP	You can export compounds as MSP files that you can then import into the NIST MS Search application.

2

Functional description of the data-processing features

For an overview of the compound detection, identification, and scoring features in the Compound Discoverer application, see the following topics:

- Chromatographic peak detection, alignment, and identification for LC Studies
- Chromatographic peak rating filter
- Peak quality factors
- Online compound databases and metabolism pathways
- Local spectral databases, mass lists, and metabolism pathways
- Best scans for composition prediction and spectral matching
- Using mzLogic to score candidates for unknown compounds
- Confidence score for an mzCloud hit
- FISh scoring for proposed structures
- Mass defect types and visualization techniques
- Neutral loss detection and visualization
- Using quality control samples to compensate for batch effects
- Batch normalization for single sequence runs
- Batch normalization for multiple sequence runs (LC studies)
- Stable isotope labeling experiments
- PFAS identification
- Methods for imputing values for missing chromatographic peaks across a set of input files

Chromatographic peak detection, alignment, and identification for LC Studies

For LC-MS/MS data, the application processes the high-resolution scan data as follows:

1. Reads the raw data files.
2. Filters the spectra by the specified filters.

   IMPORTANT If the input files are from a FAIMS-MS experiment and any of them include spectra for more than one FAIMS CV value (also known as CV switching), you must specify the CV value that you want to process, and all the input files must include spectra for the user-specified CV value.

   If the input files are from an experiment with mass range switching, you must specify the mass range that you want to process, and all the input files must include spectra for this mass range.

3. Aligns the input files by their alignment features when the analysis includes multiple input files and the processing workflow includes the Align Retention Times (ChromAlign) node or the Alignment Retention Times node.

   Note Most of the processing workflow templates in the Common Templates folder use the Align Retention Times (ChromAlign) node.

   The Align Retention Times (ChromAlign) node is new in the Compound Discoverer 3.3 application. This node automatically selects the first sample file in the Files for Analysis area of an analysis as the reference alignment file. A sample file is an input file assigned any of the following sample types: Sample, Control, or Standard. After you add input files to the Files for Analysis area of the analysis, you can select a different sample file as the reference file.

   The legacy Align Retention Times node individually aligns each feature ((m/z × RT)) as follows:

   - When the set of input files includes only one sample group, the node uses the input file with the most features (landmarks) as the reference file.
   - When the set of input files includes multiple sample groups, the node aligns the features (m/z value × RT) within a group first. Then, aligns the features among the groups based on which group has the most features.

   The new Align Retention Times (ChromAlign) node builds correlation matrices based on spectral similarities. Then, creates regression curves by using the optimal path in the correlation matrix.

   Tip Use the Retention Time Corrections view and the File Alignments table to review the corrected retention time of each detected compound in a result file.

4. Detects the XIC traces and chromatographic peaks by doing the following:

   - For an untargeted processing workflow that includes the Detect Compounds node, the analysis detects the chromatographic peaks in the XIC traces.
   - For a targeted processing workflow that includes the Expected Compounds node, the analysis searches for the expected compounds in the XIC traces.

   Both the Detect Compounds node and the Find Expected Compounds node calculate the chromatographic peak areas (for relative quantitation) according to the following parameter settings:

   - Use Most Intense Isotope Only:
     - True: Displays the area of the chromatographic peak in the XIC trace for the most intense isotope in the isotope pattern for the compound.
     - False: Displays the combined area for all the detected isotopes in the isotope pattern for the compound.

     The Detect Compounds node automatically detect the isotope pattern for organic compounds with the following elements: C, H, N, O, and S. You have the option to add Cl and Br to this list.
   - Remove Baselines:
     - True: Does not include the extra area caused by integrating the area under the XIC trace down to the baseline.
     - False: Drops a perpendicular tangent line from the start and end points of the chromatographic peak down to the baseline and includes this additional area in the reported peak area.

5. Groups the compounds across the input files as follows:

   - An untargeted processing workflow groups each compound across the input file set by its MW × RT dimensions.
   - A targeted processing workflow groups each expected compound across the input file set by its formula × MW × RT dimensions.

   When you turn on the peak rating filter, the grouping nodes (Group Compounds and Group Expected Compounds) store only the compounds that pass the filter in the analysis result. In addition, they do not send these failing peaks to the downstream nodes (Fill Gaps, Peak Area Refinement, Identification, Pathway Mapping, Compound Scoring) for further processing, which speeds up the processing time.

   Even when you do not turn on the peak rating filter, you can use the Result Filters view to filter the compounds in the analysis result by using the Peak Rating column or by any of the peak quality factor (PQF) columns in the compounds tables. By default, the PQF columns are hidden.

   For details, see "Chromatographic peak rating filter."

6. For an untargeted workflow, fills the gaps for missing chromatographic peaks when the processing workflow includes the Fill Gaps node.

   Filling the gaps with nonzero values is necessary for the statistical analyses.

7. For an untargeted workflow, predicts the elemental composition of the compounds when the processing workflow includes the Predict Compositions node.

8. Assigns annotations to the compounds by using the available information from the identification and pathway mapping nodes when the processing workflow includes the Assign Annotations node.

Chromatographic peak rating filter

The new Group Compounds and Group Expected Compounds processing workflow nodes include a peak rating filter. This filter allows you to remove low-quality chromatographic peaks without setting an overly restrictive minimum peak intensity threshold in the Detect Compounds node or the Find Expected Compounds node.

Note An appropriate intensity threshold for chromatographic peaks is difficult to estimate, especially for untargeted experiments. So, attempting to remove noise-level peaks by setting a minimum intensity threshold commonly removes low-intensity peaks that must then be gap-filled to perform statistical analyses.

The new processing workflow templates for untargeted analyses perform the initial peak detection at a very low minimum peak intensity threshold of 10 000 (minimum intensity, in ion counts, at the chromatographic peak apex). This low-intensity threshold filters out very few chromatographic peaks. To remove low-quality or non-reproducible peaks, you can set up a peak rating filter in the Group Compounds node. This peak rating filter combines peak quality and peak reproducibility across the input file set.

Note When you submit 10 or more input files (assigned the Control, Standard, Sample, or Blank sample type) for processing and the analysis includes one or both of the grouping nodes, the application prompts you to set up a peak rating filter.

The application considers only the following sample types when it calculates the total number of files for the analysis: Control, Standard, Sample, and Blank. It excludes the following sample types from the total number of files: Identification Only and Labeled.

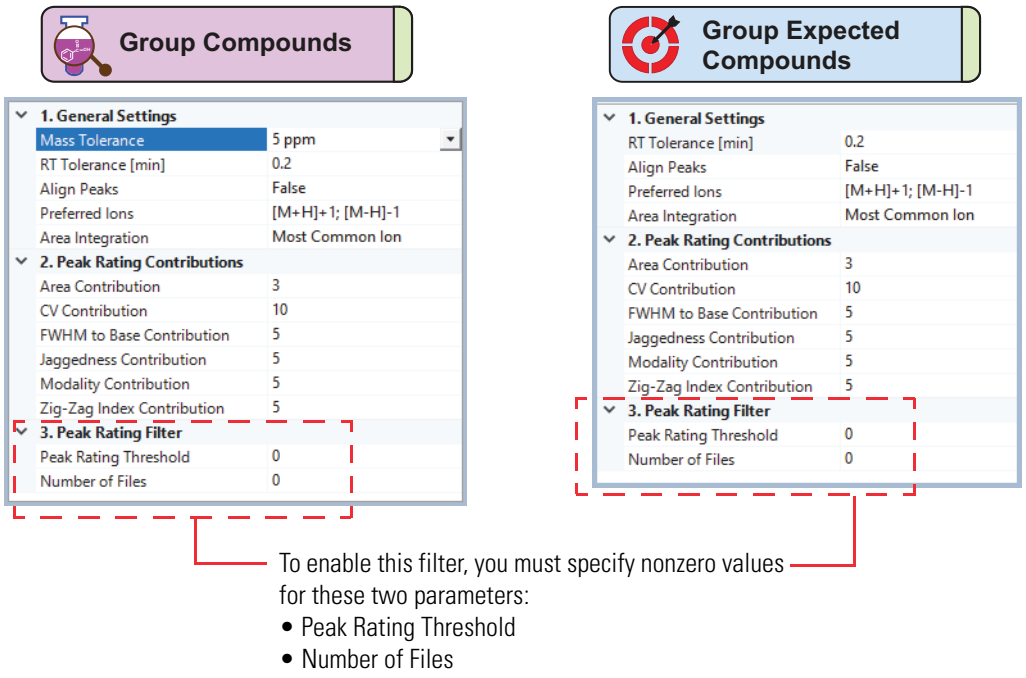
The processing workflow templates for targeted analyses still include a relatively high minimum peak intensity threshold of 1 000 000. So, these templates automatically remove low-intensity noise-level chromatographic peaks for most analyses. However, when you are analyzing large data sets with similar samples, you might find it useful to set up a peak rating filter to remove spurious compounds that are present in only a small subset of the samples.

Note Removing chromatographic peaks that do not pass the peak quality threshold in a specified number of input files at the grouping stage of the analysis decreases the overall processing time by streamlining other processing steps, such as gap filling and identification.

By default, the peak rating filter in the processing workflow templates is not enabled. See Figure 10.

To enable the filter, you must specify the minimum number of input files (number greater than or equal to 1) where the chromatographic peak for a putative compound meets or exceeds the specified peak rating value (0.1 to 10). You can also modify the various peak quality factors that contribute to the overall peak rating value. See "Peak quality factors."

Figure 10. Group Compounds node and Group Expected Compounds node parameters



Peak quality factors

The peak quality factors that contribute to the overall rating (0 to 10) for a chromatographic peak are as follows:

- FWHM2Base quality factor
- Jaggedness quality factor
- Modality quality factor
- Zig-Zag Quality Factor

The Group Compounds and Group Expected Compounds nodes calculate the peak rating of the chromatographic peaks for each compound across the set of input files. The Differential Analysis node recalculates the peak rating values for each chromatographic peak before it performs a differential analysis based on the peak areas.

For information about the peak rating values in the result tables, see "Peak Rating columns." You can filter the compounds in the compounds tables by the Peak Rating column.

For information about the peak quality factor columns in the result tables, see "Peak quality factor (PQF) columns in the result tables." You can filter the compounds tables in the analysis results by the PQF columns.

Note The Detect Compounds (Legacy) node and the Detect Compounds node use different approaches for isotope grouping:

- The Detect Compounds node uses the peak quality information to group the XIC traces for common isotopes of C, H, N, O, and S and optionally for Cl and Br. It ignores XIC traces with low-quality chromatographic peaks for isotope grouping.
- The Detect Compounds (Legacy) node does not use the peak quality information during grouping. It uses the peak quality information only for filtering after grouping.

When used in a processing workflow that runs only a targeted analysis, the Find Expected Compounds node includes hard-coded peak quality thresholds for isotope pattern detection:

- PQF: J (Jaggedness) ≤ 0.4
- PQF: ZZI (Zig-Zag Index) ≤ 0.25
- PQF: M (Modality) ≤ 0.9

When used in a processing workflow that includes a targeted analysis and an untargeted analysis, the Find Expected Compounds node uses the user-specified peak quality thresholds in the Detect Compounds node.

The Find Expected Compounds (Legacy) node does not use peak quality information.

When a processing workflow includes untargeted and untargeted analyses, it can include the Detect Compounds node and the Find Expected Compounds node or the Detect Compounds (Legacy) node and the Find Expected Compounds (Legacy) node.

FWHM2Base quality factor

The peak quality factor for the separation of the chromatographic peaks compares the peak width at half-maximum (height) to the peak width at its base.

$$\mathrm{FWHMB2Base} = \frac{W_h}{W_b}$$

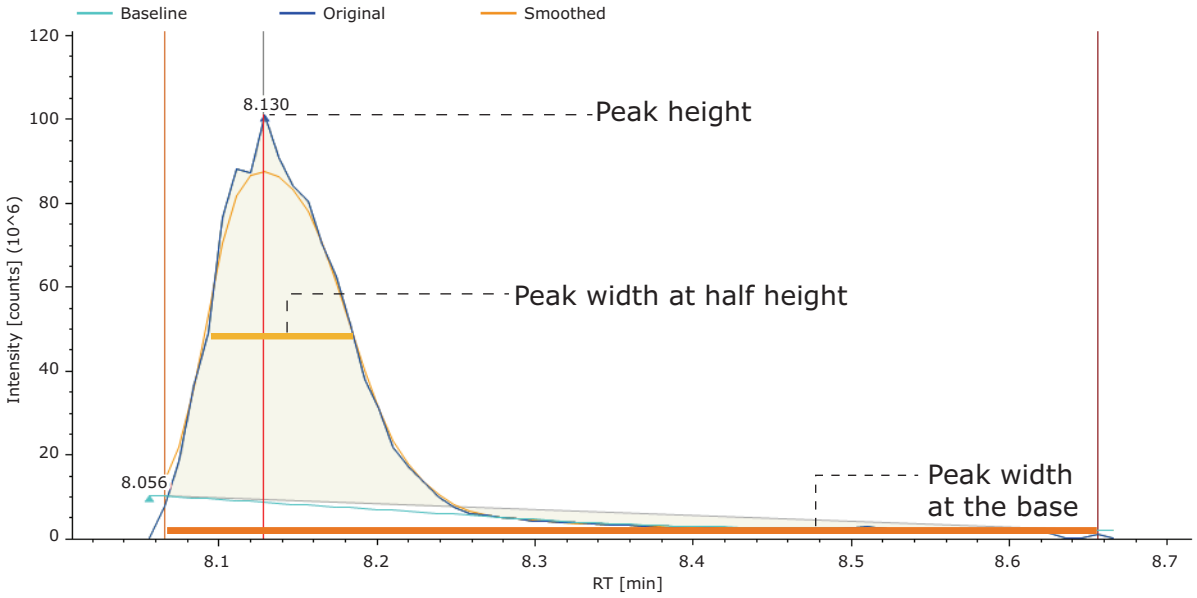
Where:

W_h = the peak width at half the maximum peak height

W_b = the peak width at the base

The calculated value ranges from 0 to 1. As the peak quality increases, the calculated value for the peak quality factor decreases.

Figure 11. FWHM to base peak quality measurement

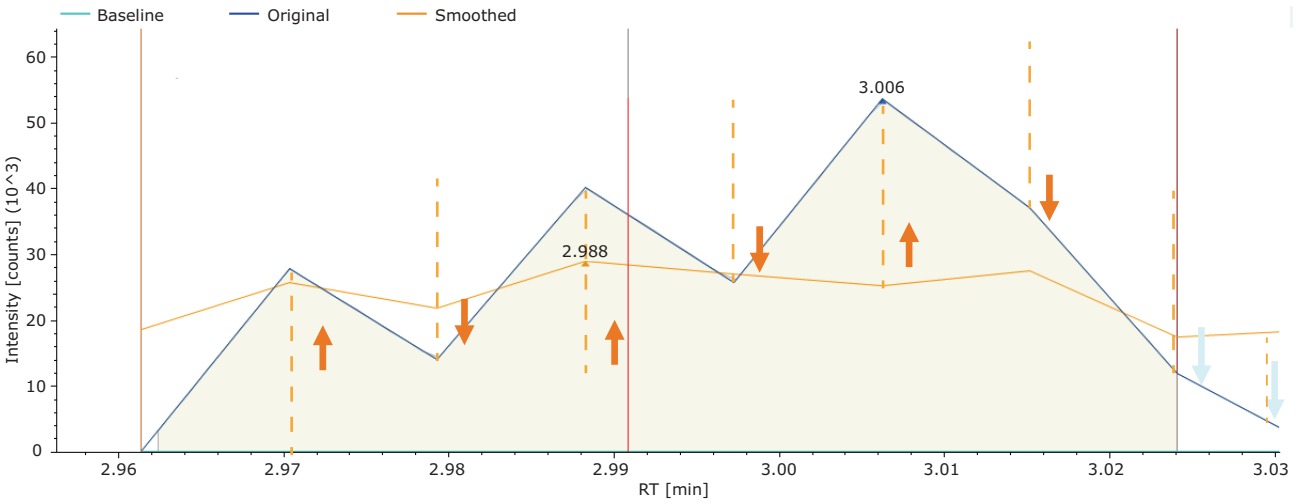


Jaggedness quality factor

The peak quality factor for jaggedness captures the quality of the chromatographic peak shape by calculating the number of changes in direction over the length of the intensity vectors.

The calculated value ranges from 0 to 1. As the peak quality increases, the calculated value for the peak quality factor decreases.

Figure 12. Jaggedness peak quality measurement



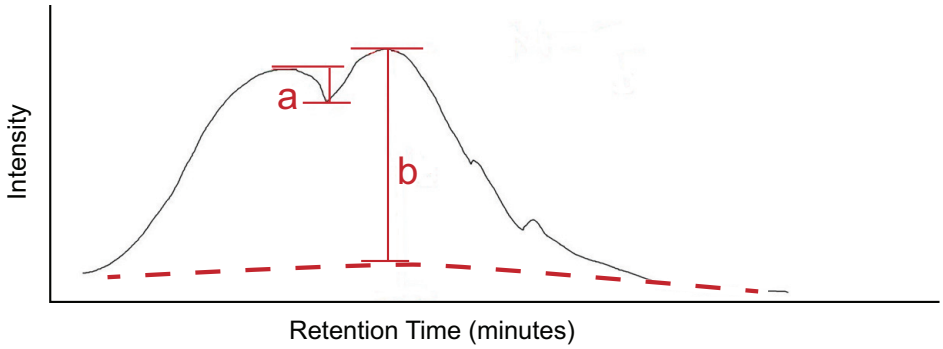
Modality quality factor

The Modality peak quality factor is the size of the deepest valley (= unexpected change) in the peak normalized by the intensity of the peak.

The calculated value ranges from 0 to 1. As the peak quality increases, the calculated value for the peak quality factor decreases.

$$\text{Modality} = \frac{a}{b}$$

Figure 13. Modality peak quality factor measurement



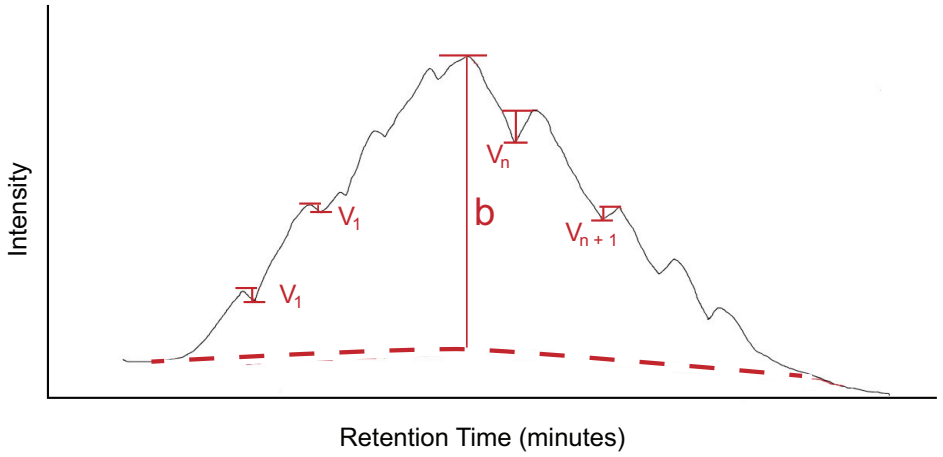
Zig-Zag Quality Factor

The zig-zag index captures the quality of the chromatographic peak shape by measuring the mean of all the valleys across the peak, which is then normalized by the intensity of the peak above the baseline.

$$\text{Zig-Zag} = \frac{\text{Mean}(V_i)}{b}$$

The calculated value is greater than zero, and in some cases it can be greater than one. As the peak quality increases, the calculated value for the peak quality factor decreases.

Figure 14. Zig-zag index peak quality measurement



Online compound databases and metabolism pathways

When the processing computer has Internet access, the Compound Discoverer application can access and use the following online databases for compound identification:

- mzCloud
- ChemSpider
- KEGG
- BioCyc

For information about checking the processing computer's access to these online databases, see Chapter 17, "Test communication to the online databases."

Local spectral databases, mass lists, and metabolism pathways

The local offline databases that you can use to identify and map compounds with the Compound Discoverer application include the following:

- mzCloud offline libraries

  For LC studies, you can create your own mzVault libraries by using the mzVault 2.3 SP1 application.

  For all studies, you can create your own mzVault libraries by exporting the mass spectral data from a compounds table in the analysis result.

- Metabolika pathways

  You can create your own Metabolika pathway drawings by using the Metabolika pathway editor. See "Create a new Metabolika Pathway file."

- Mass lists

  You can create your own mass lists by using the mass lists editor. See "Create and edit mass list files."

Best scans for composition prediction and spectral matching

For each set of raw data files that you submit for processing, the application can select the best MS1 scan and the best MS2 scan for each compound from different input files. This selection is done within the compound consolidation nodes—that is, by the Group Compounds node and the Group Expected Compounds node.

For information about how the application determines and uses the best scans, see these topics:

- Best MS1 scan for isotope pattern matching
- Best MS2 scan for fragments matching and spectral comparison

Best MS1 scan for isotope pattern matching

To determine the best MS1 scan to use for a compound across a set of input files, the consolidation nodes select the MS1 scan with the highest resolution and retention time closest to the peak apex for a compound.

The application sends the isotope pattern information from the best MS1 scan to the following workflow nodes for further processing:

- The Predict Compositions node for isotope pattern matching
- The Apply Spectral Distance node for calculating the spectral distance between the assigned elemental composition and the experimental isotope pattern

Best MS2 scan for fragments matching and spectral comparison

To identify compounds by fragmentation data or to determine the spectral similarity between the fragmentation scans for two different compounds, the application uses the best MS2 scan for each compound.

To determine which MSn scans to attach to a compound, the application does the following:

1. Searches for MS2 scans for the precursor ion within the RT range of the peak apex ± FWHM for a compound.
2. If it finds no MS2 scans for the precursor ion within this range, it searches for scans within the start and end points of the chromatographic peak for a compound, as determined by the Parameterless Peak Detection (PPD) algorithm.
3. To determine the best MS2 scan, it does the following:
    a. Selects the MS2 scan for the preferred ion.
    b. If it finds multiple spectrum trees for the preferred ion, it uses the MS2 scan from the MS1 scan with the highest precursor intensity.

For each compound, the Group Expected Compounds and the Group Compounds nodes send all the MS2 scans associated with that compound to the following nodes:

- Search mzCloud node
- Search mzVault node

For each compound, the Group Compounds node sends the best MS2 scans to the Apply mzLogic node.

Using mzLogic to score candidates for unknown compounds

mzLogic uses all the fragmentation scans (full MSn depth) for an unknown compound to score possible matching candidates.

There are two ways to run the mzLogic scoring algorithm:

- Running an untargeted analysis that includes the mzLogic node
- Running an mzLogic analysis from the mzLogic Analysis view

For information about setting up and running an analysis, see Chapter 4, “Set up, run, and reprocess analyses.”

Running an untargeted analysis that includes the mzLogic node

Processing workflow templates (processing methods) that include the following terms—Online Database Searches or mzLogic—in their file names include the Apply mzLogic node and one or more of the compound identification nodes and pathway mapping nodes.

Tip For information about selecting a processing workflow template for an analysis, see "Start a new analysis from within an existing study."

When an mzCloud search yields no identity matches for an unknown compound, the mzLogic algorithm provides a ranking score for the compound hits from the identification nodes and pathway mapping nodes.

The mzLogic algorithm can provide a ranking score for the various database search results when an unknown compound has available data-dependent MS2 scans and similarity results from an mzCloud similarity search.

Note The ranking score is not a probability score. It is only a measure of how similar the fragmentation spectra for a putative compound are to closely matching spectra in the mzCloud spectral database.

During data processing, the Apply mzLogic node does the following:

1. Runs a forward search and a reverse search using the mzCloud service.
2. For compounds that have available MS2 scans, scores all the structure candidates (or the specified maximum number of candidates) from the attached input nodes.

   Note The following nodes can supply structures to the Apply mzLogic node: Search ChemSpider, Search Mass Lists, Map to BioCyc Pathways, and Map to Metabolika Pathways.

   The mass lists that you select for the Search Mass Lists node must include structures. The Endogenous Metabolites database 4400 Compounds.masslist file does not include structures.
3. Adds the following columns to the result tables:
   - Adds the #Similarity Results column to the Compounds table. By default, this column is hidden.
   - Adds the mzLogic Score column to the following related tables as applicable: ChemSpider Results, Mass List Search Results, Metabolika Results, and BioCyc Results.

Running an mzLogic analysis from the mzLogic Analysis view

If the processing workflow for a result file did not include the Apply mzLogic node, or if you suspect that the online mzCloud spectral database now includes more spectral data, use the mzLogic Analysis view to rank the putative structures for your unknown compounds.

Because the mzLogic Analysis view includes a link to the ChemSpider database where you can select putative structures, the result file does not need to include structure annotations.

For details, see "mzLogic Analysis view."

Confidence score for an mzCloud hit

The application provides two scores for comparing a query spectrum to its library hits—the Confidence score and the Match score.

For details about these scores, see the following topics:

- Factors that affect the Confidence score
- How to use the Confidence score

Factors that affect the Confidence score

The Confidence score is a probability-based library searching and scoring algorithm, primarily developed to reduce the likelihood of a false positive identification. In essence, it is a measure of the probability of a correct compound identification calculated from a Bayesian network extensively trained on searching against the mzCloud database.

The scoring model is based on extracting six observables from a query versus library spectral pair:

- Spectral similarity (expressed as the spectral match value)
- Relative difference in the collision energies for the query and library spectra
- Polarity of the spectra
- Number of peaks in the spectra
- Relative energies of the query spectrum and library spectrum
- Identity of the compounds that produced the library spectrum and the query spectrum

The final score for a query spectrum versus library spectrum pair is based on the likelihood of two spectra belonging to the same compound given the observed spectral match, the collision energy of the unknown, the number of peaks in each spectrum, the polarity of each spectrum, and the difference in the relative collision energies of the two spectra.

The following examples illustrate how to use the confidence score and the match score for a query versus library spectrum comparison.

Example 1: Comparison of spectra with non-specific features (fragment ions)

Suppose that you are identifying 6-hydroxynicotinic acid in your sample and assume that the representative query spectrum for your sample exactly matches the mzCloud library spectrum, producing a match score of 100.

When you search the mzCloud library using the standard ID search, which is restricted only to the product spectra with a matching precursor ion, you find very similar spectra for related compounds. Because the spectrum is non-specific, any molecule with the same molecular weight and adduct is likely to have the same non-fragmented spectrum at the lower end of activation energies. The Confidence algorithm severely penalizes these library search results because they are based on a non-specific spectral fingerprint (only 1 precursor peak), making the probability of a correct ID very low.

Figure 15. MS2 HCD 20 product spectrum of 6-hydroxynicotinic acid

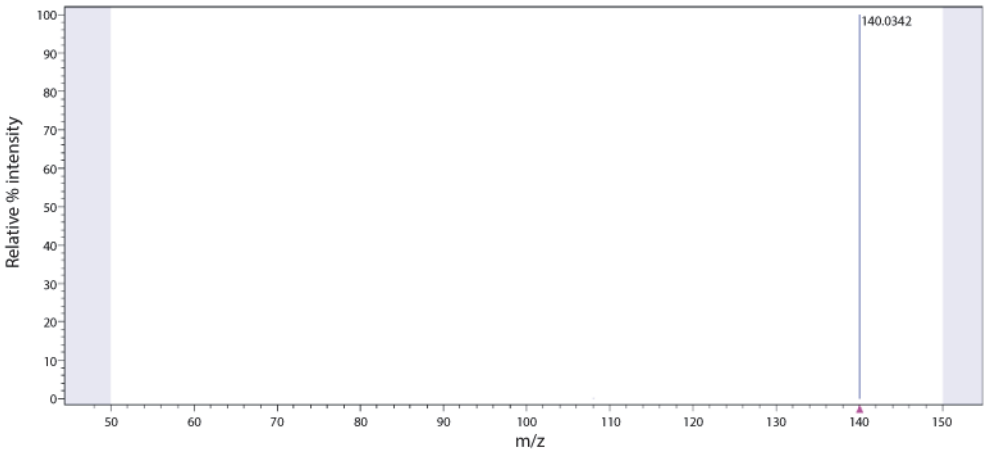
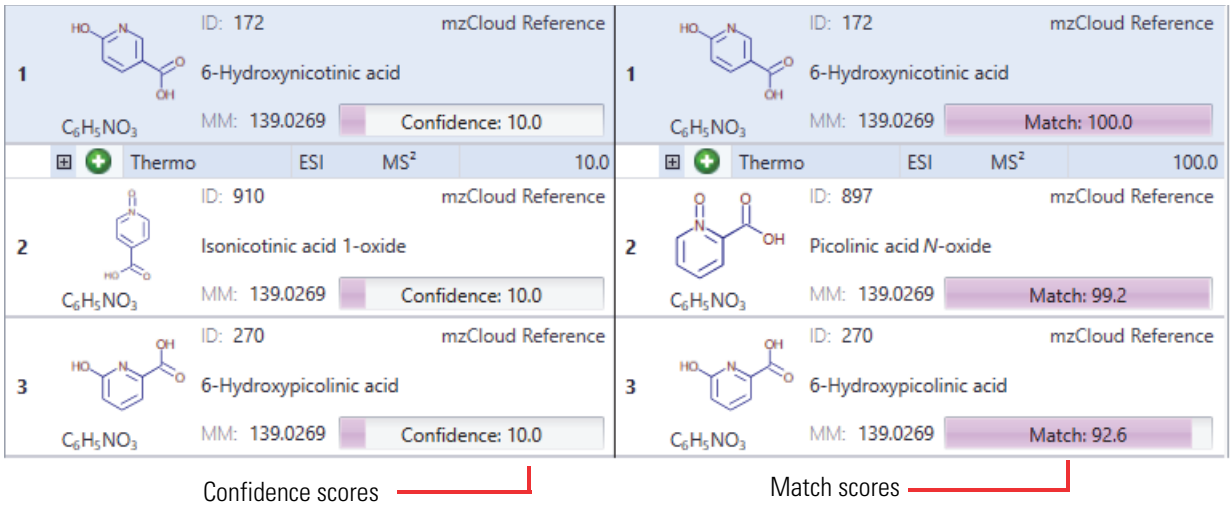


Figure 16 shows the Confidence and Match scores for the three top hits for the low-energy fragmentation scan of 6-hydroxynicotinic acid. Because the query and library spectra are so non-specific (with only one fragment peak), the Confidence scores are extremely low compared to the Match scores.

Figure 16. mzCloud search results for a query spectrum of 6-hydroxynicotinic acid obtained at a collision energy of 20 HCD



Example 2: Comparison of fragmentation-rich spectra

At a higher collision energy of 100 HCD, the fragmentation of 6-hydroxynicotinic acid produces a much richer fragmentation spectrum. The breakdown curves in Figure 17 show that this fragmentation energy is close to the optimum for generating characteristic fragments.

Figure 17. Breakdown curves for the HCD fragmentation of 6-hydroxynicotinic acid

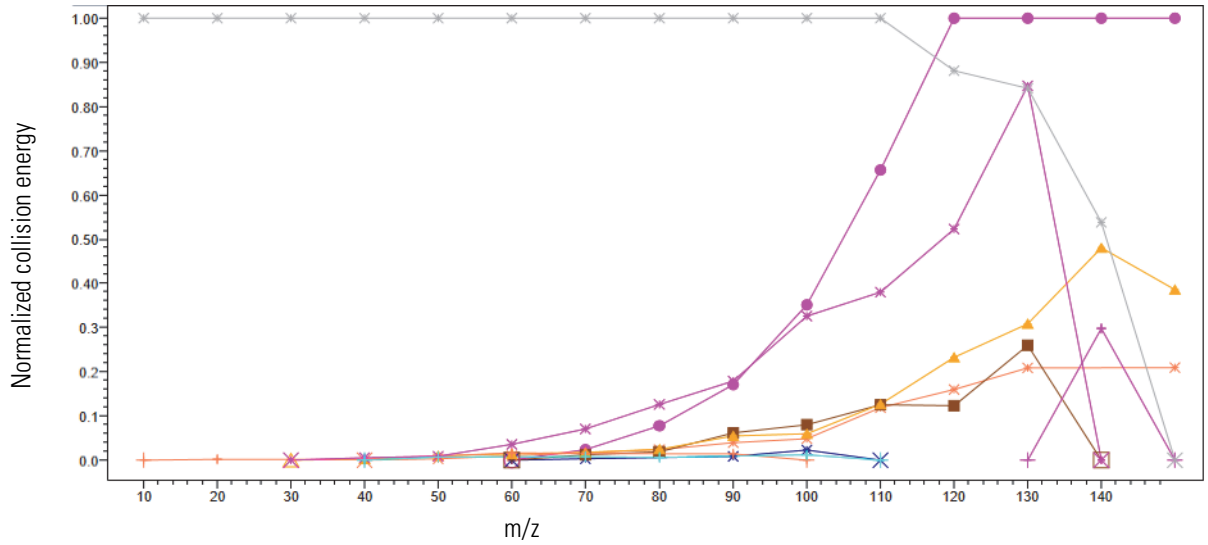
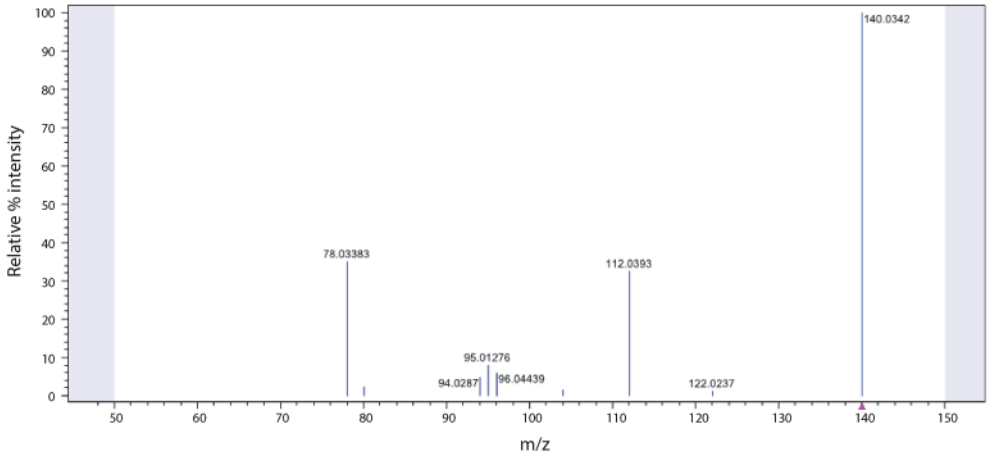


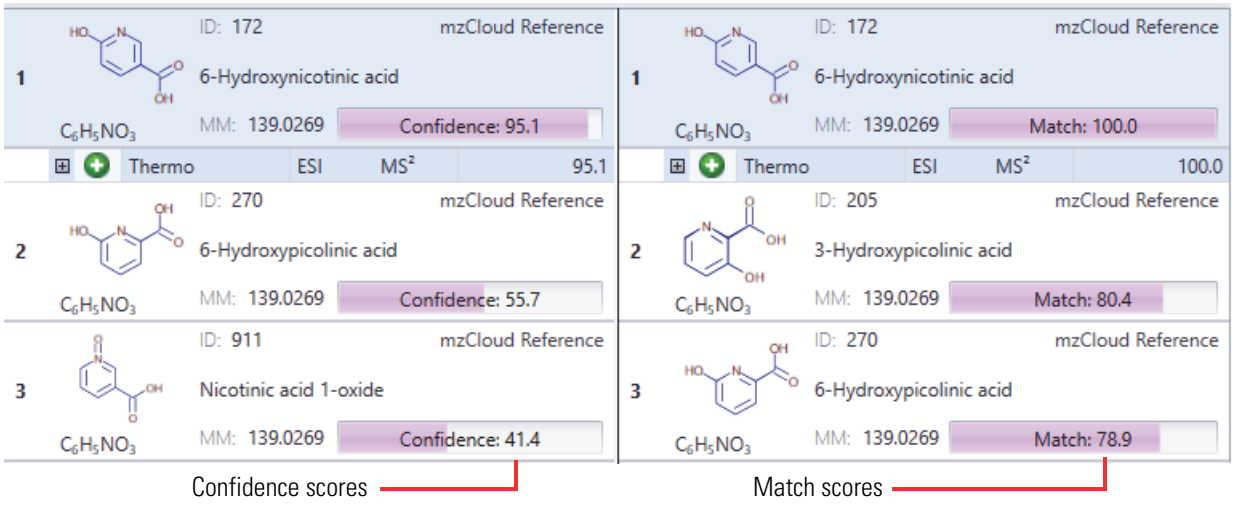
Figure 18 shows the fragmentation spectrum for 6-Hydroxynicotinic acid at the higher fragmentation energy (HCD 100).

Figure 18. MS2 HCD 100 product spectrum of 6-hydroxynicotinic acid



The search results against the mzCloud database look very different from the first example at the lower fragmentation energy. In Figure 19, you see greater separation in the scores between the true hit (6-hydroxynicotinic acid) and its analogs (false hits). The separation is even more pronounced in the Confidence score ranking.

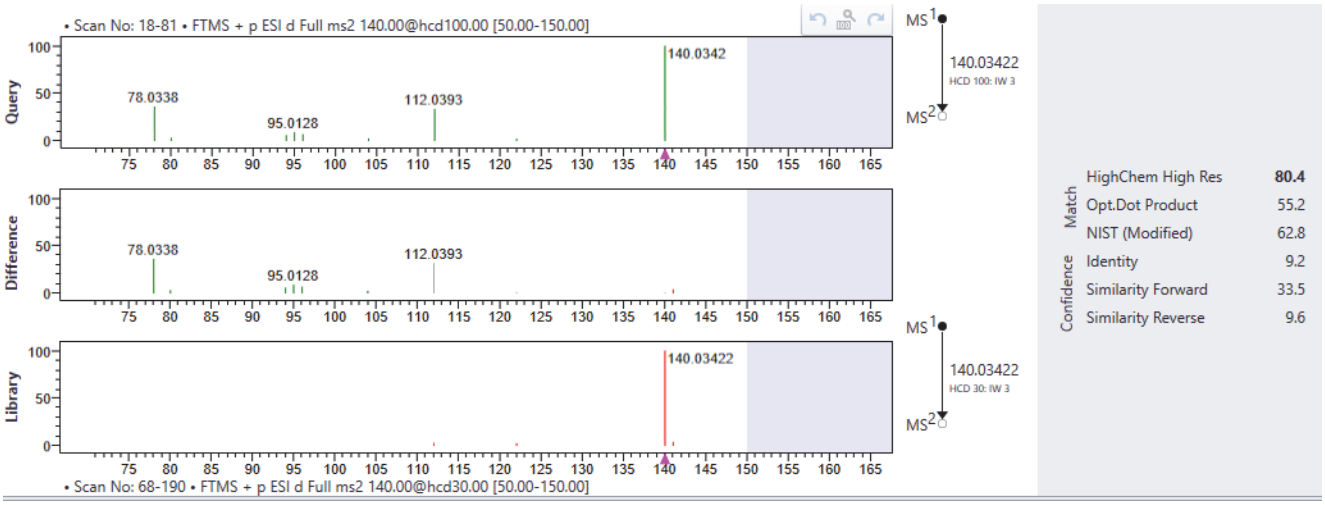
Figure 19. mzCloud search results for a query spectrum of 6-hydroxynicotinic obtained at a collision energy of 100 HCD



When you look at the next best library hit, 3-hydroxypiconilic acid, which is a positional isomer of the true hit, you see different fragmentation energies for the query spectrum (HCD 100) and the library record (HCD 30). The assumption is that identical compounds at similar fragmentation energies produce similar fragmentation spectra. So, if you observe

similar fragmentation spectra (= a high spectral match score) at different collision energies, it might mean that the original assumption of identical compounds is incorrect, which the heavily penalized Confidence score (80.4 spectral match score versus 9.2 confidence score) reflects for this particular result.

Figure 20. Query spectrum (HCD 100) versus library spectrum (HCD 30)



How to use the Confidence score

Use the Confidence score as an additional metric to prevent conclusions based on poor input data. Many applications display library search results in a tabular format with only a spectral match score. But a good match score can be misleading if the fragmentation fingerprint is non-specific.

When the Confidence score is significantly lower than the Match score, evaluate the possible reason for this difference.

When the Match score and the Confidence score are both greater than 80%, the confidence that you are identifying the compound correctly is relatively high.

FISh scoring for proposed structures

The FISh scoring algorithm works with both LC/MSn data and GC CI data.

The FISh scoring algorithm compares the experimental fragmentation spectra for a compound to the expected fragmentation spectra based on the structure of the compound.

Note In the 3.1 and later versions of the application, the FISh scoring algorithm uses all the fragmentation scans (in the spectrum tree for a compound), compared to earlier versions of the application that only used MS2 scans. Therefore, if you reprocess data sets that you already processed with an earlier version of the application, and these data sets include MSn scans (where n > 2), the FISh coverage scores might be lower.

For targeted compounds (expected compounds), you can add FISh scoring to the automated analysis.

For untargeted compounds, you can apply FISh scoring to your proposed structures or compounds with structures and MS2 or higher spectra.

The FISh scoring algorithm matches the fragment structures in a list of expected fragments to the centroids in the fragmentation scans of the precursor ions.

When a precursor ion scan is followed by only one fragmentation scan, the node calculates the FISh coverage score as follows:

$$\text{FISh coverage score} = \frac{\#\text{ matched centroids}}{\#\text{ used centroids}} \times 100$$

where:

matched centroids represents the number of matched centroids.

used (matched + unmatched) centroids represents the number of centroids in the fragmentation scan that are above the user-specified signal-to-noise threshold. The algorithm skips centroids below the user-specified signal-to-noise threshold.

When a precursor scan is followed by more than one fragmentation scan, the node calculates a composite score as follows:

$$\text{FISh coverage score} = \frac{\left(\Sigma_{\text{per all scans}} \#\text{ matched centroids}\right)}{\left(\Sigma_{\text{per all scans}} \#\text{ used centroids}\right)} \times 100$$

The FISh scoring algorithm annotates the centroids in the fragmentation scans with the matching fragment structures. It also provides a FISh Coverage score for data-dependent scans in the Mass Spectrum view legend and a FISh Coverage score in the compounds table.

Mass defect types and visualization techniques

In the Compound Discoverer application, you can use the mass defect of an elemental composition to do the following:

- Filter the spectral data during processing to keep or remove expected and detected compounds by their mass defect.
- Calculate the mass defect of each detected compound by using multiple calculation methods during processing, and then sort the resulting table of detected compounds by their mass defect.
- View a plot of the mass defects for the detected compounds versus their molecular weights to visualize the similarity between the compounds.

Table 11 lists the formulas that the application uses to calculate the mass defect of an elemental composition.

Table 11. Mass defect types

Mass defect type	Formula
Fractional mass	exact mass – floor of the exact mass where: exact mass = monoisotopic mass of the elemental composition
Standard mass defect	exact mass – nominal mass where: nominal mass = integer mass of the elemental composition The application calculates the integer mass by using the selected rounding function: • Floor rounds down • Ceiling rounds up • Round rounds to the nearest integer value
Relative mass defect	$1e^6$ × (exact mass – nominal mass)/exact mass
Kendrick mass defect	Kendrick mass – nominal Kendrick mass where: Kendrick mass = a × (b/c) a = exact mass of the elemental composition b = nominal mass of the Kendrick formula c = exact mass of the Kendrick formula

For more information about using the mass defect feature, see these topics: "Filter By Mass Defect node," "Calculate Mass Defect node," and "Mass Defect Plot view."

Neutral loss detection and visualization

The identification of neutral loss fragments in the fragmentation spectra for an unknown compound adds confidence to the identification of the compound.

For LC studies, follow these steps to report neutral loss fragments and to visualize the spectral peaks that are due to neutral losses from higher-mass precursor ions in the fragmentation scans for compounds in the Compounds table:

1. Add the Search Neutral Losses node to the processing workflow and specify the neutral losses for the search. See "Search Neutral Losses node."

   The Group Compounds node automatically connects to the Search Neutral Losses node.

   Note The *m/z* value of an expected fragment ion equals the *m/z* value of the best MS2 ion minus the user-specified neutral loss.

   Tip Because the Search Neutral Losses node is downstream of the Group Compounds node, you can quickly run a neutral loss search by reprocessing a previous analysis. See "Reprocess an analysis."

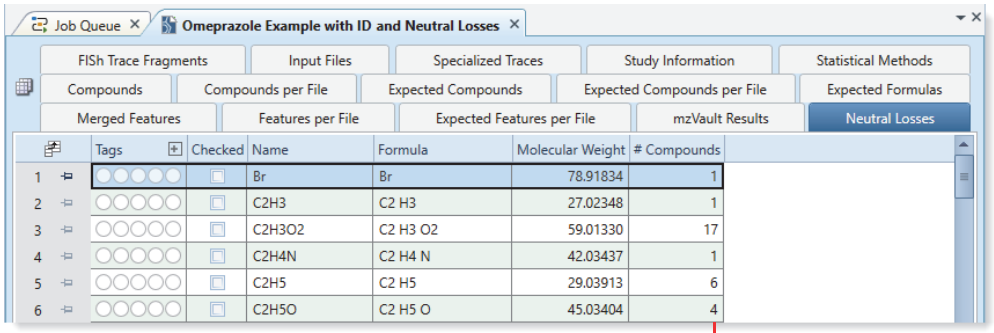
2. After you run an analysis with a processing workflow that includes the Search Neutral Losses node, open the result file.

   The Search Neutral Losses node generates the following:

   - The Neutral Losses column in the Compounds table
   - The main Neutral Losses table (see Neutral Losses table)
   - A related Neutral Losses table for each detected compound

3. To check how many compounds the analysis found for each specified neutral loss, click the **Neutral Losses** tab in the main result tables pane.

Figure 21. Neutral Losses table for an analysis with two specified neutral losses



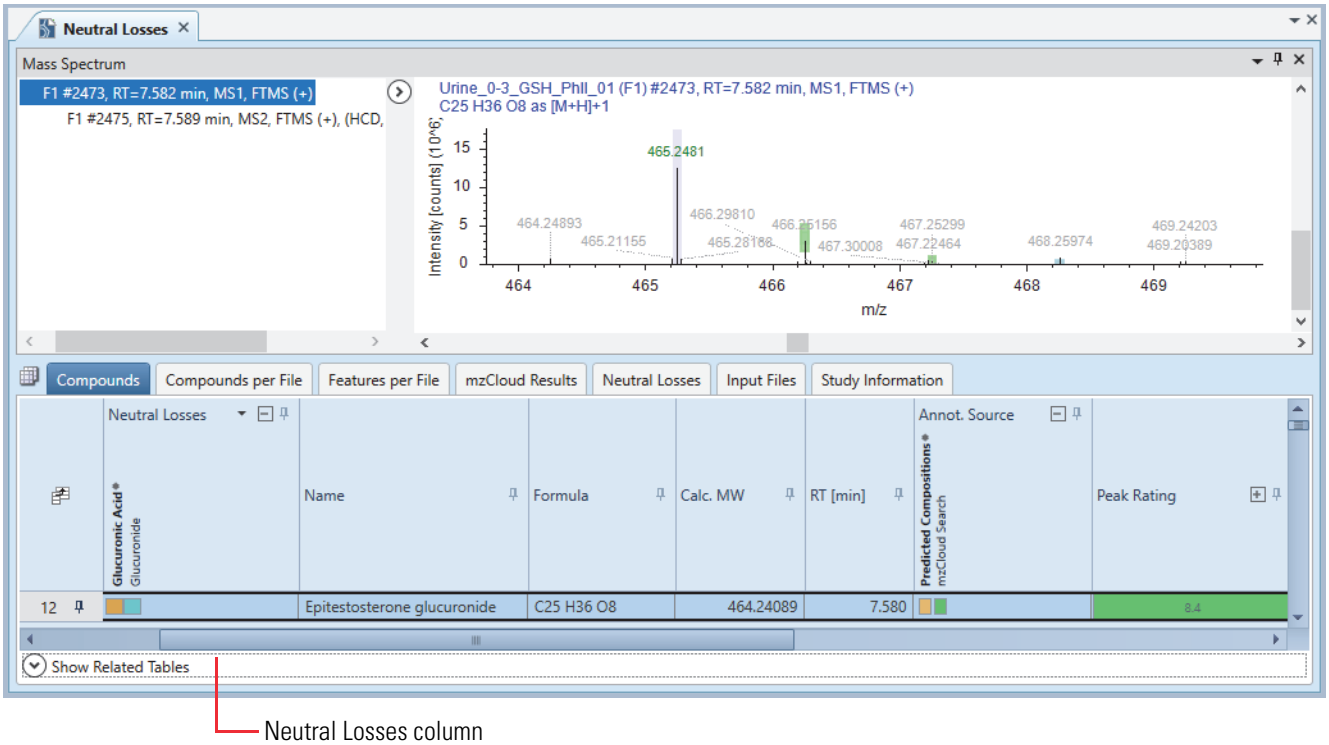
4. To make it easier to review the neutral losses for compounds of interest, modify the layout of the result page as follows:
   a. Close the Chromatograms view by clicking the close icon in the upper-right corner of the view.
   b. Click the **Compounds** tab to open the Compounds table.
   c. Right-click the Compounds table and choose **Enable Column Fixing**. Then, scroll to the right and click the pin icon to the right of the Neutral Losses column header.

      The Neutral Losses column moves to the leftmost column position.
   d. Right-click the Compounds table and choose **Expand All Column Headers**.

      The selected neutral losses are visible as subheadings in the Neutral losses column.
   e. To sort the neutral losses by one of the neutral losses, select the specific (vertical) neutral loss heading. Then, click the **Neutral Losses** column header until the arrow points down.
   f. (Optional) To pin compounds of interest to the top of the table, click the pin icon to the right of their row numbers.

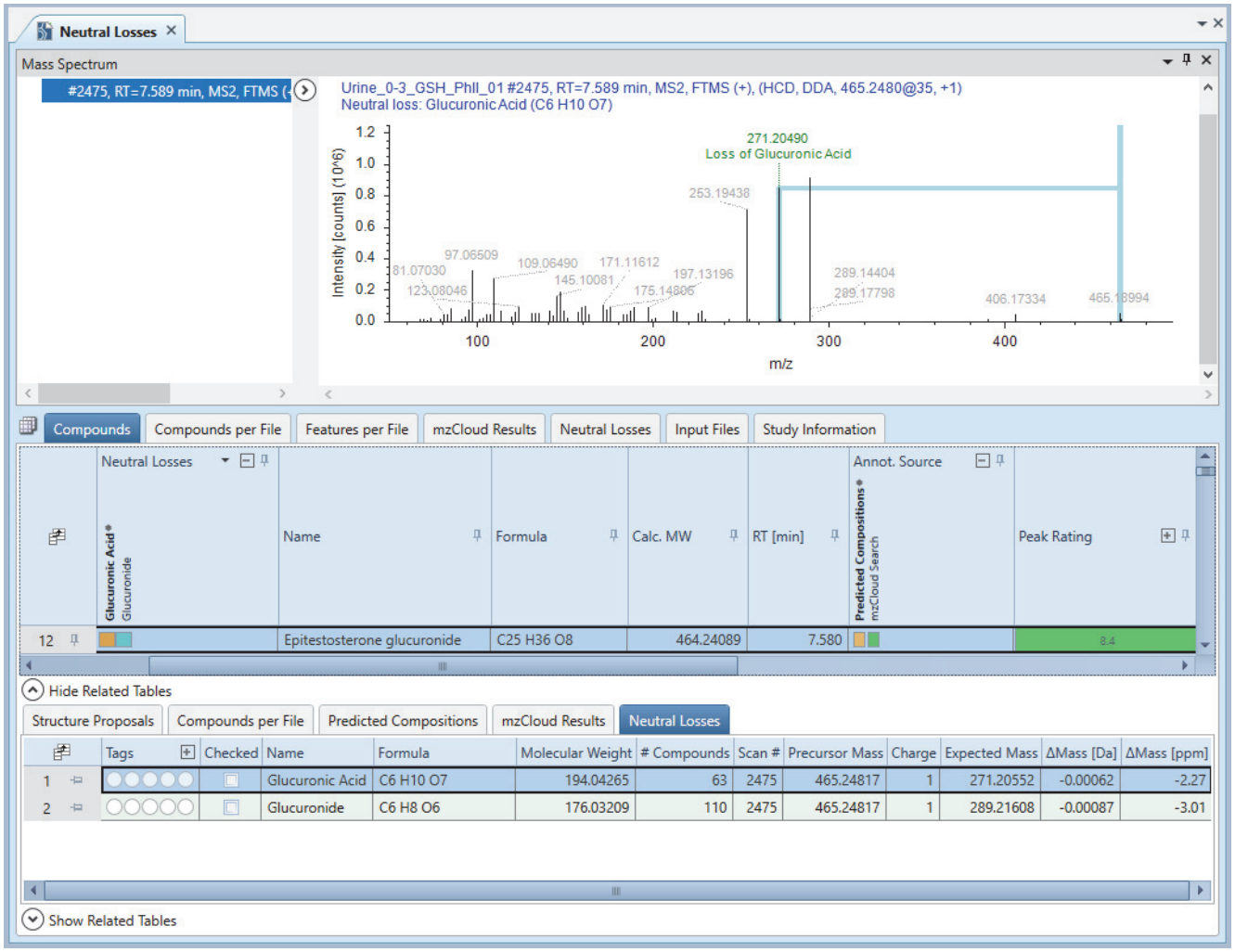
Figure 22 shows a result table from a processing workflow with the Search Neutral Losses node with two neutral losses selected: glucuronide and glucuronic acid. The Neutral Losses column is fixed at the left, and a compound is pinned to the top of the table.

Figure 22. Result file from a processing workflow with the Search Neutral Losses node (with column fixing enabled and a compound pinned to the top of the table))



5. To view specific neutral losses for a compound in the Mass Spectrum view, do the following:
   a. Select the compound in the main Compounds table.
   b. Click **Show Related Tables** at the bottom left of the result page.
   c. In the first related tables pane, click the **Neutral Losses** tab.
   d. In the Neutral Losses table, select the neutral loss that you want to visualize in the mass spectrum.
   e. In the Mass Spectrum view, review the fragmentation spectrum with the selected neutral loss.
6. To return the Mass Spectrum view to the normal view, click another row in the Compounds table.

Figure 23. Fragmentation spectrum with annotated neutral loss



Using quality control samples to compensate for batch effects

When acquiring raw data files for a large sample set by running an uninterrupted acquisition sequence, you can use pooled quality control samples to compensate for time-dependent batch effects. For information about batch effects, refer to the following article: *Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry*.[5]

To create a pooled quality control sample, combine a small aliquot from each sample in the processing batch (input file set to be processed to create one result file). When setting up an acquisition sequence, bracket the unknown samples by injecting this pooled quality control sample at regular intervals.

For details about processing the raw data files from a sequence with quality control samples, see these topics:

- Batch normalization for single sequence runs
- Batch normalization for multiple sequence runs (LC studies)

Batch normalization for single sequence runs

When the processing workflow includes the Apply QC Correction node and the input file set includes QC samples, an analysis uses the QC samples to create a regression curve of area versus acquisition time for each detected compound.

Note For information about setting up a processing workflow for a QC-corrected sample set, see "Apply QC Correction node." For information about reviewing the corrected compound areas for a QC-corrected sample set, see "Compound Area Corrections view."

An analysis does not create a regression curve for a particular compound and does not correct the areas in the non-QC samples unless all three of these conditions are met:

- It detects the compound in the user-specified minimum percentage of the QC samples.
- The relative standard deviation of the detected peak areas for the compound in the QC samples before and after correction does not exceed the user-specified thresholds.
- The number of samples acquired between the QC samples does not exceed the user-specified number.

You can view the results of the batch normalization process in the main compounds result table (Compounds table) and the Compound Area Corrections view. The Norm. Area column in the compounds table displays the corrected compound areas. The Compound Area Corrections view shows the effect of the signal correction on the absolute compound areas.

[5] Dunn, W.B.; Broadhurst, D.; Begley, P.; Zelena, E.; Francis-McIntyre, S.; Anderson, N.; Brown, M.; Knowles, J.D.; Halsall, A.; Haselden, J.N.; Nicholls, A.W.; Wilson, I.D.; Kell, D.B.; Goodacre, R. Human Serum Metabolome (HUSERMET) Consortium. *Nat Protoc*. **2011**, 6(*7*), 1060-83.

When the application excludes the selected compound during the QC signal correction step, the Compound Area Corrections view is empty. In addition, the Norm. Area column for the compound is empty across all the input files, and a filter icon appears on the compounds table tab. Pointing to the tab displays a tooltip with the number of displayed compounds, detected compounds, and filtered-out compounds. Clicking the filter icon displays all the detected compounds, including the compounds with uncorrected peak areas.

For additional information, see Chapter 4, "Set up, run, and reprocess analyses," and "Compound Area Corrections view."

Batch normalization for multiple sequence runs (LC studies)

For LC studies, use the Apply SERRF QC Correction workflow node when you are processing input files from batches acquired with more than one sequence run, and the time lapse between the sequence runs was greater than the time lapse between individual sample runs. SERRF stands for systematic error removal with random forests.

IMPORTANT The input files can comes from different batches, but the parameter settings for the instrument methods used in these different batches must be the same.

The node determines how to divide the input files into batches as follows:

1. The node orders the input files by their acquisition times.
2. After the node groups the input files by time and determines the largest time gaps, it attempts to divide the input files into the number of user-specified batches, while maintaining a minimum of five QC samples per batch. The node assumes that the biggest gaps in the series of acquisition times are due to the time gaps between batches.
3. If a batch (as determined by a time gap) contains fewer than five QC samples, the node merges it with the smallest neighboring batches. If the node cannot create multiple batches with five QC samples each, it assigns all the input files to the same batch. The SERRF algorithm can process one batch without problems.
4. The node numbers the detected batches, starting with 0, and reports the sequential batch number (0 to the maximum user-specified batch number) in the Batch column of the Input Files result table.

For information about adding the Apply SERRF QC Correction node to a processing workflow, see "Peak area refinement node connections." For information about the node parameters, see "Apply SERRF QC Correction node."

Stable isotope labeling experiments

Stable isotope labeling experiments are fundamental to understanding metabolic pathways and the turnover rate (flux) for the molecules in these pathways. Where traditional approaches are usually limited to targeted analyses, which detect and quantify known compounds and their labeled downstream metabolites, the Compound Discoverer application makes full use of continuous high-resolution accurate-mass (HRAM) full scan data from the Orbitrap™ MS (coupled to a liquid chromatograph).

Using an unlabeled reference sample, the application detects unknown compounds above a specified minimum intensity threshold, determines their elemental composition and identity, and then determines the labeled counterparts (isotopologues) of these compounds in the samples marked as labeled.

You can use any isotopic label in your experiments; however, when you use a label other than carbon-13, you must specify the labeled element in the processing workflow.

The application reports the isotopologues and the fractional label incorporation (exchange rate) for each compound. You can overlay the exchange rate as well as other statistical data onto pathways using Metabolika™, which is directly integrated into the Compound Discoverer application.

To acquire and process stable isotope labeled data, do the following:

1. Acquire LC/MS/MS data for a set of samples where at least one sample corresponds to the unlabeled state of the system.
2. In the Compound Discoverer application, select the following sample types:
   - For unlabeled samples, select **Sample**, **Identification Only**, **Quality Control**, or **Blank** as appropriate. You must select Sample (or Control or Standard) for at least one sample.

     Note Currently, the application treats Sample, Control, and Standard samples the same way. This functionality is subject to change in future releases.

   - For labeled samples, select **Labeled**.
3. Select one of the processing workflows in the following folder:

   Common Templates\Workflow Templates\LC\Stable Isotope Labeling
4. When using a label other than carbon-13, customize the parameter settings for the Analyze Labeled Compounds node in the processing workflow. See "Analyze Labeled Compounds node."

During data processing, the application does the following:

1. Detects and identifies the compounds in the unlabeled samples.
2. Submits the compounds with assigned formulas to the Analyze Labeled Compounds node which does the following:
    a. Generates isotopologues for each detected compound by replacing one occurrence of an atom at a time by its specified isotope. The formula of the compound or the user-specified limit defines the number of exchangeable atoms, whichever is smaller.
    b. Simulates the isotope pattern for each isotopologue by using its formula and the spectral resolution of the raw data.
    c. Consolidates the isotopologue patterns for each compound to get the final set of expected masses, considering the specified mass tolerance and the spectral resolution of the raw data.
    d. Generates an XIC trace for each expected mass and detects the chromatographic peaks.
    e. Deconvolves the chromatographic peaks to determine the relative amount of each isotopologue.
    f. Flags compounds containing contaminating masses in unlabeled samples, as well as unusual isotopologue distributions and insufficient pattern fits.

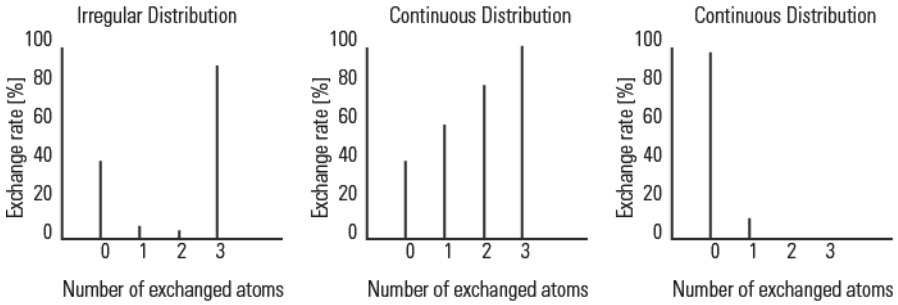
The Analyze Labeled Compounds node adds the following columns to the Compounds table in a result file: Labeling Status, Ave. Exchange, and Rel. Exchange Rate. See "Compounds table (LC studies)."

To determine the presence of contaminating masses, the Analyze Labeled Compounds Node evaluates the measured isotope pattern versus the fitted isotope pattern (for the expected isotopologues). It also evaluates the distribution of the measured exchange rates for the expected isotopologues. If the distribution is not continuous, for example, if the compound has three exchangeable atoms and chromatographic peak area for the M+2 isotopologue is significantly less than the chromatographic peak area for the M+1 and M+3 isotopologues, the node assigns an Irregular Exchange status to the input file.

These flags indicate the following states:

- () Red—Contaminating Mass—The average exchange for the unlabeled sample is above the 0.1 threshold.
- () Orange—Low Pattern Fit—The measured pattern significantly differs from the fitted pattern. The SFit value is below the threshold of 20%, the Fitted Coverage value is below the threshold of 60%, or the Measured Coverage value is below threshold of 60%. To review these values, see the "Labeled Features table."

- (■) Blue—Irregular Exchange—The isotopologue exchange rates are discontinuous; for example, there is a significant valley in the exchange rates profile. This might indicate an incorrect analysis or a special type of kinetics. However, if this is the typical behavior expected for your experiments, consider changing the setting for Mark Irregular Exchanges in the Analyze Labeled Compounds node to False.



- (■) Green—No Warnings—The measured isotope patterns and the exchange rates are within acceptable limits.
- (■) Gray—Compound was not detected in this sample.

PFAS identification

Per- and polyfluoroalkyl substances (PFAS) are a highly stable group of small molecules that have a wide range of commercial applications. PFAS are highly soluble in water, chemically stable, persistent in the environment, and can accumulate in the human body over time, leading to adverse human health effects and potential human health risks. Due to these health risks and the pervasiveness of PFAS in common household items, some compounds in the PFAS family have been banned and analytical tests have been developed to check for their presence.

LC-MS/MS analysis is a common analytical technique used for determining the presence of per- and polyfluoroalkyl substances in extraction solutions. The Compound Discoverer application supports the identification of PFAS in raw data files acquired with a Thermo Scientific high-resolution accurate-mass (HRAM) mass spectrometer. The data files must include high-quality MS1 full scans and data-dependent MS2 fragmentation scans.

These topics describe how to use the processing workflow template for PFAS analysis that is provided with the application and how to review the analysis result:

- PFAS processing workflow template
- Review the results of a PFAS analysis

PFAS processing workflow template

Use the following processing workflow template to identify per- and polyfluoroalkyl substances in raw data files acquired with a Thermo Scientific high-resolution accurate-mass (HRAM) mass spectrometer:

PFAS Unknown ID w Database Searches and Molecular Networks.cdProcessingWF

You can find this processing workflow template in the following folder for LC studies:

Common Templates\Workflow Templates\PFAS\

Note For information about selecting a processing workflow for an analysis, see "Select a processing workflow for the analysis."

The PFAS processing workflow template processes the raw data files as follows:

- Performs retention time alignment, unknown compound detection, and compound grouping across all samples.

  Table 12. Customized parameter settings for the Detect Compounds node in the PFAS processing workflow template

Parameter	Default setting for the node	Custom setting for PFAS
Min. Peak Intensity	10,000 (1e4)	1,000 (1e3)
Ions	[M+H]+1; [M+K]+1; [M+Na]+1; [M-H]–1	[2M+FA–H]–1; [2M–H]–1; [2M–H+HAc]–1; [M+Cl]–1; [M+FA–H]–1; [M–2H+K]–1; [M–H]–1; [M–H+HAc]–1; [M–H–H2O]–1

- Predicts elemental compositions for all compounds, fills gaps across all samples, and hides background compounds (by using the Blank samples).

  In the Predict Compositions node, the maximum number of fluorine atoms in the elemental composition of the compound is limited to 50.

  Minimum Element Counts: C H F

  Maximum Element Counts: C90 H190 Br3 Cl4 F50 N10 O18 P3 S5

- Identifies compounds by using the following:
  - The mzCloud™ mass spectral database (data-dependent MS2)
  - The EPA DSSTox database in the ChemSpider chemical structure database (formula or exact mass)
  - The following mass lists, which are provided with the application:
  - PFAS_NEG, PFAS_NIST, and PFASSTRUCT-2022-04-20

- Flags unknown compounds that share common set of fragments by using the Compound Class Scoring node.

  Uses the following compound class files, which are provided with the application: PFAS General from FluoroMatch Suite.cLib and \PFAS Fine signature fragment_lib.cLib.

- Generates mass defect values in the Compounds table that are based on the selected mass defect type (Kendrick for identifying homologous series).

  Uses the following Kendrick mass: C F2.

- Generates a molecular network to visualize compounds that might be related.

  Uses the following transformation: PFAS Chain Shortening (C F2 ->) under Other.

- Supports the optional scripting node that is available on AnalyteGuru.

  https://www.analyteguru.com/t5/Scientific-Library/Compound-Discoverer-PFAS-Scripting-node/ta-p/20051

For optimal performance of the analysis, do the following:

- Make sure that your raw data files include high-quality MS1 full scans and full scan data-dependent MS2 scans
- For optimum performance, add at least one blank sample to the input file set.

  For matrices where no blank is available, use a suitable sample containing relatively low levels of PFAS and modify the parameter settings in the Mark Background Compounds node. For example, increase the ratio for the Max. Sample/Blank parameter setting. The default ratio is 5 to 1.

- Use three replicates per sample to simplify peak filtering.

Review the results of a PFAS analysis

After you run an analysis using the PFAS processing workflow template that is provided with the Compound Discoverer application, open the analysis result and review the results.

Note For more information about reviewing the results from an analysis that used the PFAS processing workflow template that is provided with the application, refer the following article:

http://assets.thermofisher.com/TFS-Assets/CMD/Application-Notes/an-001826-lsms-pfas-analysis-workflow-compound-discoverer-an001826-na-en.pdf

❖ To review the results of a PFAS analysis

1. Open the analysis result by double-clicking the job on the Job Queue page or by clicking the analysis result on the Analysis Results page of a study.

2. Apply the following result filters to filter the Compounds table to display only high confidence candidates with matched fragments as follows:

   a. Set the following filters:

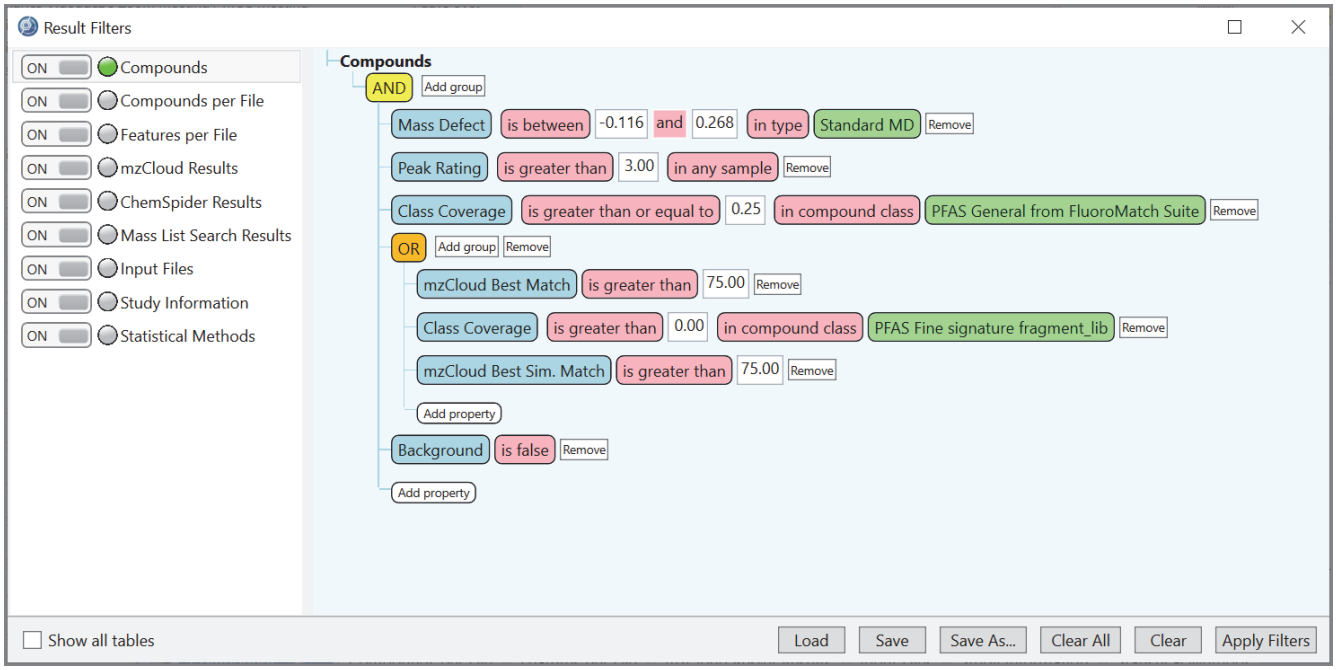
      AND (All of these conditions must be true.)

      - Mass Defect Is Between –0.116 and 0.268 In Type Standard MD
      - Peak Rating Is Greater Than 3.00 In Any Sample
      - Class Coverage Is Greater Than or Equal To 0.25 In Compound Class PFAS General from FluoroMatch Suite
      - Background is False

      OR (One of these conditions must be true in addition to the four AND filters)

      – mzCloud Best Match Is Greater Than 75.00
      – Class Coverage Is Greater Than 0.00 In Compound Class PFAS Fine Signature Fragment_Lib
      – mzCloud Best Sim Match Is Greater Than 75.00

   Figure 24. Result filter to reduce the number of compounds displayed in the Compounds table to high confidence candidates with matching fragments



   b. Click **Apply**.

      Only compounds with a high confidence of belonging to the PFAS family remain visible in the Compounds table.

3. Visualize the relationship among the remaining compounds in a scatter plot as follows:
   a. In the application menu bar, choose **View > Result Charts**.

      The Scatter Chart plot opens.

   b. In the Data Source list, select **Compounds**.

   c. Make the following selections for the three axes:

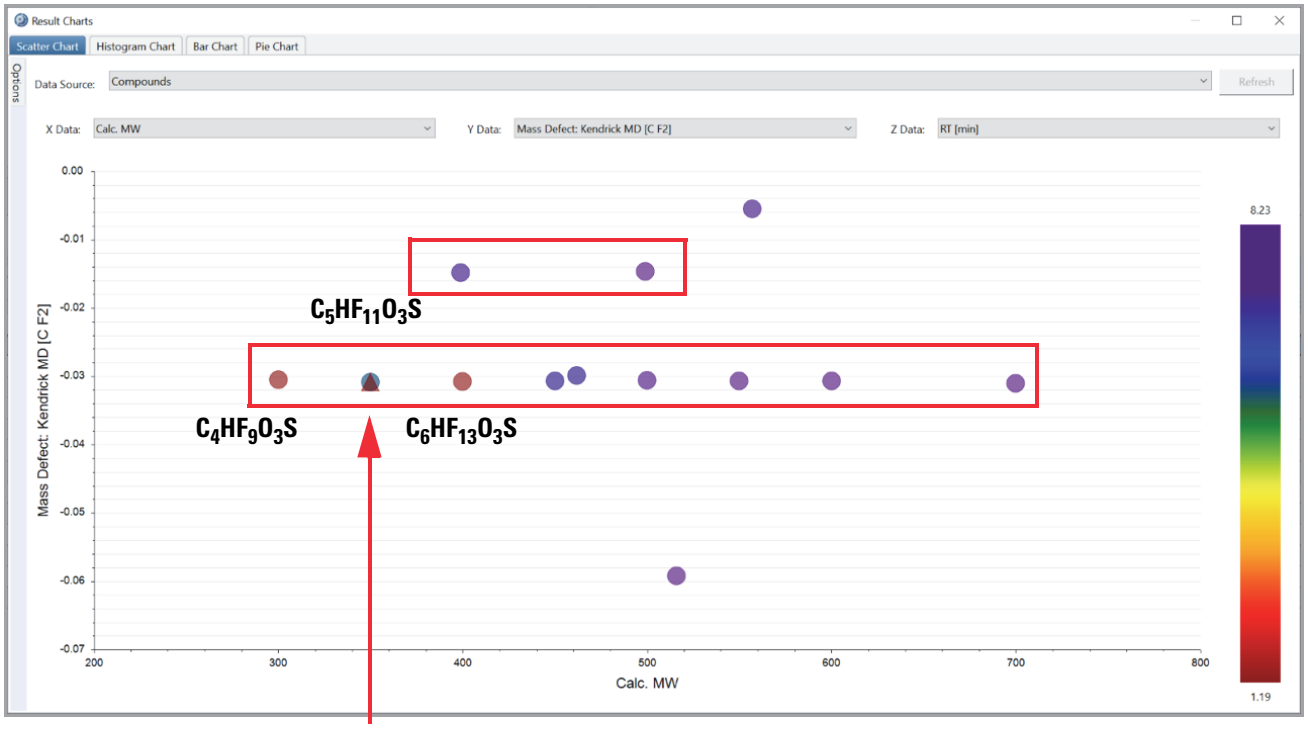
      - For X Data, select **Calc. MW**.
      - For Y Data, select **Mass Defect: Kendrick MD [CF2]**.
      - For Z Data, select **RT [min]**.

   d. Click **Refresh** to display the plot.

   In Figure 25, data points from the filtered Compounds table are plotted in three dimensions using the Kendrick MD of approximately 50 Da or exactly one CF2 to elucidate the presence of homologous PFAS series. Homologous PFAS series will share the same Kendrick MD but differ in molecular weight by 50 Da and have increasing retention time based on PFAS chain length. The retention time is color coded as a third dimension to provide a simple verification of this trend.

   Two homologous series are identified at Kendrick MD [CF2] of -0.03 and -0.015 (highlighted by the two red rectangles in Figure 25). In the longer series, there are two overlapping PFAS with a molecular weight of 349.9471 Da, which corresponds to perfluoropentanesulfonic acid. To resolve this overlap, one data point is plotted as a triangle instead of a circle. The compound that corresponds to the blue circle does not follow the retention time trend of increasing retention with increasing chain length. This retention time deviation is most likely explained by an alternate branching structure.

Figure 25. Scatter chart with a plot of the Kendrick mass defect for C F2 (y axis) against the Calc. MW of the compound (x axis) and the retention time of the compound (z axis)



4. After you filter the Compounds table to display only potential PFAS, visualize the molecular network between the compounds as follows:

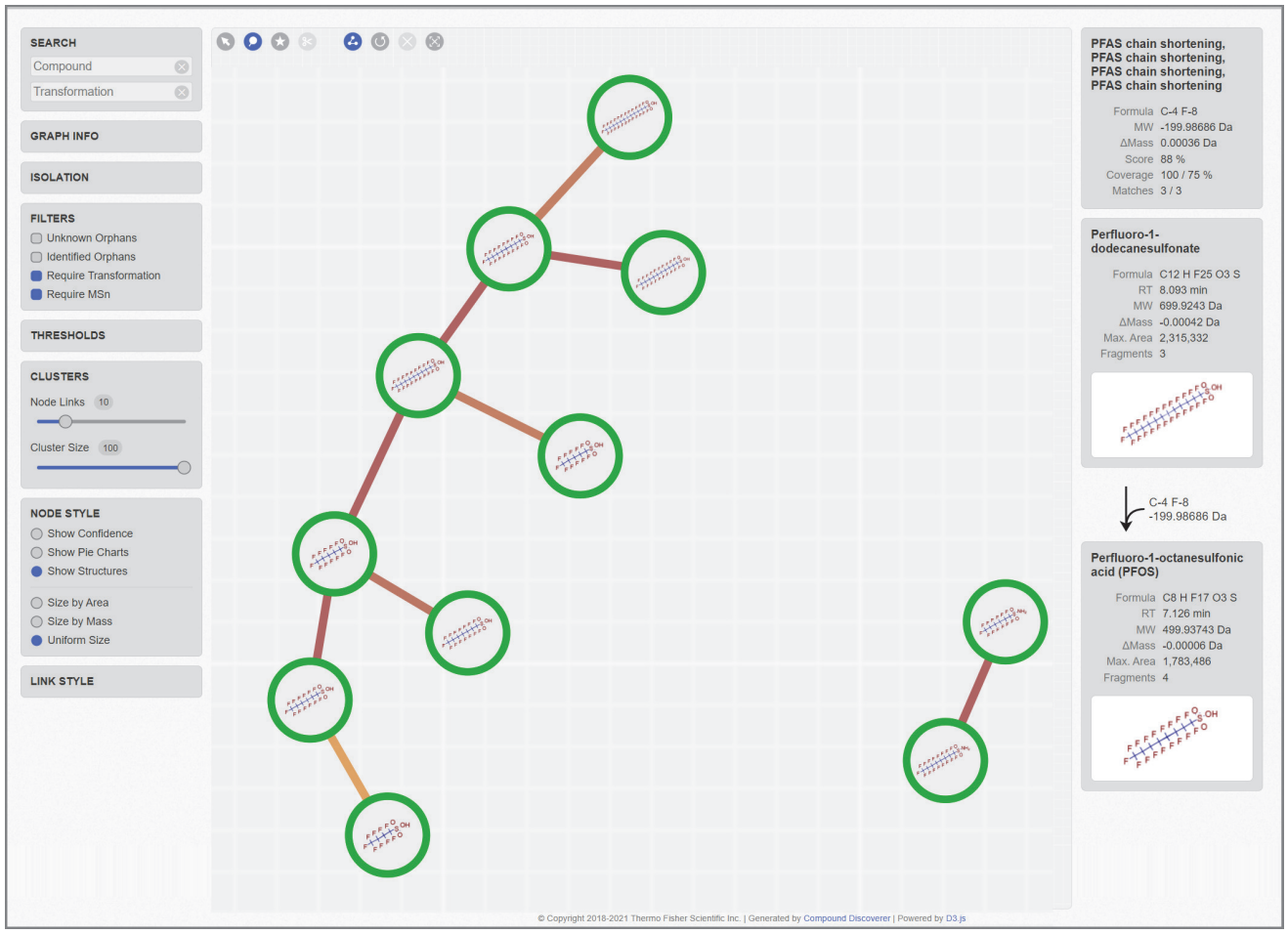
   a. Right-click the Compounds table and choose **Molecular Networks > Send to Viewer**.

      The Export Molecular Networks dialog box opens.

   b. Select the **Open Viewer After Export** check box, and then click **Export**.

      The viewer opens in a web browser where you can adjust the settings to optimize clustering. For PFAS, class-based clustering is based on fragmentation and the detection of homologous series by selecting the PFAS chain shortening transformation in the Generate Molecular Networks node. This transformation accounts for the addition or removal of up to ten CF2 moieties that correspond with the expected differences in chain length for PFAS homologous series.

Figure 26. Molecular Networks viewer with PFAS



Methods for imputing values for missing chromatographic peaks across a set of input files

For various statistical analyses, zero values within a sample set can lead to erroneous results. To avoid this type of error, the Compound Discoverer application provides methods for imputing missing chromatographic peak areas for detected compounds across the set of input files that you submit for analysis.

For LC studies, you can add one of the following two nodes to the processing workflow to impute missing peak areas: Fill Gaps or Apply Missing Value Imputation. The processing workflow templates for LC studies use the Fill Gaps node, which fills the gaps for missing chromatographic peaks by revisiting the original XIC traces and searching below the noise threshold. Use the Apply Missing Value Imputation node only if the Fill Gaps node does not give you the expected results. The Apply Missing Value Imputation node is a peak area refinement node that does not revisit the original data stream.

For details, see these topics:

- Random Forest imputation method
- Median + Small Value imputation method
- Gap filling method

Random Forest imputation method

The Random Forest method that you can select in the Apply Missing Value Imputation workflow node of a processing workflow uses a machine learning algorithm that trains itself on the set of peak profiles of the compounds detected across all input files. For this method, you specify the number of trainings (iterations) and the number of decision trees for each training.

Median + Small Value imputation method

The Median + Small Value method that you can select in the Apply Missing Value Imputation workflow node of a processing workflow uses one of two calculation methods to impute the area of a missing chromatographic peak. The method it uses depends on whether all or only some of the samples in each study group are missing the chromatographic peak for a compound.

- Partially missing peak area—If the compound is detected in one or more input files in a study group—that is, if the compound is only partially missing from the study group, this method imputes a value for the missing areas that is close to the mean of the non-missing values within the same study group. The imputed value is calculated so that the coefficient of variation (CV) for all the peak areas in the groups (imputed and experimentally acquired) is similar to the CVs for this compound in other study groups.
- Completely missing peak area—If the compound is not detected in any of the input files in a study group—that is, the compound is completely absent from the group, the Median + Small Value method imputes the area for a missing peak by dividing the smallest chromatographic peak area detected in the input file by 2.

To avoid distorting the CVs of the sample groups with missing or partially missing peaks, this imputation method does the following:

- Adds a corresponding variability to the mean for a partially missing group.
- Adds the smallest value detected in the input file divided by 2 for a completely missing group.

- Calculates the typical (or local) standard deviations by using local estimations (depending on the median of the areas) of the compound CVs. It uses a maximum number of 50 neighbors to estimate a local CV. The number of neighbors is lower than 50 if there are fewer than 100 compounds with at least three sample-replicate values in the dataset. After it estimates the local CVs, it removes the local outliers and estimates the local median CVs with the remaining data.
- Calculates the mean (or minimum value) plus the added variability as a random value (positive or negative). The added variability follows a Gaussian distribution that is centered at the mean (or minimum value) with a standard deviation that corresponds to the estimated typical standard deviation for similar area values for other study groups in the analysis.

Gap filling method

For LC studies, the Fill Gaps node of a processing workflow calculates the area of missing chromatographic peaks as follows.

1. Calculates the detection limit for each missing ion as an area of a simulated Gaussian peak that starts and ends at a zero intensity baseline. To calculate the area of the Gaussian peak, the node uses the expected peak width and the maximum spectrum noise in the expected retention time range multiplied by the S/N threshold.
2. Searches for the missing ion with the expected *m/z* × RT dimensions against all detected ions (in the mass list generated by the Detect Compounds node) while ignoring the assigned adduct type. If it finds a match (ion with the expected *m/z* × RT dimensions), it uses the ion's area to fill the gap and displays **Filled by Matching Ion** for the Fill Status.
3. If the node does not find a matching ion, it attempts to detect the peak at a lower intensity threshold by using the new peak detection algorithm in the detect compounds node (the new Detect Compounds node or the Detect Compounds (Legacy) node. If it detects a chromatographic peak at a lower threshold, it uses the integrated peak area to fill the gap and displays **Re-detected Peak** for the Fill Status.
4. If the node does not find a chromatographic peak by using a lower intensity threshold, it fits a Gaussian peak to the XIC trace for the expected *m/z* range and displays **Filled by Simulated Peak** for the Fill Status.
5. If the filled area is still zero or lower than the detection limit, the node uses the detection limit value to fill the gap and displays **Filled by Spectrum Noise** for the Fill Status.
6. If the node cannot fill the gap, it displays **Area Could Not Be Filled** for the Fill Status.

For details about the parameter settings for the Fill Gaps node, see "Fill Gaps node."

Create a new study and an analysis by using the wizard

Use the New Study and Analysis Wizard to create a new study and set up a new analysis. Before you start the wizard for the first time, review the available sample types and the directory structure for studies.

Note For information about the terminology used in the Compound Discoverer application, see "Terminology used in the Compound Discoverer application."

Preliminary information:

- Available sample types
- Directory structure for Compound Discoverer studies
- Create a study template file that contains all the study information

To set up a new study and a new analysis, follow these steps:

1. Start the New Study and Analysis Wizard.
2. Define the study type, name the study, and optionally select a study template and a processing workflow.
3. Add input files to the new study.
4. Characterize the new input files.
5. (Optional) Extract study factor values from the file names of the input files.
6. (Optional) Set up the sample groups and ratios for a new analysis.
7. Prepare to submit the analysis to the job queue.

Available sample types

Table 13 describes the sample types that the application supports and how it uses these sample types.

For information about selecting the sample types, see "Select the sample types."

Table 13. Sample types

Sample type	Application use
Sample[a]	Detects the compounds in the sample.
Control[a]	Detects the compounds in the sample.
Blank	Detects the compounds in the sample. When the processing workflow includes one or both Mark Background Compounds nodes, marks these components as background compounds.
Identification Only (LC studies only)	Does not report the chromatographic peak areas for the compounds detected in this sample type. Uses the fragmentation scans in this sample type for component identification when the processing workflow includes the Group Compounds node.
Quality Control	Detects the compounds in the sample. Pools the QC samples to determine a group area for each detected compound for area normalization.
Standard[a]	Detects the compounds in the sample.
Labeled (LC studies only)	Determines the formulas for the compounds in the labeled samples.

[a] The application attributes the same functionality to the Sample, Control, and Standard sample types. You can use the Control and Standard sample types to label your control or standard samples; that is, you can use these sample types as an additional study variable for grouping.

Directory structure for Compound Discoverer studies

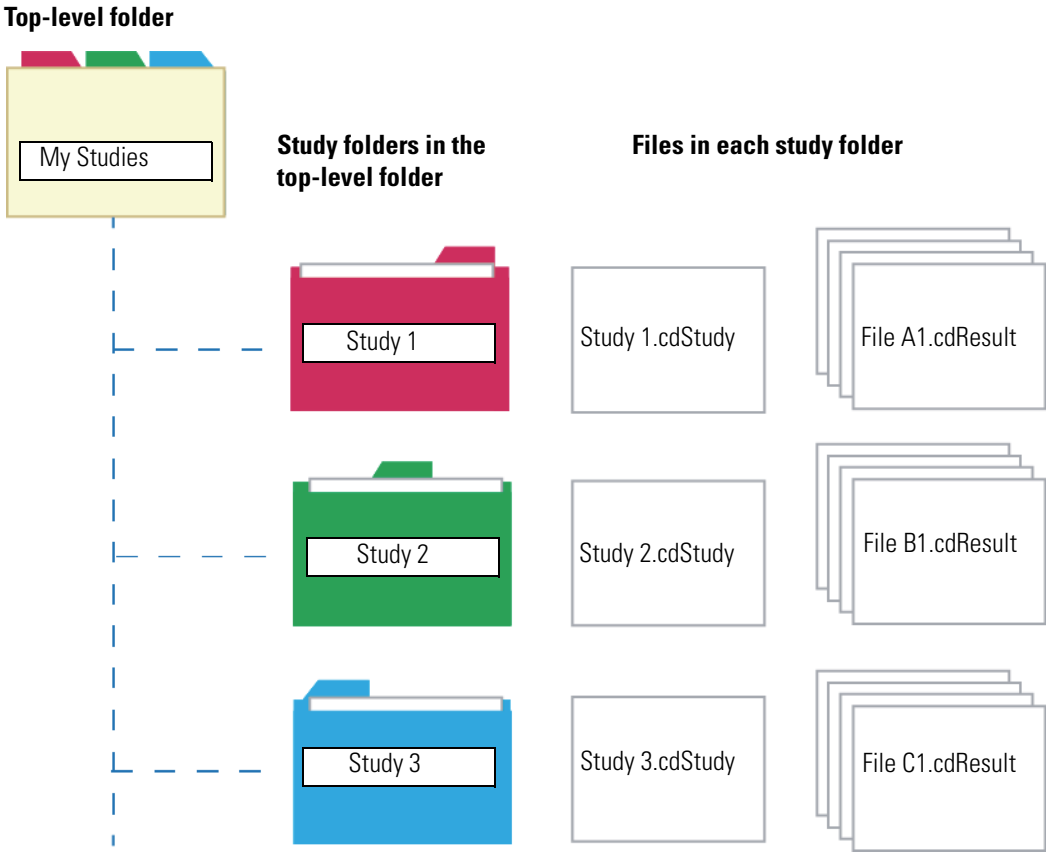
Figure 27 shows the hierarchy of the study folders. The studies folder is the top-level folder for all your studies or a particular set of studies. Each study folder within the studies folder holds one study file (.cdStudy) and one or more result files (.cdResult).

Note You can create more than one top-level folder for your studies. Each time you open the New Study and Analysis Wizard, it opens to the last opened top-level folder.

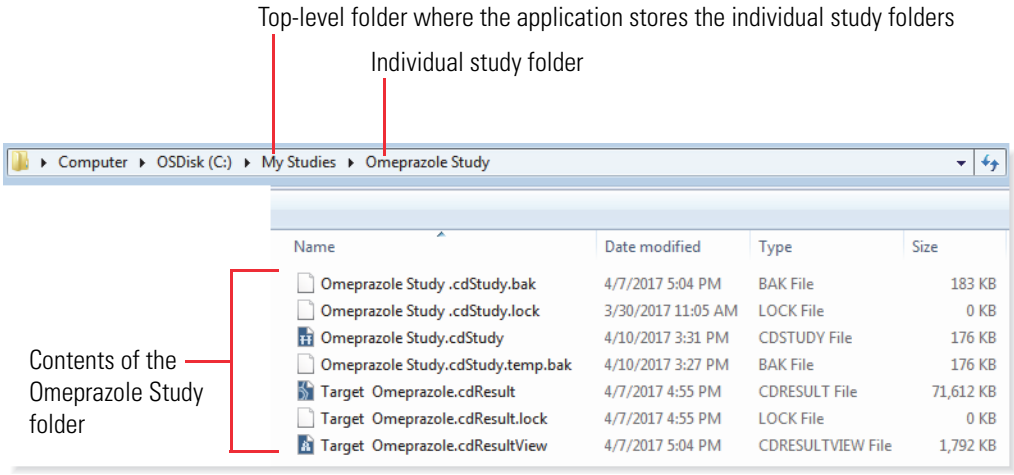
Study files include a list of input files with their location, the sample information for each file, and a list of the analyses run within the study. The sample information includes the file name, study factor values, and sample type for each sample.

Result files contain the results of an analysis in tabular form. In addition, you can access multiple views for visualizing the analysis results when you open a result file in the application window.

Figure 27. Studies folder structure



This figure shows an example of the directory hierarchy for a study named Omeprazole Study with one result file. The individual study folder and the study file share the same name.



Create a study template file that contains all the study information

There are two ways to create a study template file.

For details, see the following topics:

- Manually create a template that includes all the study information
- Edit a spreadsheet for use as a study template

For information about selecting a study template file for a new study, see "Define the study type, name the study, and optionally select a study template and a processing workflow."

Manually create a template that includes all the study information

If you have already run an analysis that includes the study information for all your input files, you can export the study information from the result file to a spreadsheet. After you export the information to a spreadsheet, you must edit the information to make it compatible with the New Study and Analysis Wizard.

❖ To export the study information in a result file to a spreadsheet

1. Open a result file that includes the study information of interest.
2. Click the **Study Information** tab.
3. Click the **Field Chooser** icon, , in the upper-left corner of the active table.
4. In the Field Chooser dialog box, clear all the check boxes except those for the CF: *study factor name*, File Name, and Sample Type. Then, close the dialog box.
5. Right-click the Study Information page and choose **Export > As Excel**.

6. In the Export to Excel dialog box, select the folder where you want to store the Excel spreadsheet, select the **All Items** option, select the **Open File After Export** check box, and then click **Export**.

   The exported spreadsheet opens in the spreadsheet application.

7. Change the File Name column heading to File.
8. Save the spreadsheet.

Edit a spreadsheet for use as a study template

If you already have a spreadsheet with all the study information you need, you can edit the spreadsheet to make the information available to the New Study and Analysis Wizard.

❖ To edit a spreadsheet for use as a study template

1. Open the Excel spreadsheet application and create a new spreadsheet.
2. Set up columns with the following column headers:
   - Column A: File
   - (Optional) Column B: Sample Type

     If the spreadsheet does not include a Sample Type column, the application assigns the Sample as the sample type for all the input files.

   - Column C and higher:
     – For a categorical study factor, type **CF: *study factor name.***
     – For a numerical study factor, type **NF: *study factor name***.

       You can append a unit to the end of a numerical study factor, for example, NF: Solution [mL].

     – For a biological replicate factor, type **BF: *study factor name***.

     If you do not label the study factor columns CF:, NF:, or BF:, the application treats them as categorical study factors.

3. Add the following information to the columns:
   - Column A: complete directory path and file name for each input file
   - Column B: sample type for each input file
   - Column C and higher: study factor value for each input file

4. Save the file as a spreadsheet file.

Start the New Study and Analysis Wizard

To create a new study, you use the New Study and Analysis Wizard. You can start the wizard in several ways.

❖ **To start the New Study and Analysis Wizard**

Do one of the following:

- From the menu bar, choose **File > New Study and Analysis**.
- In the toolbar, click the **Create a New Study and Analysis** icon,  .
- On the Start page under What Would You Like to Do?, click **New Study and Analysis**.

The New Study and Analysis Wizard opens to the Study Name and Processing Workflow page (step 1 of 5).

The wizard has embedded "How To" instructions that you open by clicking the light bulb icon,  , in the lower-left corner. In addition, there is a context-sensitive Help topic for each page of the wizard. To open the context-sensitive Help for the current page of the wizard, press the **F1** key on your computer keyboard.

Define the study type, name the study, and optionally select a study template and a processing workflow

To start the New Study and Analysis Wizard, see "Start the New Study and Analysis Wizard." The wizard opens to the Study Name and Processing Workflow page.

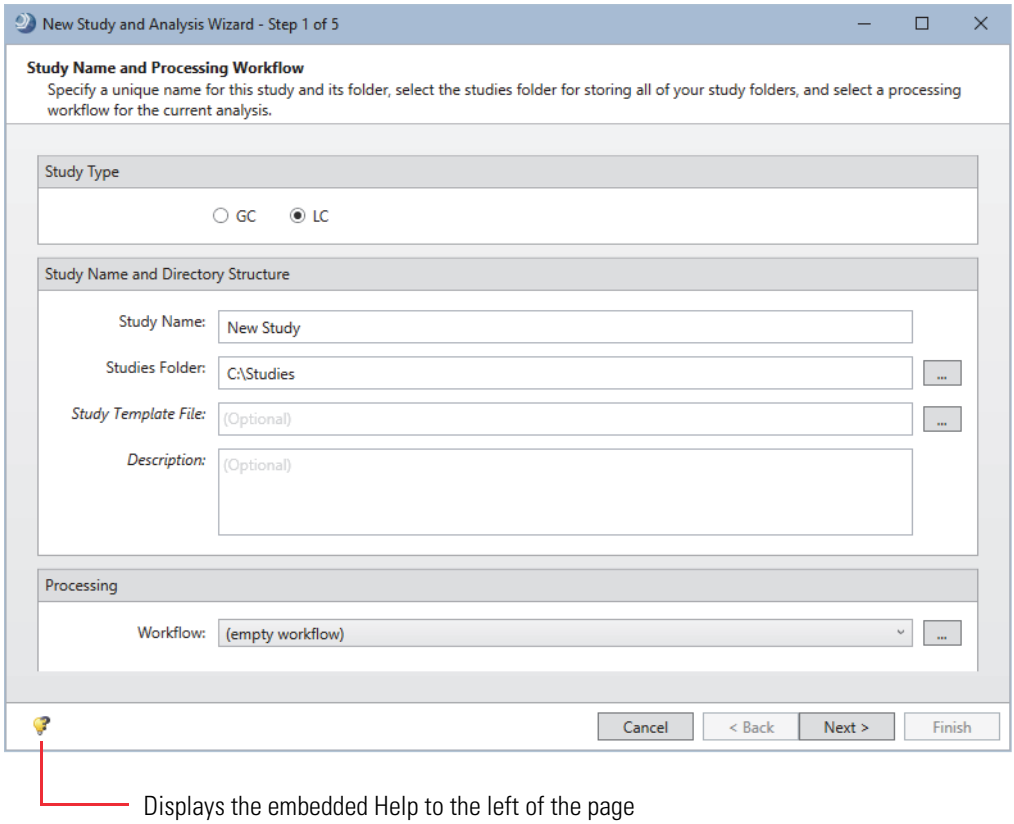
Use the Study Name and Processing Workflow page (step 1 of 5) of the New Study and Analysis Wizard to do the following:

- Select the study type: LC or GC (chromatography type = liquid chromatography or gas chromatography).
- Name the current study. This step automatically creates a study folder and a study file with the same name. See "Directory structure for Compound Discoverer studies."
- Select a current folder or create a new top-level folder for storing all the study folders or a subset of the study folders.
- (Optional) Select a template file for the study.

  A study template file is either a study file that includes defined study factors or a tab-delimited text file or spreadsheet file that includes all the study information. The study information includes the location, sample types, and study factors for all the input files in a study.
- (Optional) Select a processing workflow for the analysis.

Note You can select a processing workflow after you create the study.

Figure 28. New Study and Analysis Wizard – Study Name and Processing Workflow page



For more information about the Study Name and Processing Workflow page of the wizard, see these topics:

- Select the study type
- Name the new study, select the top-level studies folder, and optionally select a study template
- Select a processing workflow for the analysis

Select the study type

The New Study and Analysis Wizard is open to the Study Name and Processing Workflow page. See "Start the New Study and Analysis Wizard."

❖ To select the study type

In the Study Type area, do one the following:

- Select the **GC** option for a GC study.
- Select the **LC** option for an LC study.

The Workflows list in the Processing area includes the processing workflow templates that are available for the study type that you selected.

Note The wizard retains this selection (LC or GC) after you close it. The next time you create a new study, the Study Type area displays your last selection.

You can process either GC/MS data or LC/MS data from within a study; you cannot process both types of data from within the same study. After you create a study, you cannot modify its study type.

You can perform step 1 through in any order—that is, naming the study, selecting the studies folder, and selecting a processing workflow are independent of each other.

Name the new study, select the top-level studies folder, and optionally select a study template

The New Study and Analysis Wizard is open to the Study Name and Processing Workflow page and you have selected the study type. See Start the New Study and Analysis Wizard and Select the study type.

❖ To name a new study, select the top-level studies folder, and optionally select a study template

1. In the Study Name and Directory Structure area, type a name for the new study in the Study Name box.

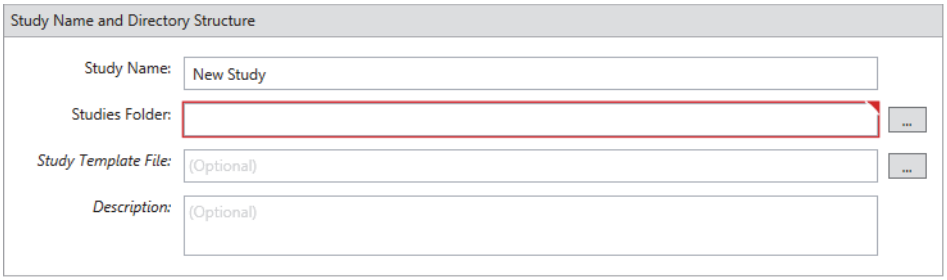
   Note When you create a new study, the application uses the study name that you specify for two items: the study file (.cdStudy) and the study folder where it stores the study file. The application stores the result files from the analyses run within the study in this named study folder. For details, see "Directory structure for Compound Discoverer studies."

Note The first time you create a study, the studies folder is undefined and the Studies Folder box is empty and outlined in red. If you have already created at least one studies folder, the Studies Folder box is populated with the name and location of the last studies folder that you created.

2. Use the current folder name and location that is displayed in the Studies Folder box or do the following to select an existing folder or create a new folder:

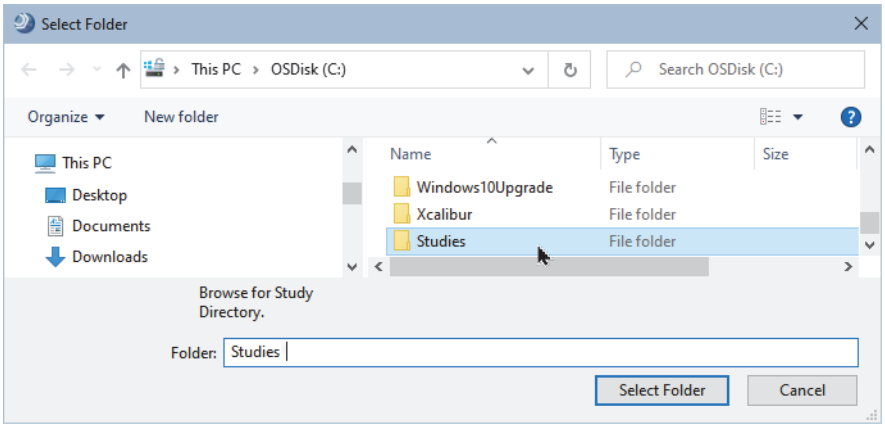
   a. Click the browse icon to the right of the Studies Folder box.

   Figure 29. Undefined studies folder



   The Select Folder dialog box opens.

   Figure 30. Select Folder dialog box



   b. Browse to an existing folder or use the New Folder command to create a new folder.

   The name and location of the new folder appear in the Studies Folder box.

Note You can store all your study folders in a single top-level folder or categorize your studies by setting up multiple top-level folders. See "Directory structure for Compound Discoverer studies."

Tip To create two studies with the same name but different data types, store the two studies in different folders.

3. (Optional) To select a study template file, click the browse icon, ..., next to the Study Template File box. Then, do one of the following:

   - To import only the study factors for the study, browse to and select a study file (.cdStudy).
   - To import all the study information, browse to and select a text file or a spreadsheet file that contains the study information in a compatible format.

     Note To create a spreadsheet that contains all the study information, see "Create a study template file that contains all the study information."

Select a processing workflow for the analysis

You can select a processing workflow (workflow template) on the Study Name and Processing Workflow page of the New Study and Analysis Wizard or on the Workflows page of an analysis.

- For information about opening the New Study and Analysis wizard, see "Start the New Study and Analysis Wizard."
- For information about starting a new analysis from within a study, see "Set up a new analysis from within an existing study."
- For information about opening th Workflows page of an analysis, see "Select a workflow template."

❖ To select a processing workflow for the current analysis

Do either of the following:

- Select a processing workflow from the Workflow list.

  The Workflow list displays the processing workflow files in the Common Templates folder for the study type that you selected in New Study and Analysis Wizard. Before you select a processing workflow on the Study Name and Processing Workflow page of the wizard, select the study type: GC or LC.

- Select a processing workflow or result file from another folder by clicking the browse icon, ..., next to the Workflow list.

  When you select a processing workflow file, the file name appears in the Workflow list. When you select a result file, the following text appears in the Workflow list:

  Imported from: *File name*

  where:

  File name is the file name of the result file

  If the processing workflow includes a description, the description appears in the Workflow Description box below the Workflow list.

If you are creating a new study and a new analysis in the New Study and Analysis Wizard, click **Next** to go to the Input File Selection page of the wizard.

Add input files to the new study

Use the Input File Selection page of the New Study and Analysis Wizard to select all the input files for the new study or only those input files that you want to process with the current analysis. If you click Finish before you add files to the study, the wizard saves the named study to the named folder and closes.

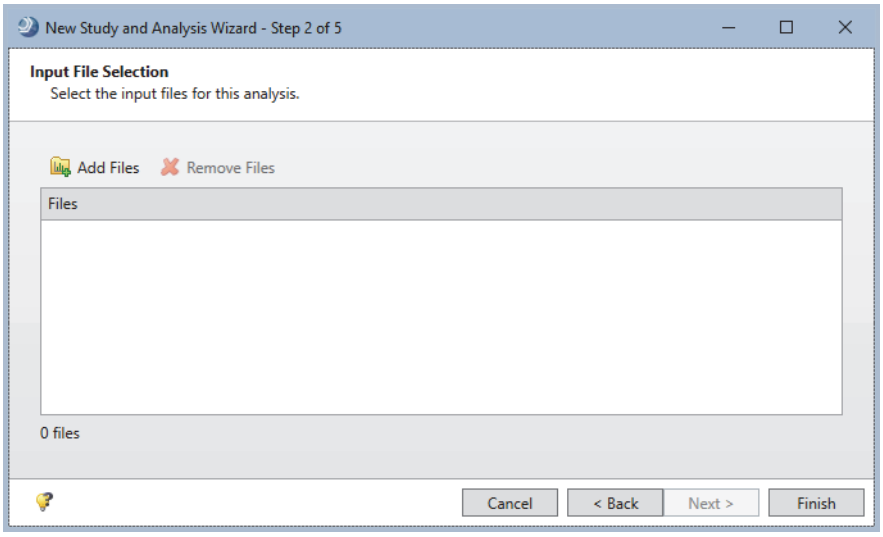
For information about starting the wizard and defining the study, see "Define the study type, name the study, and optionally select a study template and a processing workflow."

Note The example Xcalibur RAW files for the tutorials are on the Compound Discoverer USB key in the software media kit or in the software media that you downloaded from the Life Sciences and Mass Spectrometry Software Download and Licensing Portal website page. The software installation process does not install the example files on your processing computer.

❖ To add raw data files

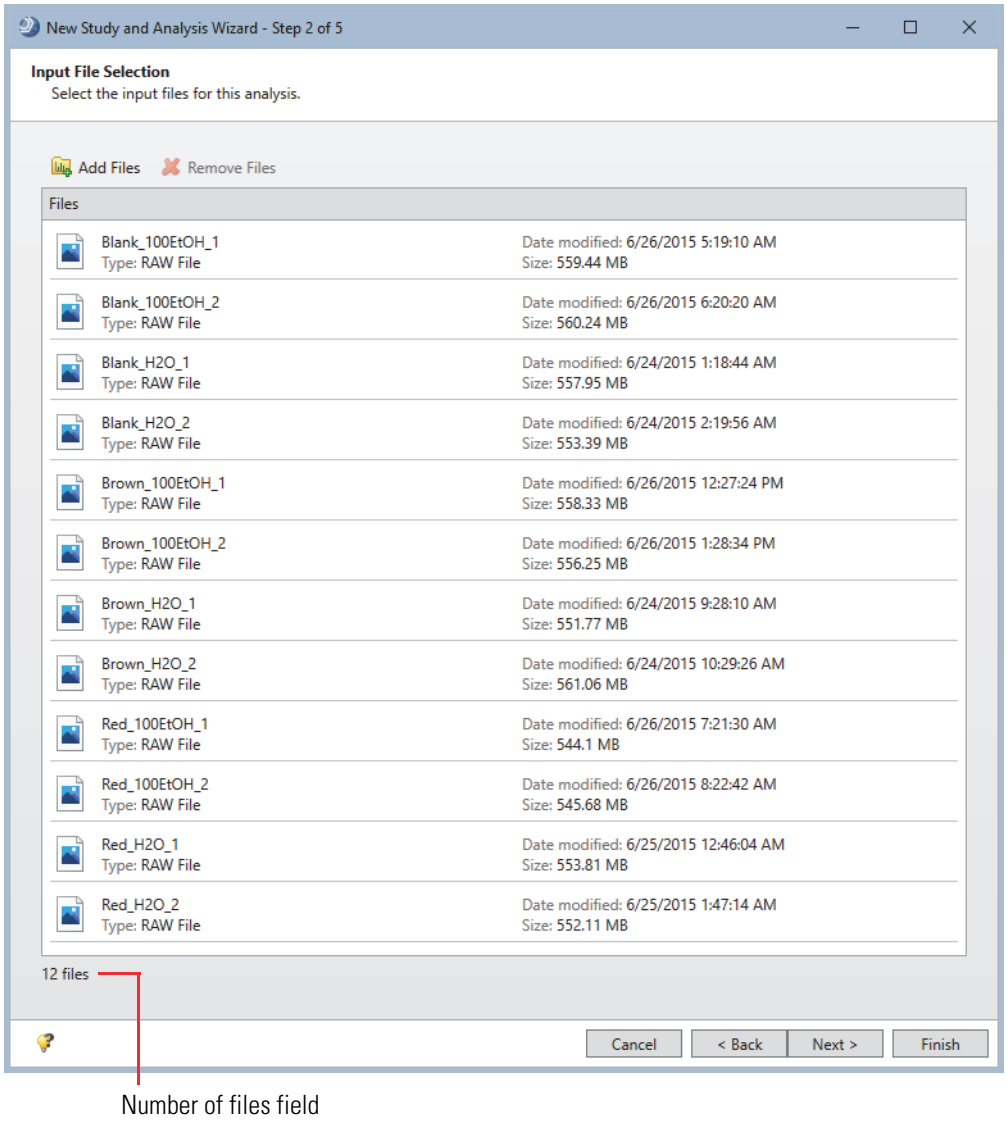
1. On Input File Selection page of the wizard, click **Add Files**.
2. Browse to the appropriate folder, select the Xcalibur RAW files of interest, and click **Open**.

Figure 31. Input File Selection page of the wizard



The file names of the selected files appear in the Files box, the number of files that you selected appears below this box, and the Next button becomes available.

Figure 32. Input File Selection page with selected files (brown O-rings and red O-rings)



Tip To remove any of the added files, select them and click **Remove Files**.

3. Do one of the following:
   - Click **Next** to continue to the Input File Characterization page.
   - Click **Finish** to create the new study and close the wizard.

Characterize the new input files

You can set up the sample information for the input files in a study in two ways:

- You can use the Input File Characterization page (step 3 of 5) of the New Study and Analysis Wizard that opens after you add new input files on the Input File Selection page of the wizard.

–or–

- You can use the Input File Characterization dialog box that opens when you add input files to an existing study.

The sample information includes the sample type and study factor values for each sample.

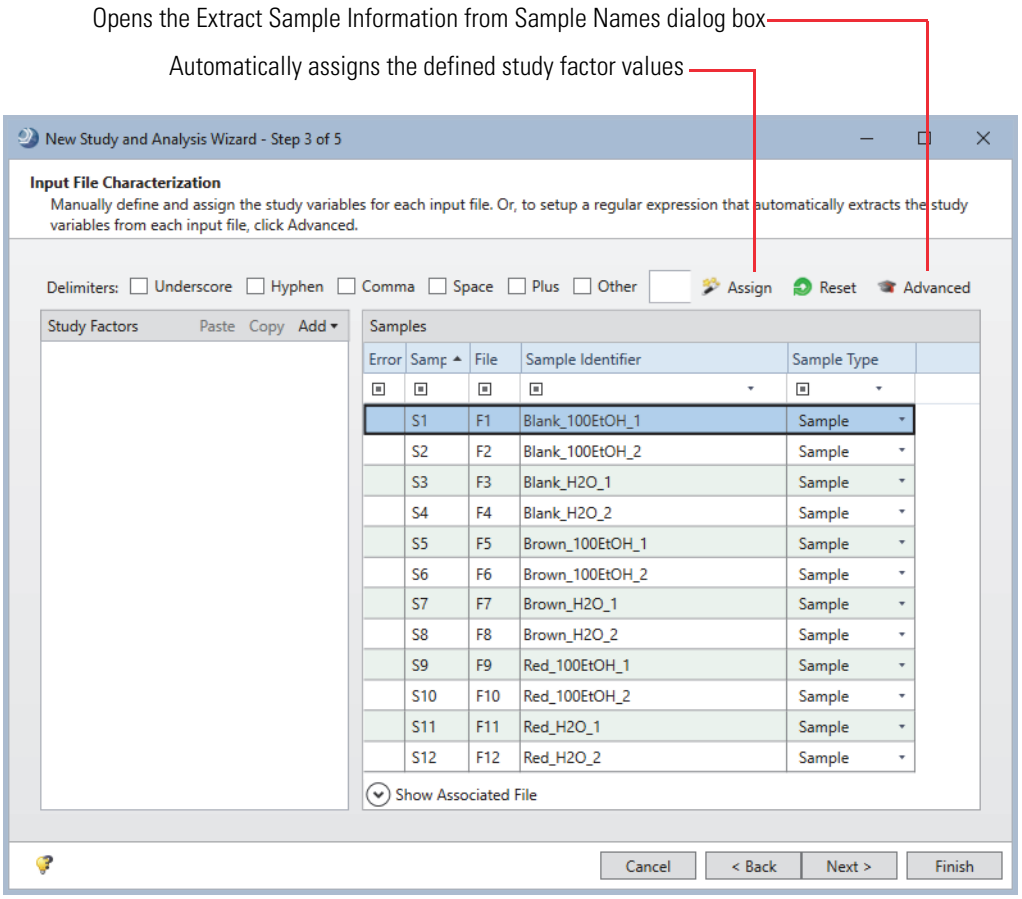
For information about starting the New Study and Analysis Wizard, see "Start the New Study and Analysis Wizard."

Note In an existing study, you can do the following:

- Use the Input File Characterization dialog box to add and edit the study factors and set up the sample information for additional input files.
- Add and edit the study factors on the Study Definition page.
- Manually select the sample types and study factor values on the Samples page.

Figure 33 shows the Input File Characterization page of the wizard.

Figure 33. Input File Characterization page of the wizard (with 12 O-rings)



To characterize the input files for a study, follow these steps as applicable:

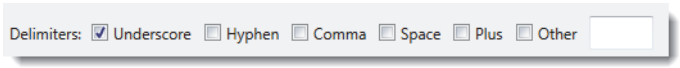
1. Select the delimiters for parsing the file names.
2. Add or edit the study factors.
3. To select or assign the study factor values to the samples (in the Samples area), see the following topics as applicable:
   - Automatically assign the study factor values
   - Manually select the study factor values
   - Reset the sample assignments
4. Select the sample types.

Select the delimiters for parsing the file names

You can select the delimiters for parsing a file name on the Input File Characterization page of the New Study and Analysis Wizard or in the Input File Characterization dialog box. For information about opening the Input File Characterization page or dialog box, see "Characterize the new input files."

❖ To select the delimiters that separate the factors in the file names

1. Select the check box or check boxes of the delimiter or delimiters for the input file names.



   For example, the underscore character is the delimiter that separates the study factors from the other parts of the file name in the following file names:

   In this case, the study factors are O-ring color and solvent. The O-ring colors are red and brown. The solvents are water and ethanol.

Blank_100EtOH_1	Blank_H2O_1
Blank_100_EtOH_2	Blank_H2O_2
Red_100EtOH_1	Red_H2O_2
Red_100EtOH_2	Red_H2O_1
Brown_100EtOH_1	Brown_H2O_1
Brown_100EtOH_2	Brown_H2O_2

2. If the delimiter is not available, select the **Other** check box and type the delimiter character in the box.

Add or edit the study factors

A study can include many study factors. You can add and edit the study factors on the Input File Characterization page of the New Study and Analysis Wizard or the Study Definition page of an existing study.

For details, see these topics:

- Add categorical study factors
- Add numeric study factors
- Add biological replicate study factors
- Delete study factors
- Duplicate study factors
- Edit study factors

Add categorical study factors

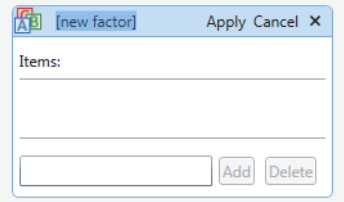
You can add study factors when you create a new study, when you add files to an existing study, and on the Study Definition page of an existing study.

❖ To add a categorical study factor to a study

1. From the menu bar at the top right of the Study Factors pane, choose **Add > Categorical Factor**.

   The categorical factor editor appears with [new factor] automatically selected.

   Figure 34. Categorical factor editor

2. Select the [new factor] text and type the name of the factor.

   For example, type **Color**.

3. For each item that you want to add to the Items list, do the following:

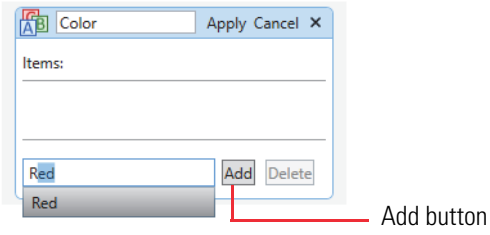
   a. In the Items box (to the left of the Add button), begin typing a factor.

      For example, type **Red** for one of the Color study factor items.

      If the file name contains a character delimiter (underscore, hyphen, comma, space, plus, or other defined character) and you selected the check box for this delimiter, the editor automatically enters the appropriate text in the Items box as you start typing. Otherwise, you must type all the characters for the item.

      Note The file name parsing feature is not available on the Study Definition page of an existing study, so you must type all the characters for the item.

      The Add button becomes available.

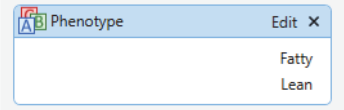
      

   b. Click **Add**.

      The current item appears in the Items list.

4. To save the study factor, click **Apply**.

   The factor editor collapses to show only the study factor name and the Items list. The items appear in ascending order.



Tip To continue editing the study factor, click **Edit**. The editor expands, providing access to the study factor name and items.

Add numeric study factors

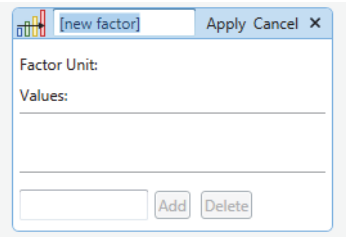
You can add study factors when you create a study, when you add files to an existing study, and on the Study Definition page of an existing study.

❖ To add a numeric factor to a study

1. From the menu bar at the top right of the Study Factors pane, choose **Add > Numeric Factor**.

   The numeric factor editor appears with [new factor] automatically selected.

Figure 35. Numeric factor editor



2. Type a factor name to replace [new factor], for example, **Replicate**.
3. Point to the right of Factor Unit and, in the box that appears, type a unit for the factor if applicable.

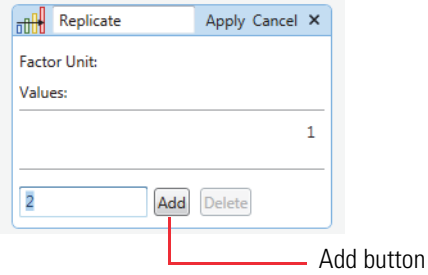
   The Factor Unit is only a text label; however, it must start with a letter.

4. For each numeric value that you want to add to the Values list, do the following:

   a. In the box next to the Add button, type a numeric value.

      The Add button becomes available.

Figure 36. Entering numeric values in the values box



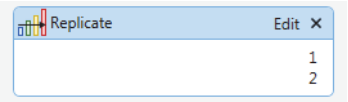
b. Click **Add**.

The value appears in the Values list in ascending order.

5. To save the study factor, click **Apply**.

The factor editor collapses to show only the study factor name and the Values list.

Figure 37. Numeric factor with a list of values



Tip To continue editing the study factor, click **Edit**. The editor expands, providing access to the study factor name and items.

Add biological replicate study factors

You can add study factors when you create a study, when you add files to an existing study, and on the Study Definition page of an existing study.

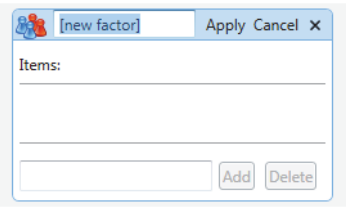
You can add only one biological replicate factor to a study. Use the biological replicate factor for nested statistical models—that is, for studies that include one study factor nested within another study factor.

❖ To add a biological replicate factor to a study

1. From the menu bar at the top right of the Study Factors pane, choose **Add > Biological Replicate Factor**.

The biological replicate factor editor appears with [new factor] automatically selected.

Figure 38. Biological replicate factor editor



2. Type a factor name to replace [new factor].
3. For each item that you want to add to the Items list, do the following:
   a. In the Items box (next to the Add button), type a study factor item.

      The Add button becomes available.

   b. Click **Add**.

      The current item appears in the Items list.
4. To save the study factor, click **Apply**.

   The factor editor collapses to show only the study factor name and the Items list. The items appear in alphabetical order.

> **Tip** To continue editing the study factor, click **Edit**. The editor expands, providing access to the study factor name and items.

Delete study factors

You can delete study factors in the Study Factors pane on the Study Definition page or the Study Factors pane on the Input File Characterization page or dialog box.

❖ To delete a study factor from a study

1. In the Study Factors pane, click X in the title bar of the factor.

> **Note** Because the application cannot recognize whether a study factor is in use, this prompt appears even when you attempt to delete an undefined study factor.

2. At the prompt, click **Yes** to delete the study factor.

Duplicate study factors

You can use the Copy and Paste commands to duplicate and create new study factors in the Study Factors pane on the Study Definition page or the Study Factors pane on the Input File Characterization page or dialog box.

❖ To create a new study factor by using the Copy and Paste commands

1. In the Study Factors pane, select the factor that you want to copy.

   The title bar of the selected factor turns blue.
2. Click **Copy**. Then, click **Paste**.

   A copy of the selected factor appears.

Edit study factors

You can edit study factors as you create a new study with the wizard, in Study Factors area of the Input File Characterization dialog box when you add more files to an existing study, and in the Study Factors area on the Study Definition page of an existing study.

❖ To edit a study factor

1. In the factor title bar, click **Edit**.

   The text entry box and the Add and Delete buttons appear. For a numeric factor, the Factor Unit box also appears.

2. To change the unit for a numeric factor, select the current unit and type a new unit.
3. To add more entries to the Items or Values list, type alphanumeric text in the appropriate box, and then click **Add**.
4. To delete an entry, select the entry and click **Delete**.

   When an entry is in use, it is unavailable. To delete a value that is in use, you must first undo its assignment to any sample.

Automatically assign the study factor values

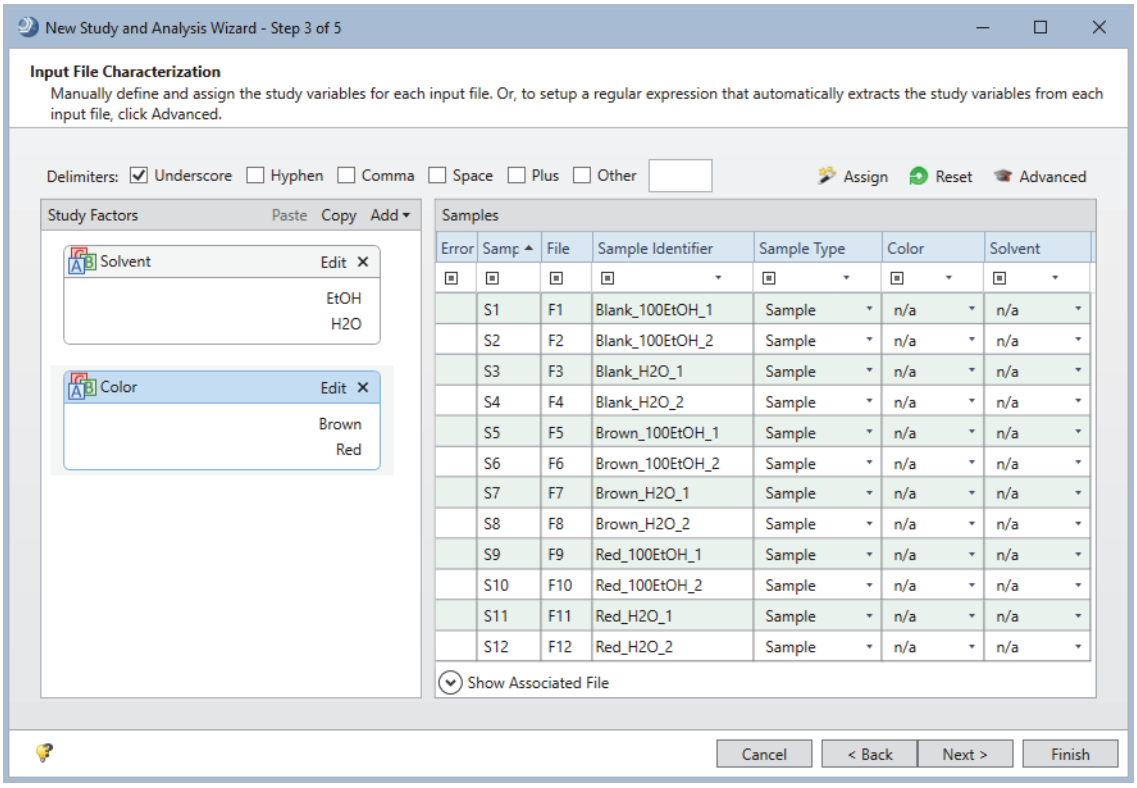
After you set up the study factors for a study, you can assign the study factor values to each sample. If the input file names follow a consistent pattern and the study factor values are completely defined, clicking Assign on the Input File Characterization page (or dialog box) assigns the study factor values to the samples.

Note You can only manually assign study factor values on the Samples page of an existing study.

❖ To automatically assign the study factor values to a sample set

1. If you have not already set up the study factors, set them up. See “Add or edit the study factors.”

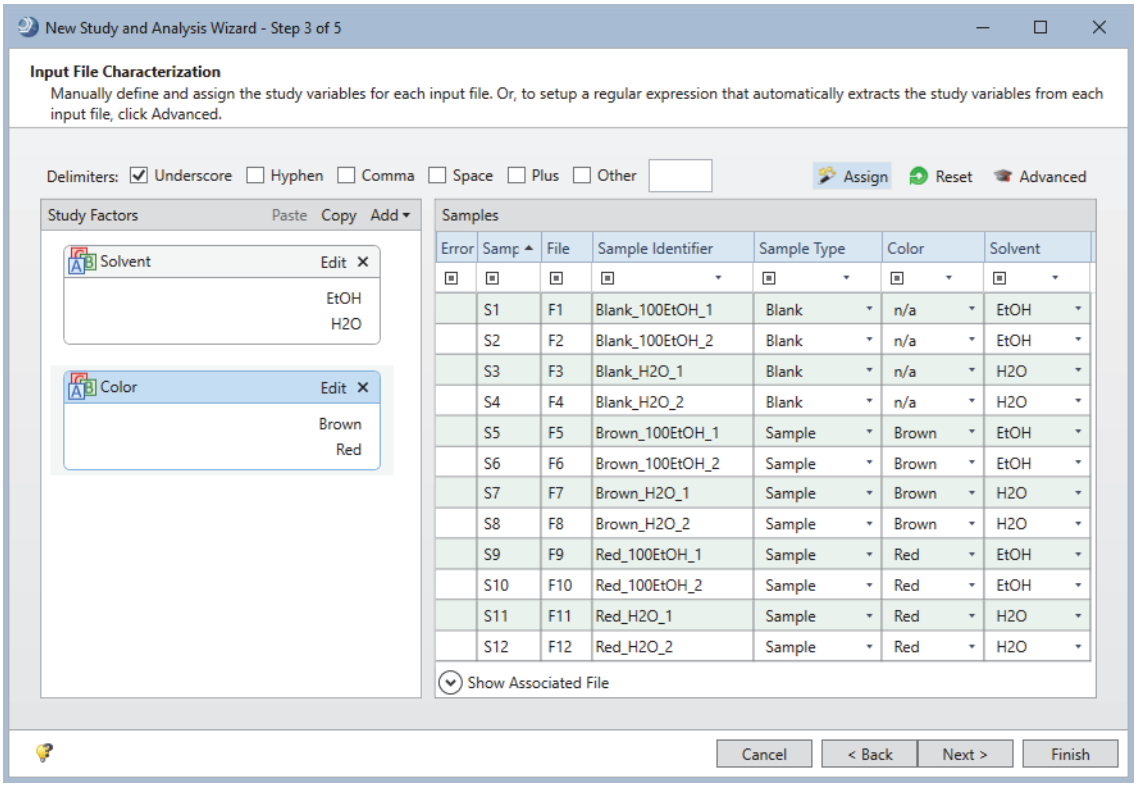
Figure 39. Input file Characterization page with two study factors—Color and Solvent



2. In the command bar of the Input File Characterization page or dialog box, click **Assign**.

   The application assigns the study factors to the samples. See Figure 40.

Figure 40. Input file Characterization page with assigned sample types and study factors



3. Check the study factor columns, verify the sample assignments, and manually assign the study factor values if necessary.

Manually select the study factor values

After you set up the study factors for the study, you can select the study factor values for each sample. If the input file names do not follow a consistent pattern or do not include the study factor values or you are selecting the values on the Samples page of an existing study, you have to manually select these values.

❖ To manually select the study factor values

On the Input File Characterization page (or dialog box) or on the Samples page of an existing study, do the following:

- To select the factor values for a single sample, select the appropriate value from the list in each factor column.
- To select the same value for a consecutive sample range, drag the pointer across the rows of interest. Then right-click and choose **Set *Factor* To > *Value***.
- To select the same value for nonconsecutive samples, hold down the CTRL key and click the samples of interest. Then right-click and choose **Set *Factor* To > *Value***.

Reset the sample assignments

On the Input File Characterization page (or dialog box), you can use the Reset button in the command bar to automatically clear the sample assignments. The Samples page of a study does not have a command bar.

❖ To clear the assignments in the Samples pane

In the command bar, click **Reset**.

Clicking Reset resets the Sample Type and study factor assignments—that is, it resets the sample type to Sample and the study factor values to n/a for all the samples.

Note To edit the values for a study factor, you must first clear the sample assignments if the values are assigned to samples.

Select the sample types

You can select the sample type for the study samples from any of these locations:

- The Samples pane of the Input File Characterization page (page 4 of the wizard)
- The Samples pane of the Input File Characterization dialog box
- The Samples page of an existing study

By default, the selected sample type for each input file is Sample. Clicking Assign on the Input File Characterization page (or dialog box) automatically assigns the Blank sample type to samples with a file name that includes "blank" as a delimited value (for example, solvent_blank_1.raw, where the underscore character is the delimiter).

❖ To select a sample type other than the default assignment

In the Samples pane (any location), do any of the following:

- To select the sample type for a single sample, select a sample type from the dropdown list in the Sample Type column. See "Available sample types."
- To assign the same sample type to a consecutive sample range, use the SHIFT key to select a range of samples. Then, right-click and choose **Set Sample Type To > *Sample Type***.
- To assign the same sample type to nonconsecutive samples, use the CTRL key to select the samples. Then, right-click and choose **Set Sample Type To > *Sample Type***.

Tip To select a row, click a column without a list.

Extract study factor values from the file names of the input files

Use the Extract Sample Information From Sample Names dialog box to automate the setup and assignment of the study factors. This dialog box is accessible from the Input File Characterization page of the New Study and Analysis Wizard or from the Input File Characterization dialog box that opens when you add input files to a study.

Note For the extraction and assignment process to work, you must select the study factor portions of an example input file name and define these portions appropriately as categorical, numerical, or biological replicate factors.

When the undefined portions of the file name are not exactly the same for all the samples that you want to characterize, you can mark the text to be ignored or you can manually assign or edit the study factor values for these samples after returning to the Input File Characterization page or dialog box.

❖ To extract the sample information from the sample names

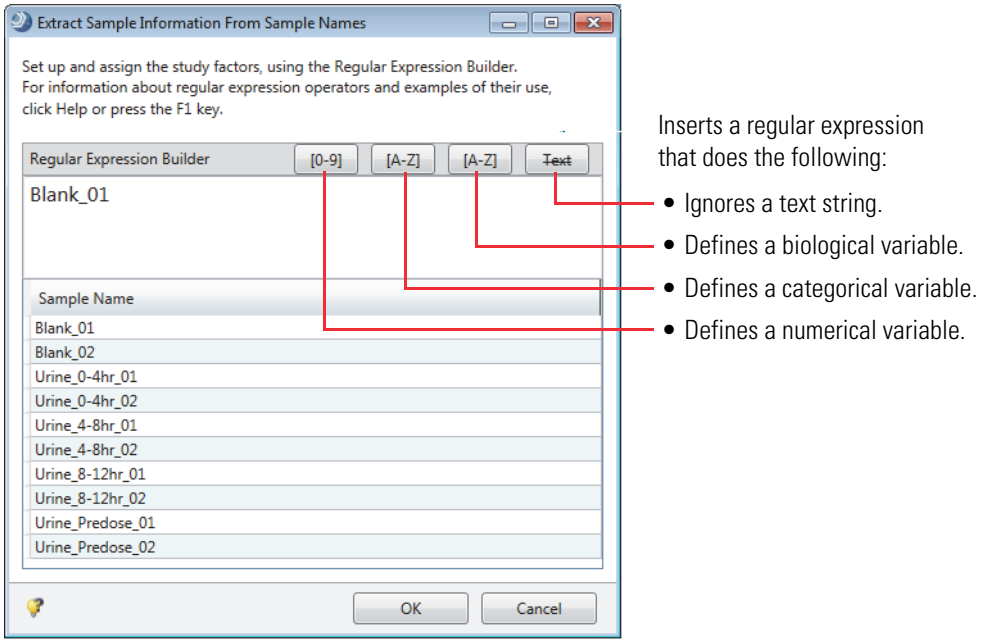
1. Open the Input File Characterization page (step 3 of 5) of the wizard or the Input File Characterization dialog box from within an existing study.

   Note When you are working within an existing study, the Input File Characterization dialog box opens when you add files to the study. You cannot open the Input File Characterization dialog box to characterize raw data files that are already linked to the study.

2. Click **Advanced**.

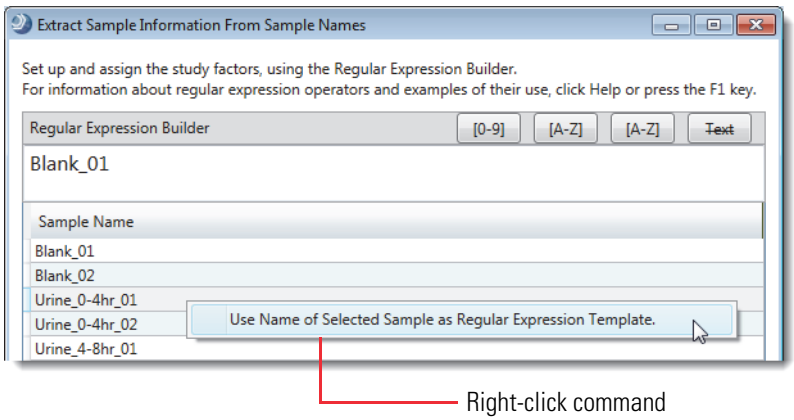
   The Extract Sample Information From Sample Names dialog box opens with the first file name displayed in the Regular Expression Builder box and the file names of all the selected input files listed below it. See Figure 41.

Figure 41. Extract Sample Information From Sample Names dialog box



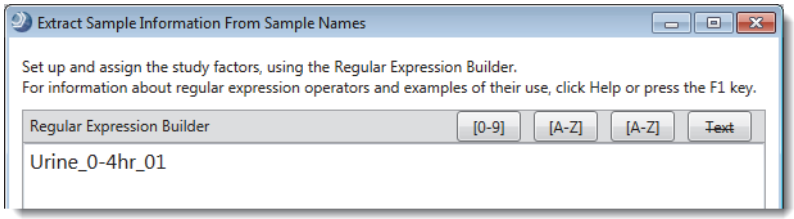
3. If the Regular Expression Builder box does not contain a representative sample name, right-click a representative sample name in the Sample Name column and choose **Use Name of Selected Sample as Regular Expression Template**.

Figure 42. Urine_0-4hr_01 sample name selected



The selected sample name replaces the nonrepresentative sample name.

Figure 43. Urine 0-4hr file name to be used as the regular expression template



4. For a representative sample name, do the following:

   - For each categorical study factor, select the corresponding study factor item and click **[A-Z]**.

     For example, select **0-4hr** and click **[A-Z]**.

     The CategoricalVariable_1 column appears to the right of the sample names. In this example, the application extracts the categorical study factor for the Urine_Predose_01 sample. The column is not populated with study factor values for the remaining samples for two reasons:

     – The remaining portions of the sample names are not the same (for example, _01 and _02).

     – The default expression for a categorical factor does not recognize the hyphen special character in the 0-4hr, 4-8hr, and 8-12hr time points.

   - For each numeric study factor, select the corresponding study factor value and click **[0-9]**. For example, select **1** and click **[0-9]**.

     For this example, the following expression replaces the file name:

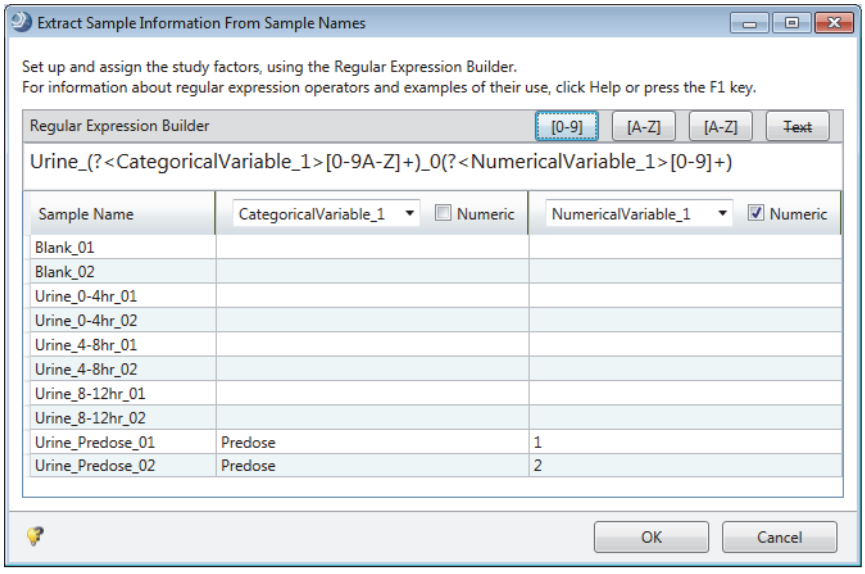
     Urine_(?<CategoricalVariable_1>[0-9A-Z]+)_ (?<NumericalVariable_1>[0-9]+)

     –and–

     Only the study factor values for these file names appear in the table: Urine_Predose_01 and Urine_Predose_02.

Figure 44 shows the new regular expression in the regular expression builder box. This expression cannot interpret the time points that include hyphens (0-4hr, 4-8hr, 8-12hr). Only “Predose” matches the expression, which is looking for an alphanumeric string.

Figure 44. Building a regular expression with the default categorical and numeric operators



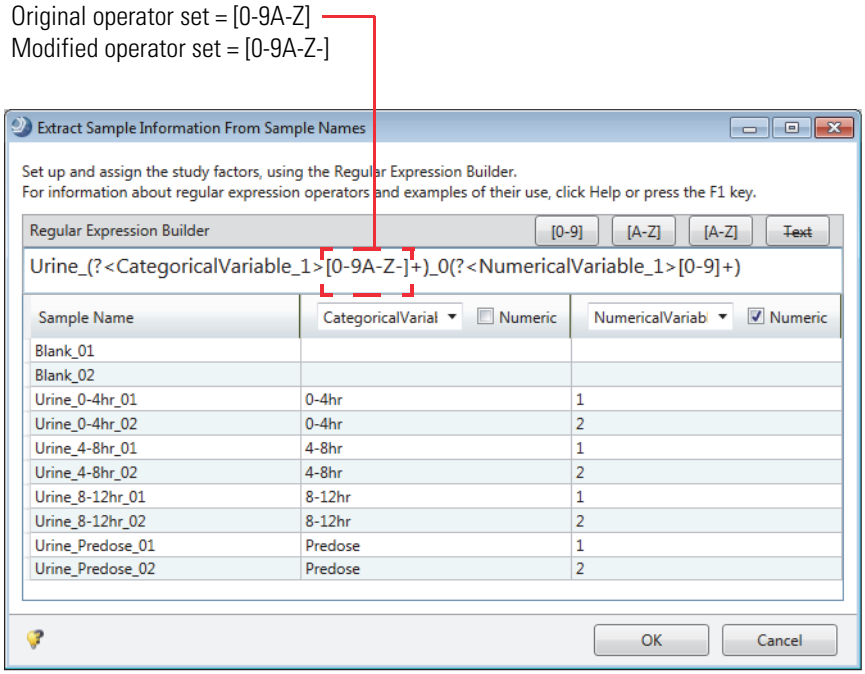
5. If the study factor columns do not populate as expected, modify the regular expression operators within the square brackets.

Table 14. Examples of regular expression operators

Operator	Quantifier	Matching pattern
[0-9]	none	A single integer
[0-9]	+	One or more integers
[A-Z]	none	One alphabetic character
[0-9A-Z]	none	One alphanumeric character
[0-9A-Z]	+	One or more alphanumeric characters
[0-9A-Z-]	+	One or more alphanumeric characters, one or more hyphens, or both (for example, 555-0000)
[0-9A-Z] [0-9A-Z]	+	One or more alphanumeric characters, a space, and one or more alphanumeric characters (for example, ABC 123)

For example, to populate the rows for the other file names with defined time periods, add a hyphen to the operators in the square brackets. Figure 45 shows the hyphen character added to the operator set for a categorical factor.

Figure 45. Hyphen building block added to the regular expression for a categorical factor

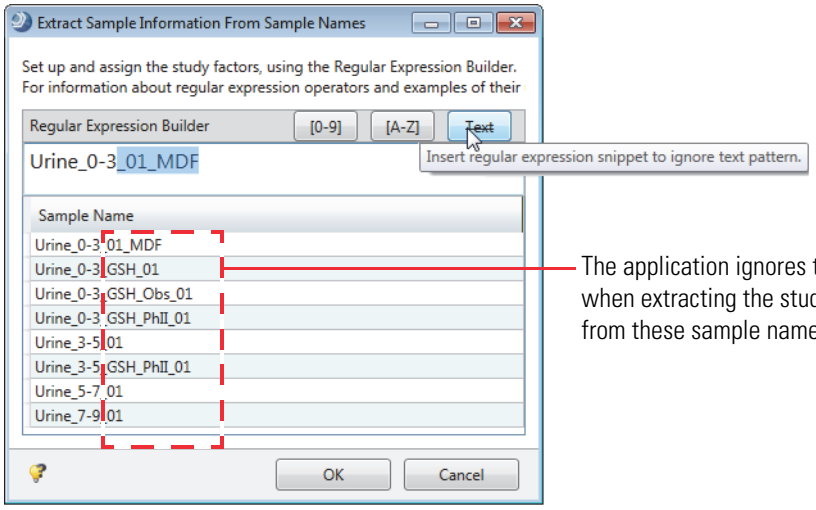


6. If the sample names include extra text that differs from sample to sample and does not define a study variable, exclude this text from the regular expression by selecting it and clicking Text.

Note Figure 46 and Figure 47 show a different sample set than the previous figures.

For example, in the sample set shown in Figure 46, exclude all the characters to the right of the categorical variable by selecting **_01_MDF** and clicking Text.

Figure 46. Selecting the text that you want to exclude from the expression



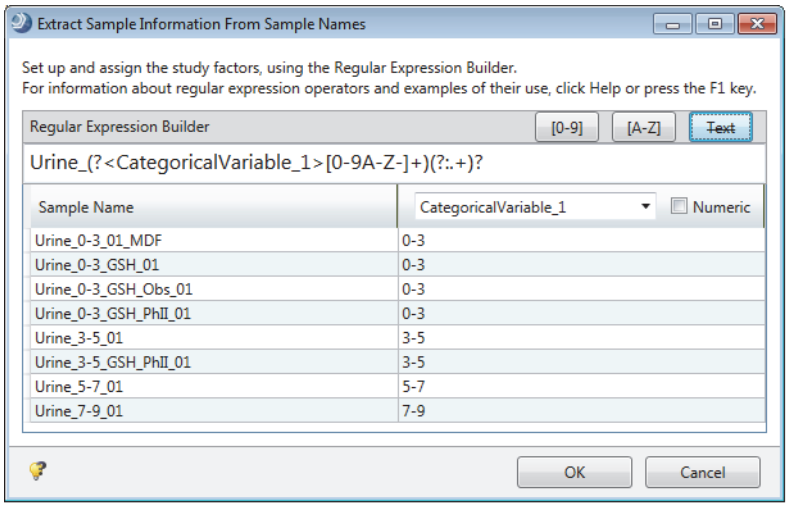
The regular expression builder replaces the selected text with the following expression:

(?:.+)?

Figure 47 shows the result of these actions:

- Selecting the time period (0-3) as a categorical variable
- Adding a hyphen to the categorical variable expression
- Selecting "_01_MDF" as text to ignore

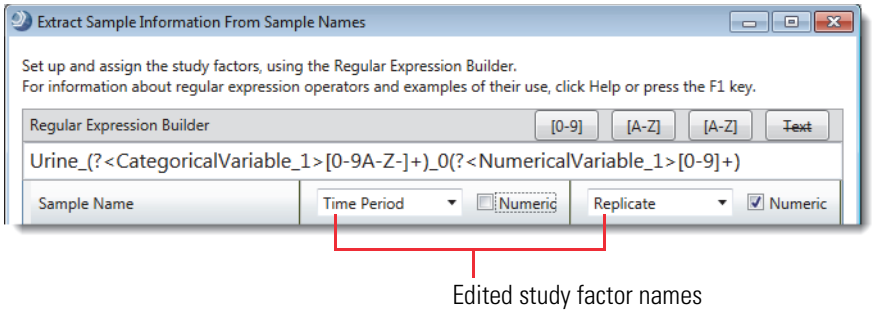
Figure 47. Regular expression that defines the categorical variable and the text to ignore



7. To enter the study factor names, type the study factor names in the column-heading boxes.

   For example, replace CategoricalVariable_1 with **Time Period** and NumericalVariable_1 with **Replicate** (Figure 45 and Figure 48).

Figure 48. Study factors renamed



Tip You can edit the study factor names in two ways:

- In the column-heading boxes, replace the default column headings with the study factor names.
- On the Input File Characterization page, edit the study factors.

8. Click **OK** to return to the Input File Characterization page where you can modify the values in the study variable columns if necessary.

Tip The Regular Expression Builder does not assign sample types. To assign Blank as the sample type, click Assign on the Input File Characterization page after selecting the appropriate delimiters.

For example, select the **Underscore** check box on the Input File Characterization page and click **Assign**, for the following file name: Solvent_Blank_1.

Table 15 describes the parameters in the Extract Sample Information From Sample Names dialog box.

Table 15. Extract Sample Information From Sample Names dialog box parameters

Parameter	Description
Regular Expression Builder	
Initially displays the first file name in the Sample Name list. Use this file name (or a different file name in the list) to build a regular expression that extracts the study factor values for the file names in the Sample Name list.	
Buttons	
[0-9]	Identifies a numeric factor. Clicking [0-9] replaces the selected text with the following expression: (?<NumericalVariable_1>[0-9]+)
[A-Z]	Identifies a categorical factor. Clicking [A-Z] replaces the selected text with the following expression: (?<CategoricalVariable_1>[0-9A-Z]+)
[A-Z]	Identifies a biological replicate factor. Clicking [A-Z] replaces the selected text with the following expression: (?<ReplicateVariable_1>[0-9A-Z]+)
Text	Excludes text that does not define a study variable and does not follow a pattern. Clicking Text replaces the selected text with the following expression: (?:.+)?
Columns	
Sample Name	Displays the file names of the selected input files.
CategoricalVariable_*1*	Displays the extracted items for this factor. You can edit the column heading.
NumericalVariable_*1*	Displays the extracted values for this factor. You can edit the column heading.
ReplicateVariable_*1*	Displays the extracted values for this factor. You can edit the column heading.

Set up the sample groups and ratios for a new analysis

Use the Sample Groups and Ratios page of the New Study and Analysis Wizard or the Grouping & Ratios page of an analysis within an existing study to set up the sample groups that you want to compare and the group ratios that you want to include in the result file.

Note The Sample Groups and Ratios page of the New Study and Analysis Wizard is the fourth page of the wizard. To open the fourth page of the wizard, you must select one or more input files on the second page of the wizard.

Note When you start a new analysis in an existing study, you must manually add the input files to the Files for Analysis area of the Analysis view.

IMPORTANT Do not create ratios with sample groups that have an n/a assignment for a study variable. To use a sample group in a ratio, you must replace the n/a assignment with a study factor value.

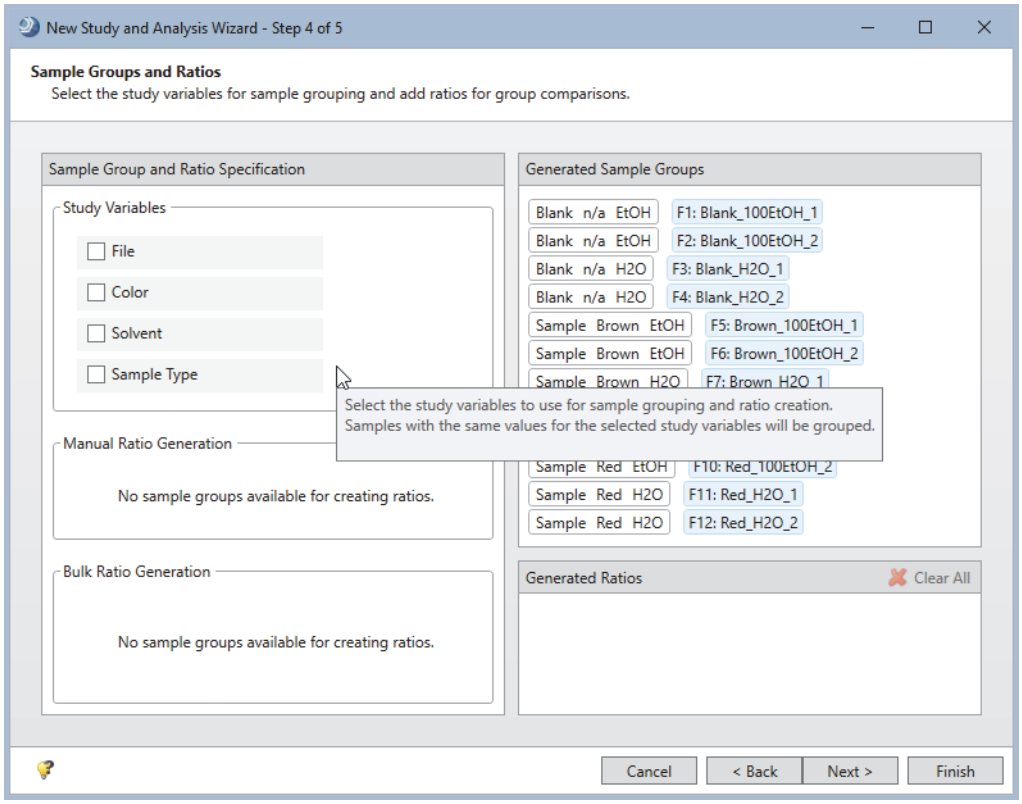
Follow these topics:

1. Set up the sample groups for an analysis
2. Set up the group ratios

The Study Variables area contains a File check box, a Sample Type check box, and an additional check box for each study factor you created on the Input Files Characterization page of the wizard or the Study Definition page of the current study.

Figure 49 shows the Sample Groups and Ratios page of the wizard. The Generated Sample Groups area lists the input files for the analysis.

Figure 49. Sample Groups and Ratios page of the wizard



Set up the sample groups for an analysis

To set up the sample groups for an analysis, follow these procedures:

1. Select the study variables for the sample groups
2. Review the generated sample groups and fix any assignment errors
3. Do the following as appropriate:
   - Change the hierarchy of the study variables
   - Change the sort order of the study variables

Select the study variables for the sample groups

You select the study variables that you want to group on one of these pages:

- Grouping & Ratios page of an existing analysis

> **Note** To start a new analysis from within an existing study, click **New Analysis** in the study command bar. Or, reprocess an existing analysis on the Analysis Results page of a study.

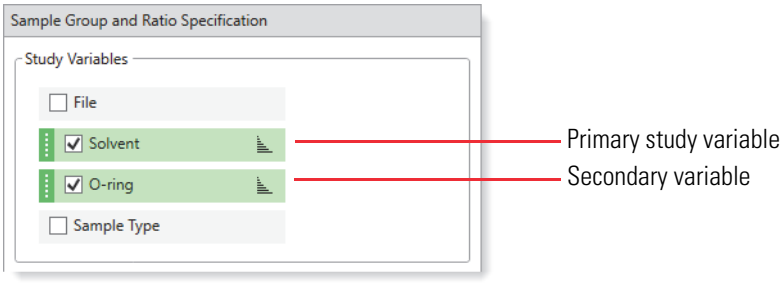
- Sample Groups and Ratios page of the New Study and Analysis Wizard

> **Note** The Sample Groups and Ratios page of the New Study and Analysis Wizard is the fourth page of the wizard. To open the fourth page of the wizard, you must select one or more input files on the second page of the wizard.

❖ **To select the study variables for sample grouping**

In the Study Variables area of the page, select the check boxes for the study variable or variables for sample grouping.

Selected study variables have a light green background, a dark green handle ( ) on the left, and a Sorting icon ( )on the right.



Review the generated sample groups and fix any assignment errors

After you select the study variables for sample grouping, the Generated Sample Groups area displays the generated sample groups.

The hierarchy of the selected study variables in the Study Variables area affects the sample group names and the denominator list for bulk ratio generation. See "Change the hierarchy of the study variables."

The naming scheme for the study groups in the Generated Sample Groups area is as follows:

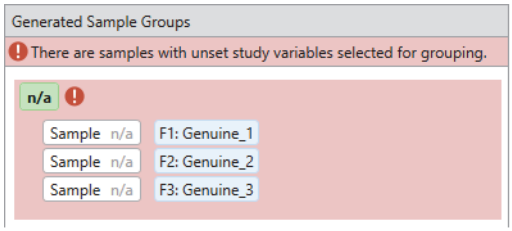
- Group names (green) consist of the common values for the selected study variables.
- Sample names (blue) consist of a unique ID and the input file name.

Following data processing, the result file displays the chromatographic peak areas for individual samples and the named sample groups.

When selecting the study variables generates an n/a sample group that includes Sample, Control, or Standard sample types, the application highlights the selected study variable and the n/a group in red and displays the following error message:

There are samples with unset study variables selected for grouping.

Figure 50. Error message for unset study variables



❖ **To fix an assignment error on the Sample Groups and Ratios page of the wizard or the Grouping & Ratios page of an analysis within an existing study**

1. Check the sample type and study factor assignments of the input files as follows:
   - If you are creating a new study, in the New Study and Analysis Wizard, return to the Input File Characterization page.
   - If you are modifying an existing study, open the Samples page.
2. Do any of the following:
   - Assign study factor values to the Sample, Control, or Standard sample types. If necessary, create new study factor values for these samples.
   - For LC studies, change the sample type assignment for samples without a study factor value to **Blank, Identification Only**, or **Quality Control** as appropriate.
3. Do one of the following:
   - In the New Study and Analysis Wizard, return to the Sample Groups and Ratios page and verify the assignments.
   - In an existing study where you have started a new analysis, return to the Grouping & Ratios page.

Change the hierarchy of the study variables

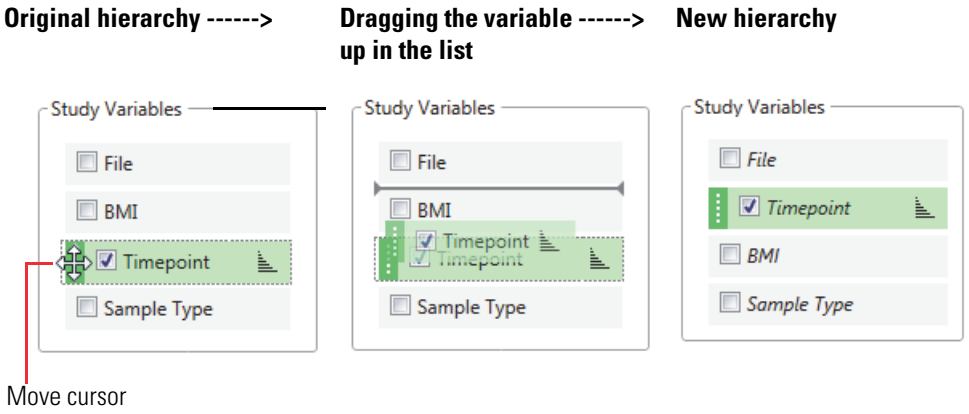
You can set up the group ratios on the Grouping & Ratios page of an existing analysis or on the Sample Groups and Ratios page of the New Study and Analysis Wizard.

The hierarchy of the selected study variables in the Study Variables area affects the sample group names and the denominator list for bulk ratio generation.

❖ **To change the hierarchy of the study variables**

Place the pointer over the handle ( ) to the left of a variable name. When the move cursor ( ) appears, drag the variable up or down in the list.

Figure 51. Changing the hierarchy of the study variables



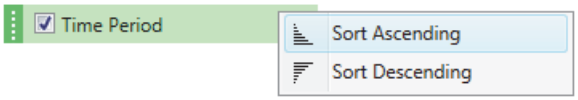
Change the sort order of the study variables

The sort order of the study variables affects the denominators to be used in the Bulk Ratio Generation area on the Grouping & Ratios page of an existing analysis or on the Sample Groups and Ratios page of the New Study and Analysis Wizard.

❖ **To change the sort order of the study variables**

Click the **Sorting** icon for the study variable that you want to sort by and choose **Sort Ascending** or **Sort Descending**.

Figure 52. Sort order shortcut menu for the study variables



Set up the group ratios

You can set up group ratios individually in the Manual Ratio Generation area or automatically by using the bulk ratio generator.

For details about setting up the group ratios, see the following topics:

- Set up the group ratios individually
- Set up the group ratios by using the bulk ratio generator

The application assumes you are setting up the group ratios for a differential analysis. When you set up at least one group ratio, information about the statistical test that the Differential Analysis node will perform appears in the Generated Ratios area.

Tip The Differential Analysis node is a post-processing node in the processing workflow for an analysis. When you set up group ratios for an analysis that does not include the Differential Analysis node, a validation prompt appears when you submit the analysis to the job queue. If you do not want the analysis to perform a differential analysis, you can click Ignore to dismiss the prompt and start the run.

The workflow templates provided with the application that include Statistics in their file names include the Differential Analysis node.

Table 16. Messages in the Generated Ratios area (Sheet 1 of 2)

Setup	Message
Non-nested design	
Two group comparison	Hypothesis test performed by a two-tailed student's t-test (which assumes that the means for the two groups are not equivalent). P-values are adjusted by the Benjamini-Hochberg algorithm.
Multi-group comparison	Hypothesis test performed by a one-way ANOVA model with Tukey as post-hoc test. P-values are adjusted by the Benjamini-Hochberg algorithm.
Nested design	
Two group comparison	Hypothesis test performed by a multivariate paired t-test (assuming equal variance). P-values are adjusted by the Benjamini-Hochberg algorithm.
Multi-group comparison	Hypothesis test performed by an unpaired ANOVA model with Tukey as post-hoc test. P-values are adjusted by the Benjamini-Hochberg algorithm.

Table 16. Messages in the Generated Ratios area (Sheet 2 of 2)

Setup	Message
Alert message with a yellow background	
Non-nested design for ratios with biological samples	Nested design is not applicable. For a nested design, the same biological samples must be present in all sample groups.

Set up the group ratios individually

You can set up the group ratios on the Grouping & Ratios page of an existing analysis or on the Sample Groups and Ratios page of the New Study and Analysis Wizard.

❖ To set up group ratios one by one

In the Manual Ratio Generation area of the page, select a group from the Numerator list, select a group from the Denominator list, and click **Add Ratio**. Repeat this step for each pair of groups that you want to compare.

Set up the group ratios by using the bulk ratio generator

You can set up the group ratios on the Grouping & Ratios page of an existing analysis or the Sample Groups and Ratios page of the New Study and Analysis Wizard.

Note The hierarchy of the selected study variables in the Study Variables area affects the sample group names and the denominator list for bulk ratio generation and the sort order of the study variables affects the denominators to be used in the Bulk Ratio Generation area. For details, see "Change the hierarchy of the study variables," and

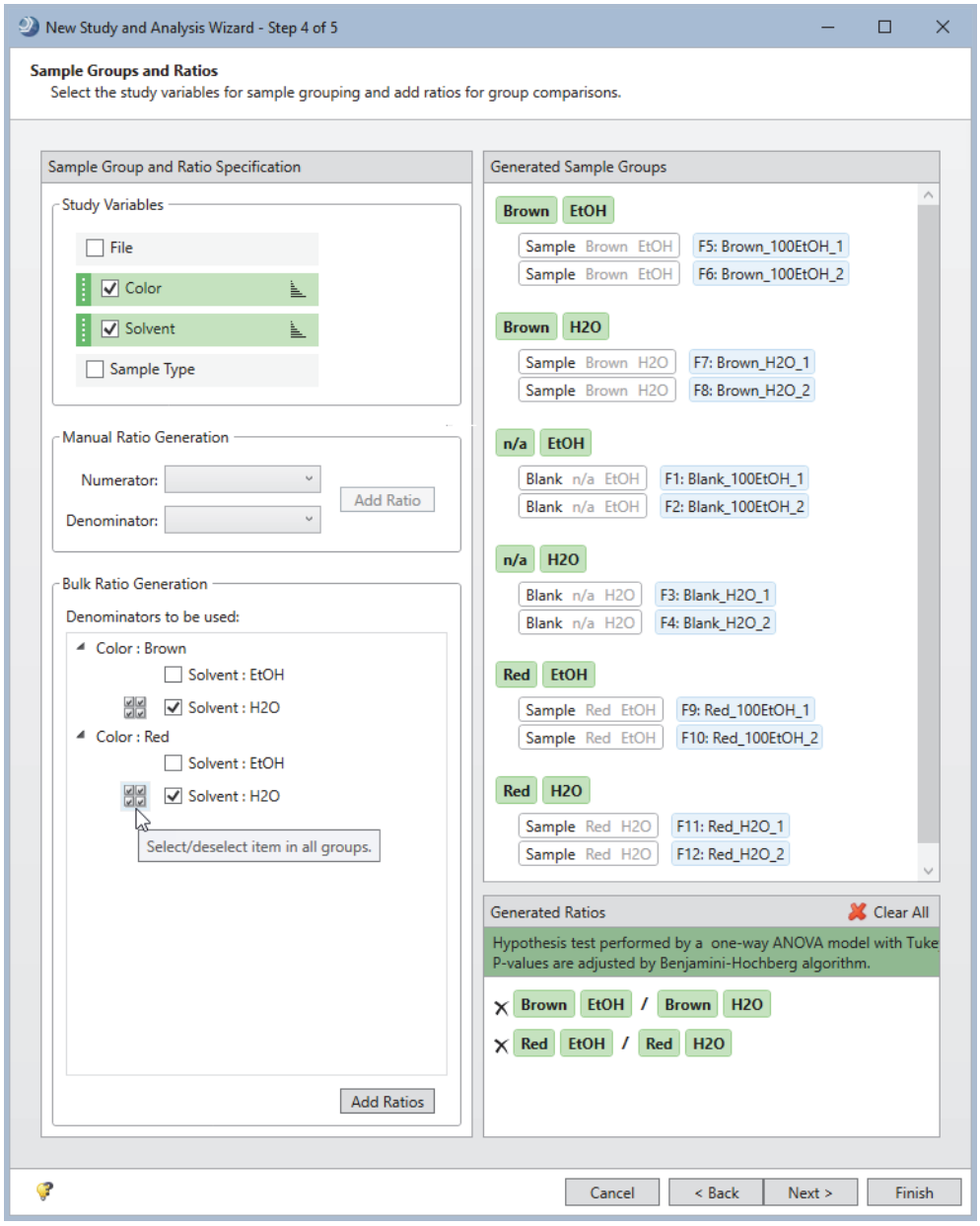
❖ To automatically set up one or more ratios

1. Modify the sort order and hierarchy of the study variables as appropriate.
2. In the Bulk Ratio Generation area, select one or more denominators and click **Add Ratios**.

   When you select more than one variable in the Study Variables area and the selected variables have multiple values, the Select/Deselect Item in All Groups icon,  , appears when you place the pointer near a denominator in the Denominators to Be Used area.

   To automatically select multiple check boxes for the same value in all groups, select one of the check boxes for the value, and then click the **Select/Deselect Item in All Groups** icon,  .

Figure 53. Two study factors and multiple groups



3. To modify the group ratio list, do either of the following:
   - To remove a ratio, click the delete icon (✕) to its left.
   - To clear the entire list, click **Clear All**.

Prepare to submit the analysis to the job queue

The first time you use the New Study and Analysis Wizard, read the instructions on the final page of the wizard (step 5 of 5).

Clicking Finish on the Input File Selection page (after selecting input files), on the Input File Characterization page, or on the final wizard page opens the study page and the Analysis view. The Analysis view contains the selected input files. If you selected a processing workflow on the Study Name and Processing page of the wizard, the Workflow box on the Analysis view displays the name of the processing workflow, and the Workflows page contains the processing workflow.

Before starting a run, you can edit the study, the processing workflow, the input file list, and the result file name. Some of the defined processing workflows require customization. For example, for a targeted analysis, you must select the target compounds for the Generate Expected Compounds node. For information about customizing a processing workflow, see "Customize the processing workflow."

If the processing workflow is valid and the Analysis view contains one or more input files, the Run command at the top right of the Analysis view is available.

If the Run command is unavailable, you must fix the analysis errors. See "Troubleshoot common analysis errors."

4

Set up, run, and reprocess analyses

To set up and submit new analyses, review the details of completed analyses, or reprocess analyses, see these topics:

- Set up a new analysis from within an existing study
- Troubleshoot common analysis errors
- Submit an analysis to the job queue and fix any validation issues
- Control the Job Queue
- Review or reprocess an analysis
- Analysis view parameters

These topics describe how to set up additional tables, lists, or files for use in a processing workflow:

- Set up individual isotope patterns by using the Isotope Ratio Editor
- Create an isotope patterns list by using the Pattern List Editor
- Extract analog and PDA traces

Set up a new analysis from within an existing study

You can set up a new analysis by beginning with an empty Workflows page, an empty Grouping & Ratios page, and an empty Analysis view. Or, you can set up a new analysis by reprocessing an analysis from the Analysis Results page.

Tip You cannot set up the sample groups and ratios on the Grouping and Ratios page without first adding the appropriate input files to the Analysis view.

To set up a new analysis from within an existing study, follow these steps:

1. Start a new analysis from within an existing study
2. Select a workflow template
3. Customize the processing workflow

4. Select the input files for the new analysis
5. Edit the file name for the result file to be generated by the analysis
6. Select the study variables and set up the group ratios for a comparison analysis

For information about reprocessing an analysis, see "Reprocess an analysis."

Start a new analysis from within an existing study

This topic describes how to start a new analysis from within an existing study. For information about reprocessing an existing analysis, see "Reprocess an analysis."

❖ To start a new analysis from within an existing study

1. Open the study. See "Open an existing study."
2. In the study command bar, click **New Analysis**.

   The Workflows tab and the Grouping & Ratios tab appear to the right of the study page tabs and an empty Analysis view opens to the right of the tabbed pages. Both the Workflows and Grouping & Ratios pages are empty.

Tip You can also start a new analysis by opening an analysis template.

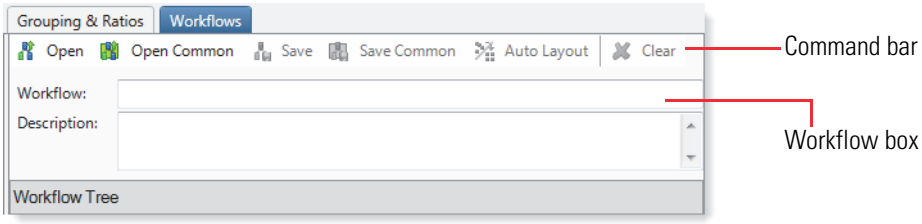
Select a workflow template

On the Workflows page of an analysis, you can select a workflow template from a directory folder, create a new processing workflow, or load a processing workflow from a result file.

The following procedure describes how to select a processing workflow template or load an existing processing workflow from a result file. For information about creating a new processing workflow from scratch, see Chapter 6, "Create and edit processing workflows."

❖ To select a workflow template

1. Click the **Workflows** tab.



2. In the Workflow Tree area on the Workflows page, create a new processing workflow or in the Workflows command bar, do one of the following to select an existing processing workflow:

   - To select a standard processing workflow from the Common Templates folder, click **Open Common**, select the folder for the field of interest, select one of the provided processing workflow templates, and click **Open**.

     The file name appears in the Workflow box, and a description of the processing workflow appears in the Description box.

   - To select a processing workflow from another folder, click **Open**, locate the processing workflow file (.cdProcessingWF) of interest, and click **Open**.

     The file name appears in the Workflow box.

   - To load the processing workflow that you previously used to process a specific result file, click **Open**, locate the result file (.cdResult) of interest, and click **Open**.

3. To customize the processing workflow, see the next topic, "Customize the processing workflow."

Customize the processing workflow

In the Compound Discoverer application, you can customize processing workflows only from within a study. To open an analysis from within an existing study, see "Start a new analysis from within an existing study."

Table 17 lists the workflow nodes in processing workflows within LC studies that require custom settings.

Table 17. Workflow nodes that require customization for an LC study (Sheet 1 of 2)

Node	Required customization
Generate Expected Compounds	From the Compound list, select library compounds. In the defined workflow templates, this selection is empty.
Create FISh Trace	From the Compound list, select a library compound. In the defined workflow templates, this selection is empty.
Create Pattern Trace	In the Isotope Ratios box, enter an elemental composition formula—for example, C15S or C17S. In the defined workflow templates, the formula has been preset to C15S.
Note If you add the Create Pattern Trace node to a processing workflow, the Isotope Ratios box is empty until you populate it.	

Table 17. Workflow nodes that require customization for an LC study (Sheet 2 of 2)

Node	Required customization
Search Mass Lists	From the Input Files list, select mass lists. In the defined workflow templates, one of the preinstalled mass lists is pre-selected, according to the vertical market.
Search mzVault	From the mzVault Library list, select mzVault libraries. In the defined workflow templates, one or more of the preinstalled mzCloud Offline for mzVault libraries are selected.
Compound Class Scoring	From the Compound Classes list, select a Compound Class file.
Pattern Scoring	For the Isotope Patterns parameter, set up an isotope pattern. In the defined workflow templates, the pattern has been set to C15S. You can define and add more ratios.

For LC studies, Thermo Fisher Scientific has optimized most of the parameter settings in the defined processing workflow templates by the area of study (vertical market). Table 18 lists the parameters that usually require a different setting, regardless of whether you use one of the defined templates or create your own processing workflow.

Table 18. Parameter modifications for workflow nodes

Node	Parameter settings to optimize or modify
Create Analog Trace	Select the trace of interest.
Create Mass Trace	Select the trace of interest.
Generate Expected Compounds	Set up the dealkylation and transformation steps and select the appropriate ions.
Search nodes	Select the libraries or lists of interest.
Detect Compounds (Legacy)	For the recommended minimum peak intensity settings for a specific mass spectrometer model, see Table 19.
Group Compounds	Set up a peak rating filter to remove low-quality chromatographic peaks from the analysis.
Group Expected Compounds	Set up a peak rating filter to remove low-quality chromatographic peaks from the analysis.

Table 19 lists the recommended range for the minimum peak intensity setting in the Detect Compounds (Legacy) node for an LC study. The optimal setting depends on the sensitivity of the mass spectrometer.

IMPORTANT Unless you are creating a new analysis for comparison with legacy analyses, Thermo Fisher Scientific recommends that you use the new Detect Compounds node instead of the Detect Compounds (Legacy) node. With the new Detect Compounds node, you can use the peak rating filter to eliminate compounds for further processing and from the analysis result unless their chromatographic peaks pass the peak quality threshold in a specified number of input files.

Table 19. Recommended minimum peak intensity range

Mass spectrometer	Minimum peak intensity (chromatographic peak height)
Q Exactive, Q Exactive Plus™, Q Exactive HF	500 000 to 1 000 000
Orbitrap Fusion, Orbitrap Lumos™, Orbitrap ID-X™	50 000 to 100 000
Exactive, Exactive Plus™, Orbitrap Elite™, Orbitrap Velos Pro™	100 000 to 500 000
LTQ Orbitrap XL™, LTQ Orbitrap Velos™	25 000 to 100 000

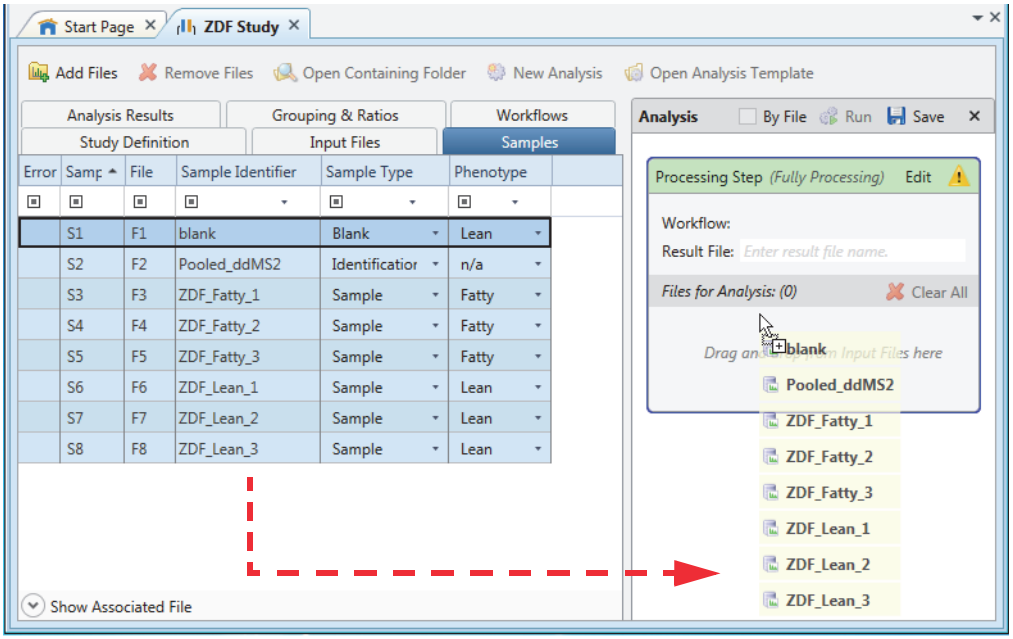
Select the input files for the new analysis

Follow this procedure to select the input files for a new analysis from within an existing study. If you are reprocessing a previous analysis, the Files for Analysis area of the Analysis view includes its input files. If you are starting a new analysis, the Files for Analysis area is empty.

❖ To select the input files that you want to process

1. Open the study of interest and start a new analysis. See "Start a new analysis from within an existing study."
2. On the Input Files page or the Samples page of the study, select the files of interest.
3. Right-click the selection and choose **Set As Input File**, or drag the files of interest to the Files for Analysis area of the Analysis view.

Figure 54. Dragging input files to the Analysis view



The following items appear in the Analysis view:

- The file name of the last input file appears in the Result File box.
- The Run command becomes available if the Workflows page contains a valid processing workflow.
- When you add more than one input file to the Files for Analysis area, the By File check box becomes available.

If the Caution symbol in the Processing Step title bar remains, the processing workflow contains an error. See "Troubleshoot common analysis errors."

Go to the next topic, "Edit the file name for the result file to be generated by the analysis."

Edit the file name for the result file to be generated by the analysis

After you add the input files to be processed to the Analysis view, the application automatically populates the Result File box with the file name of the first input file. You can edit the file name.

❖ To change the name of the result file for an analysis

In the Analysis view, select the default file name in the Result File box and type the new name.

Go to the next topic, "Select the study variables and set up the group ratios for a comparison analysis."

Select the study variables and set up the group ratios for a comparison analysis

To run a differential analysis automatically, you must define the sample groups and ratios for the new analysis.

Note When the processing workflow includes the Differential Analysis node, the Analysis Validation confirmation box opens if the analysis does not include defined sample groups and ratios on the Grouping & Ratios page of the analysis.

❖ To set up sample groups and ratios for a new analysis

1. If you have not already opened an existing study and started a new analysis, do the following:
   a. Open an existing study. See "Open an existing study."
   b. Click **New Analysis** in the study command bar.
   c. On the Workflows page of the analysis, select a workflow template or set up a processing workflow. See "Select a workflow template."
   d. Select the input files for the analysis. See "Select the input files for the new analysis."
2. On the Grouping and Ratios page of the analysis, select the study variables and set up group ratios.

For details about selecting the variables for the analysis and setting up group ratios, see "Set up the sample groups and ratios for a new analysis," which describes how to set up the sample groups and ratios on the Sample Groups and Ratios page of the New Study and Analysis Wizard.

Go to the next topic, "Troubleshoot common analysis errors."

Troubleshoot common analysis errors

After you set up an analysis, you must troubleshoot the analysis if a Caution symbol appears in the Analysis view and the Run button is unavailable.

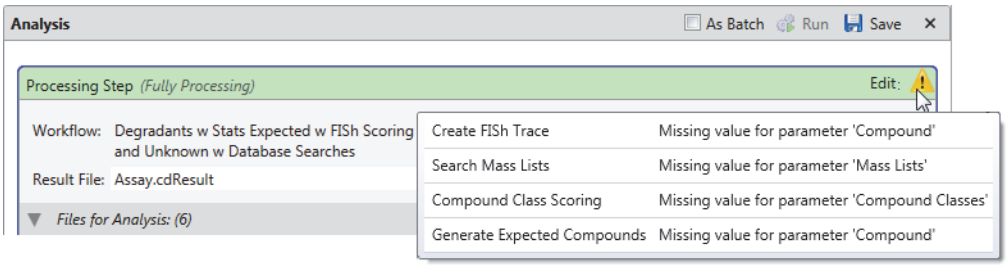
Tip For LC studies, the application does not know the polarity of the scan data or whether the data contains data-dependent or data-independent fragmentation (acquisition) scans. For best results, check the following:

- When the processing workflow contains any of these nodes—Create Mass Trace, Create FISh Trace, or Create Pattern Trace—verify that the ion polarity setting matches the data.
- When the processing workflow contains the Create FISh Trace node, verify that the setting for Fragmentation Mode matches the data.

❖ To troubleshoot an analysis

1. In the Analysis view, point to the Caution symbol, ⚠, to display the list of missing analysis items, or check the error information in the Current Workflow Issues pane (Figure 56) below the Post-Processing pane on the Workflows page.
2. Using the information provided in the list of missing items, fix the analysis errors until the Caution symbol disappears. See Table 20.

Figure 55. Error messages for a defined processing workflow in an LC study



For example, Figure 55 shows the error message that appears before you customize the defined processing workflow provided in the Common Templates folder:

> Degradants w Statistics Expected w FISh Scoring and Unknown ID w Online and Local Database Searches.cdProcessing WF

Figure 56 shows the corresponding error messages in the Current Workflow Issues pane.

Figure 56. Current Workflow Issues pane with issues for an LC study

Current Workflow Issues

Node Name	Issue Description	Parameter Name	Value
Create FISh Trace	Missing value for parameter 'Compound'	Compound	
Search Mass Lists	Missing value for parameter 'Mass Lists'	Mass Lists	
Compound Class Scoring	Missing value for parameter 'Compound Classes'	Compound Classes	
Generate Expected Compounds	Missing value for parameter 'Compound'	Compound	

In addition, each workflow node that is missing a value for one of its parameters has an exclamation mark, ❗, in its upper-right corner.

To fix the analysis errors for this example, you must select a compound for the Create FISh Trace node, one or more compounds for the Generate Expected Compounds node, and a mass list for the Search Mass Lists node.

> **Tip** You can update all the libraries and lists when an analysis is open—that is, the available selections in the workflow nodes that include selections from these libraries and lists automatically update when you modify the associated libraries and lists.

Go to "Submit an analysis to the job queue and fix any validation issues."

To troubleshoot common analysis errors, see Table 20.

Note To troubleshoot validation issues, which occur after you submit a run, see "Common validation issues."

Table 20. Common analysis errors

Error message	Error	Solution
The workflow does not contain a start node.	You have not added the Input Files node to the workflow.	Add the Input Files node to the beginning of the workflow.
No input files defined.	You have not added input files to the Files for Analysis area.	Add input files from the Input files or Samples page to the Files for Analysis area.
The current workflow does not contain any nodes.	You have not set up a processing workflow on the Workflows page.	Select or set up a processing workflow on the Workflows page.
Node Name Missing value for parameter "*Parameter Name*"	The processing workflow contains a node that requires a custom parameter setting.	Make the appropriate selections in the affected workflow nodes.
Node Name Missing connection for "*Connection Information*"	You have not connected node to the processing workflow.	Make the appropriate node connections.

Submit an analysis to the job queue and fix any validation issues

To submit an analysis to the job queue, understand the validation issues that might occur, and control the job queue, see these topics:

- Submit an analysis to the job queue
- Common validation issues

Submit an analysis to the job queue

After you set up an analysis and troubleshoot any analysis errors, the Run command becomes available.

❖ To submit an analysis to the job queue

1. Decide whether you want to create one result file for the entire set of input files or one result file for each input file.
   - To create a single result file, leave the **By File** check box clear.
   - To create a separate result file for each input file, select the **By File** check box.
2. (Optional) In the Result File box, type a name for the result file to overwrite the default name.

3. In the Analysis command bar, click **Run**.

   If the analysis contains no validation issues, the Job Queue page opens. See "Control the Job Queue."

   If the analysis contains issues, the Analysis Validation Issues prompt opens.

4. If a warning prompt appears, do the following:

   a. Read the warning message. See "Common validation issues."

   b. Do one of the following:

      - To modify the analysis, click **Abort** and remedy the error.
      - To start data processing, click **Ignore**.

Common validation issues

If the Analysis Validation Issues prompt appears when you submit and analysis, see Table 21 to troubleshoot common validation issues.

Table 21. Validation issues (Sheet 1 of 2)

Validation issue	Remedy
The peak rating filter in the Group Compounds node, the Group Expected Compounds node, or both nodes is not enabled.	When appropriate, set up an appropriate peak rating filter in the Group Compounds node, the Group Expected Compounds node, or both nodes.
The processing workflow includes the Differential Analysis node, but you have not set up sample groups and ratios.	• On the Sample Groups and Ratios page, set up the appropriate sample groups and ratios. • On the Workflows page, delete the **Differential Analysis** node. –or– • Do not change the analysis settings and click **Ignore**.
The analysis includes sample groups and ratios, but the processing workflow does not include the Differential Analysis node.	On the Workflows page, add the **Differential Analysis** node to the workflow.
IMPORTANT If the analysis does not include sample ratios or the Differential Analysis node, the application does not run a differential analysis, and the Compounds and Expected Compounds tables in the result file does not include the following columns: Ratios, Log2 Fold Change, P-value, and Adj. P-value.	

Table 21. Validation issues (Sheet 2 of 2)

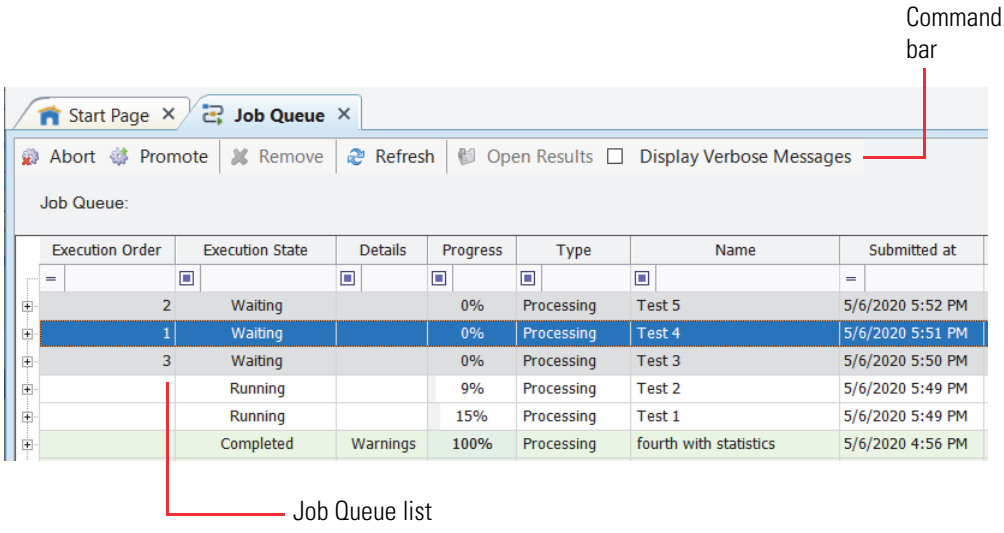
Validation issue	Remedy
The processing workflow includes Compound Identification nodes or Pathway Mapping nodes, but it does not include the Assign Compound Annotations node.	On the Workflows page, add the **Assign Compound Annotations** node to the workflow.
IMPORTANT For an untargeted analysis in an LC study, the application does not assign names or formulas to compounds in the Compounds table of a result file if the processing workflow does not include the Assign Compound Annotations node.	
The processing workflow includes the Assign Compound Annotations node, but the processing workflow does not include any of the compound identification or pathway mapping nodes.	Click **Ignore**. –or– Add one or more compound identification or pathway mapping nodes to the processing workflow.

Control the Job Queue

When you submit an analysis for processing, the Job Queue page opens (Figure 57). You can also open the Job Queue page by choosing View > Show Job Queue from the menu bar.

The application can process two runs simultaneously. If you submit a second run while the first run is being processed, the status of the second run changes to Not Queued, Running, or Execution Failed. If you submit a third run while the application is processing the first two runs, its status changes to Waiting.

Figure 57. Job Queue list with runs in various processing states

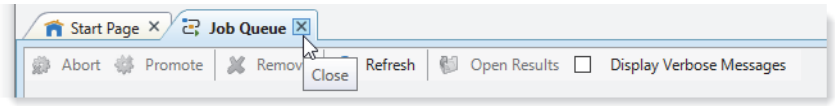


To work with the jobs on the Job Queue page, see the following instructions.

Open the Job Queue page

The Job Queue page automatically opens when you submit a job for processing. You can close the page by clicking the Close icon on the right side of its tab.

Figure 58. Command bar on the Job Queue page



❖ To open a hidden Job Queue page

From the Compound Discoverer menu bar, choose **View > Show Job Queue**.

The Job Queue page opens as a tabbed document.

Cancel a run

You can cancel a run before it ends—that is, you can cancel a run when it is in the Waiting or Running state.

❖ To cancel a run that is being processed

1. On the Job Queue page, select the run that you want to cancel.
2. In the command bar on the Job Queue page, click **Abort**.

   When you cancel a run, its status changes to Aborted, and the application does not create a result file for the run.

Promote a run

If the application has not started processing a job, you can promote the job one position at a time. You cannot promote a job to a position in front of a job that is already running—that is, you cannot pause a run in progress to promote a job in front of it.

❖ **To promote a run**

1. On the Job Queue page, select a job that is waiting in the job queue list.
2. Click **Promote**.

Remove completed or failed jobs from the Job Queue

❖ **To remove completed or failed jobs from the Job Queue list**

1. On the Job Queue page, select the jobs that you want to remove.
2. In the command bar on the Job Queue page, click **Remove**. Then, at the prompt, click **OK**.

   The selected jobs disappear from the Job Queue list. The application does not remove the result files from the study.

Refresh the Job Queue list

❖ **To refresh the Job Queue list**

In the command bar on the Job Queue page, click **Refresh**.

Open a result file from the Job Queue page

❖ **To open a result file from the job queue list**

On the Job Queue page, do one of the following:

- Select the completed run of interest and click **Open Results** in the command bar.
- Double-click a completed run of interest.

The Results page for the selected run opens as a tabbed document in the application window.

Display verbose messages on the Job Queue page

By default, the application only displays high-level processing information on the Job Queue page. To display all the available processing information, you can display the verbose messages.

❖ **To display verbose messages in the Job Queue list**

Select the **Display Verbose Messages** check box.

View the processing steps for a job

By default, the application displays one entry for each job in the job queue, but you can expand each entry for the job to display its processing steps.

❖ **To view the processing steps for a job**

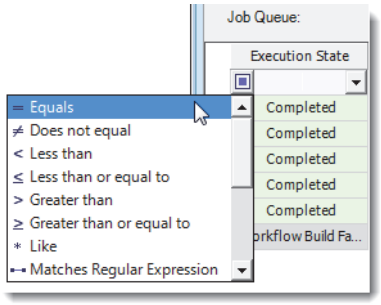
On the Job Queue page, click the expand icon, ⊞, to the left of the job row.

Filter the Job Queue list

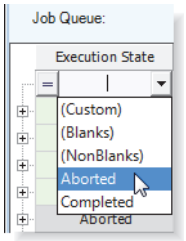
❖ **To filter the job queue list**

Note Use the filters for the column that you want to sort by. For example, to display only the runs that you ended before completion, follow this procedure.

1. Click the icon, ▣, to the left of the Execution State filter list and select **Equals**.



2. In the Execution State filter list, select **Aborted**.



The job queue list displays the canceled runs only.

3. To undo filtering, close and reopen the Job Queue page.

Job Queue page parameters

Table 22 describes the command bar and progress table on the Job Queue page.

Table 22. Job Queue page features (Sheet 1 of 2)

Command or table column	Description
Command bar	
Abort	Stops processing and removes the selected job from the queue. Selecting a job that is being processed makes this button available.
Promote	Promotes the selected job to the next earlier and available run position. For example, if you have queued four jobs with two actively running and two waiting, promoting the fourth job after moves it to the third position, where it is still waiting. As soon as the application completes one of the first two jobs, it starts the promoted job. You cannot promote a job in front of a job that is already running. You can promote a job multiple times, but you can only promote it one position at a time.
Remove	Selecting one or more completed jobs makes this button available. Removes the selected jobs from the job queue, but does not remove the runs from the Analysis Results page of the study.
Refresh	Refreshes the job queue list.
Open Results	Opens the result files for the selected, completed jobs.
Display Verbose Messages	Displays more messages of less importance. When this check box is clear, the Job Queue displays no more than a few messages for each workflow node.
Table columns	
Execution Order	Displays the execution order of the submitted jobs that are waiting to start. The application does not display an execution order for the jobs that are currently running. When multiple jobs are waiting to run, you can promote any of the runs with an execution order greater than 1.

Table 22. Job Queue page features (Sheet 2 of 2)

Command or table column	Description
Execution State	Displays the status of the job. • Not Queued—The application takes a finite length of time to start a job after you click the Run command. • Running—The application is currently processing the job. The application can process two jobs simultaneously. When you submit an analysis as a batch, each input file is processed as a separate job. • Aborted—You canceled the job while the application was processing the analysis. • Execution Failed—The application was unable to complete the job. • Waiting—The application has not begun to process the job. • Completed—The application has completed the analysis and you can open the result file.
Details	Displays whether the job ran with or without warnings.
Progress	Displays the progress of the run as a percentage.
Type	Displays the job type.
Name	Displays the name of the result file.
Submitted At	Displays the date and time when you submitted the run to the job queue.
Study	Displays the name of the study.
Data Source	Displays the location and file names of the input files for the current job.
Description	Displays the description that you typed in the Description box on the Workflows page.

Review or reprocess an analysis

When you submit a run to the job queue, the run appears in the list of analyses on the Analysis Results page of the current study.

Use the Analysis Results page of a study to review or reprocess a completed analysis or to open a result file. An analysis consists of a processing workflow, optional sample groups and ratios, and the selected input files.

Note The Execution State on the Job Queue page updates more quickly than the Execution State on the Analysis Results page.

For details, see these topics:

- Analysis Results page parameters
- Review an analysis
- Reprocess an analysis
- Reprocess a legacy analysis result from an untargeted analysis

Analysis Results page parameters

Table 23 describes the command bar and progress table on the Analysis Results page of a study.

Table 23. Analysis Results page parameters (Sheet 1 of 2)

Feature	Description
Command bar	
Selecting an analysis in the list on this page makes these commands available.	
Open Result	Opens the selected result file.
Reprocess	Opens the Analysis view with the list of input files that were used for the selected analysis. The Workflows page contains the processing workflow, and the Grouping & Ratios page contains the sample groups and ratios used for the selected analysis.
Search box	Use this box to type text to search for.
Search For	Use this dropdown list to select the column to search by.
Table columns	
Execution State	Displays the status of the analysis.
Creation Date	Displays the date and time when you submitted the run to the job queue.
File Name	Displays the file name of the result file.

Table 23. Analysis Results page parameters (Sheet 2 of 2)

Feature	Description
Description	Displays the description of the processing workflow that you or the originator typed in the Description box on the Workflows page.
Below the table	
Show Associated Analysis/Hide Associated Analysis	Opens a locked Processing Step area that shows the names of the processing workflow and result file and a list of the input files for the analysis.
Shortcut menu commands	
Copy with Headers, Copy, Clear Selection, Cell Selection Mode, and Enable Row Grouping	See these topics: • Copy table entries to the clipboard • Group table rows
Open Result	Opens the selected result file.
Open Containing Folder	Opens the folder that contains the result file.
Show Details	Opens the Analysis Sequence Details window where you can view the analysis processing workflow in the Workflow Tree pane and the Processing Step information in the Analysis view. You cannot start runs from this window.
Reprocess	Same functionality as the Reprocess command in the command bar.

Review an analysis

Use the Analysis Sequence Details window to review an analysis.

❖ To review an analysis

1. On the Analysis Results page of a study, right-click the analysis and choose **Show Details**.

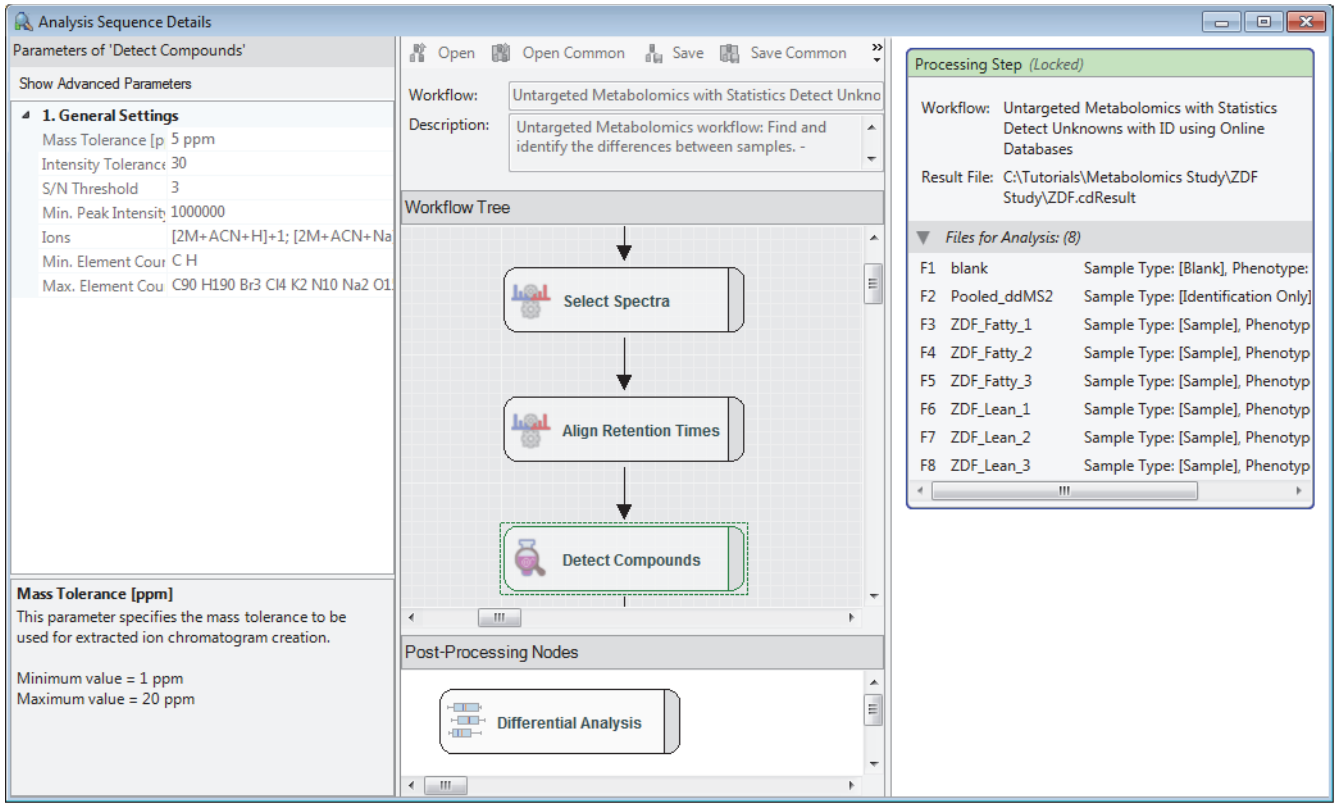
   The Analysis Sequence Details window opens and displays the processing workflow in the Workflow Tree pane and the result file name and input files in the Processing Step pane.

2. To view the parameter settings for a workflow node, select it in the Workflow Tree pane.

   The parameter settings appear in the Parameters pane at the left.

   Note The Processing Step is locked, preventing you from reprocessing the analysis from this window.

Figure 59. Analysis Sequence Details window showing the parameter settings for the Detect Compounds node (LC study)



Reprocess an analysis

You can reprocess an entire analysis or only the post-compound detection portions of an analysis.

Note Because result files (analysis results) for untargeted analyses from previous versions of the Compound Discoverer application contain an obsolete Detect Compounds node, you cannot partially reprocess these legacy analysis results. You can fully reprocess these legacy analyses after you replace the "not available" node with the current Detect Compounds node or the Detect Compounds (Legacy) node. See "Reprocess a legacy analysis result from an untargeted analysis."

❖ To reprocess an analysis

1. On the Analysis Results page of a study, right-click the analysis and choose **Reprocess**.
   - If the Analysis view is open and contains information for an analysis that you have not yet submitted to the job queue, the following prompt appears:

     The analysis was not started. Do you really want to discard the analysis?

- If the Analysis view is closed, it reopens with the settings from the selected analysis. In addition, the Grouping & Ratios tab and Workflows tab appear to the right of the study tabs.

2. If prompted, do the following:
   a. Check the Analysis view and decide whether you want to discard the current settings.
   b. Click **Yes** to replace the current settings in the Analysis view with the settings from the selected analysis. Otherwise, click **No** to return to the in-progress analysis.
3. Do one of the following:
   - To reprocess the entire analysis, go to step 5.
   - To reprocess only part of the processing workflow, go to step 4.

> **Note** For LC studies, you can add or reprocess any of the Peak Area Refinement nodes, Pathway Mapping nodes, Search nodes, and Compound Scoring nodes without reprocessing the entire workflow.
>
> You must reprocess the entire workflow to reprocess any of the nodes for Spectrum Processing, Trace Creation, Compound Detection, or Expected Compounds (except for the Merge Features node).

4. To reprocess only part of the processing workflow or add workflow nodes downstream of the core processing workflow, do the following:
   a. Click the **Workflows** tab.

      The processing workflow appears in the Workflow Tree (Reprocess) area. All the nodes are white with a gray tab, which indicates that they are not set for reprocessing.

      > **Tip** When you attempt to reprocess an analysis result from a previous version of the Compound Discoverer application, some of the processing workflow nodes are obsolete and unavailable for reprocessing. The gear icon and n/a label indicate obsolete workflow nodes.
      >
      > You cannot directly reprocess analysis results with obsolete processing workflow nodes. To reprocess analysis results from previous versions of the Compound Discoverer application, you must replace the obsolete workflow nodes with comparable nodes on the Workflow Nodes page.

   b. Do any of the following:
      - Right-click any of the nodes currently in the workflow that you want to reprocess and choose **Reprocess**.
      - Add downstream workflow nodes.

      The selected nodes and any related nodes revert to their original color, and the Run command becomes available in the Analysis view.

Note If you are only partially reprocessing the existing input files, the Source File row appears in the Analysis view. You cannot edit the source file name.

c. If you are partially reprocessing the data, consider changing the result file name.

   If you do not change the result file name, the application automatically appends a number to the file name when you submit the run.

d. Go to step 7.

5. To reprocess the entire processing workflow, right-click the Input Files node and choose **Reprocess**. Then, at the prompt, click **OK**.
6. If necessary, make changes to the sample groups and ratios on the Grouping & Ratios page and the settings in the Analysis view.

   Note When you change any of the settings on the Grouping & Ratios page or the files for analysis in the Analysis view, the application automatically reprocesses the entire processing workflow.

7. To start the analysis, click **Run**.

Reprocess a legacy analysis result from an untargeted analysis

You cannot partially reprocess an analysis result from a previous version of the Compound Discoverer application if the processing workflow for the analysis includes the (n/a) Detect Compounds node.

❖ To fully reprocess the analysis result from a legacy analysis

1. On the Analysis Results page of the legacy study, right-click the analysis and choose **Reprocess**.
   - If the Analysis view is open and contains information for an analysis that you have not yet submitted to the job queue, the following prompt appears:

     The analysis was not started. Do you really want to discard the analysis?

   - If the Analysis view is closed, it reopens with the settings from the selected analysis. In addition, the Grouping & Ratios tab and Workflows tab appear to the right of the study tabs.
2. If prompted, do the following:
   a. Check the Analysis view and decide whether you want to discard the current settings.
   b. Click **Yes** to replace the current settings in the Analysis view with the settings from the selected analysis. Otherwise, click **No** to return to the in-progress analysis.
3. To open the Workflows page of the analysis, click the **Workflows** tab or click **Edit** to the right of Processing Step (Partially Reprocessing).

4. Review the processing workflow:
   - If the processing workflow includes the (n/a) Detect Compounds node, you must replace the node.
   - If the processing workflow also includes the Find Expected Compounds (Legacy) node, you must replace the (n/a) Detect Compounds node with the Detect Compounds (Legacy) node.
   - If the processing workflow does not include the Find Expected Compounds (Legacy) node, you can replace the (n/a) Detect Compounds node with the Detect Compounds node or the Detect Compounds (Legacy) node.
5. Replace the (n/a) Detect Compounds node with an available detect compounds node as follows:
   a. Click the **(n/a) Detect Compounds** node to select it and press the **Delete** key.
   b. Click the **Workflow Nodes** tab at the bottom right of the Workflow Tree area.

      Note If the processing workflow includes the Find Expected Compounds (Legacy) node, only the Detect Compounds (Legacy) node is available.

   c. On the Workflow Nodes page, drag one of the detect compounds nodes to the Workflow tree area.

      The detect compounds node automatically connects to the Merge Features node and the Group Compounds node, but the Align Retention Times node does not automatically connect to the detect compounds node.

      Note When you replace the (n/a) Detect Compounds node with the Detect Compounds (Legacy) node and you want the node to yield results that are similar to the previous version of the Compound Discoverer application, keep the default setting of False for the Use Peak Quality for Isotope Grouping parameter.

      The User Peak Quality for Isotope Grouping parameter is an advanced parameter under Isotope Pattern Detection.

   d. Connect the Align Retention Times node to the detect compounds node.
6. Make other changes to the processing workflow as appropriate.
7. To start the analysis, click **Run**.

Analysis view parameters

The Analysis view appears to the right of the analysis pages when you start a new analysis or open an existing analysis template. Table 24 describes the parameters in the Analysis view.

Table 24. Analysis view parameters (Sheet 1 of 2)

Parameters	Description
Title bar	
By File check box	Available when you add more than one input file to the Files for Analysis area. • Clear (default setting)—The application creates one result file as it processes the input files in the Files for Analysis area. • Selected—The application creates one result file for each input file in the Files for Analysis area.
Run command	Submits the analysis to the job queue. Available when the Workflow Tree pane on the Workflows page contains a valid processing workflow and the Files for Analysis area contains a list of input files.
Save command	Opens the Save Analysis Template dialog box where you can provide a file name for the analysis template and save it to an appropriate directory.
	Closes the Analysis view, the Workflows page, and the Grouping & Ratios page.
Processing Step area	
Edit	Opens the Workflows page.
	If the analysis includes errors, such as missing parameter settings or no input files, a Caution symbol appears to the far right of the Processing Step. To display the error list, point to the Caution symbol. For more information, see Table 20.
Workflow	By default, the text matches the text in the Workflow box on the Workflows page. You cannot change the text in the Analysis view. To change the name of the processing workflow, edit the text on the Workflows page. To select a different processing workflow, see "Start a new analysis from within an existing study."
Result File	Specifies the file name for the result file. This box is empty until the Files for Analysis area lists at least one input file. The name of the first input file automatically populates the Result File box. If the analysis creates only one result file, you can type a name for the result file in the Result File box.

Table 24. Analysis view parameters (Sheet 2 of 2)

Parameters	Description
Source File	Displays the filename of the original result file. Available when you set up an analysis for partial reprocessing.
Files for Analysis: (#)	Displays the number of input files in the Files for Analysis area.
Files for Analysis area	After you add the input files from the Input Files page or the Samples page of the study to this area, this area displays the names of the input files. See "Select the input files for the new analysis."

Set up individual isotope patterns by using the Isotope Ratio Editor

For LC studies, use the Isotope Ratio Editor dialog box to set up the pattern and the required isotopes for the Create Pattern Trace node or the Pattern Scoring node.

For LC studies, you can access the Isotope Ratio Editor dialog box from the Create Pattern Trace node or the Pattern Scoring node.

To set up an isotope pattern, see the following topics as applicable:

- Open the Isotope Ratio Editor
- Define an isotope pattern from an elemental composition
- Copy an elemental composition from the Expected Compounds library
- Set up a custom isotope pattern
- Export a mass spectrum from a raw file to the Clipboard
- Isotope Ratio Editor parameters

Open the Isotope Ratio Editor

Use the Isotope Ratio Editor dialog box to set up isotope patterns.

❖ To open the Isotope Ratio Editor dialog box

1. Open or create a processing workflow on the Workflows page of an analysis.

   For information about starting a new analysis, see "Set up a new analysis from within an existing study."

2. For LC studies, add one or both of these nodes to the processing workflow: **Create Pattern Trace** or **Pattern Scoring**.

3. For LC studies, click the **Create Pattern Trace** node or the **Pattern Scoring** node in the Workflow Tree pane.

The parameters for the node appear in the Parameters pane.

4. To display the browse icon, click the **Isotope Ratios** box.
5. Click the browse icon,  .

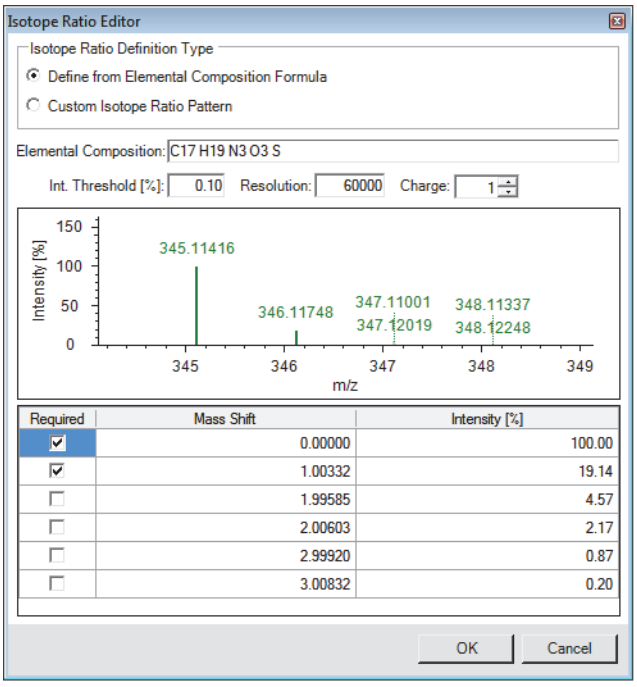
   For the Create Pattern Trace node, the Isotope Ratio Editor dialog box opens. For the Pattern Scoring node, the Pattern List Editor dialog box opens.
6. To open the Isotope Ratio Editor dialog box for the Pattern Scoring node, click **Add Patterns** in the Pattern Editor dialog box.

Define an isotope pattern from an elemental composition

❖ To set up the pattern for a compound by using its elemental composition

1. Open the Isotope Ratio Editor dialog box. See Open the Isotope Ratio Editor.
2. In the Isotope Ratio Definition Type area of the Isotope Ratio Editor dialog box, select the **Define from Elemental Composition Formula** option.

   Figure 60. Isotope Ratio Editor dialog box with an isotope pattern for a defined elemental composition



3. In the Elemental Composition box, type or paste the alphanumeric elemental composition of the compound of interest.

   The application automatically populates the Mass Shift and Intensity [%] columns by using these default settings:

   - Intensity threshold: 0.10%

- Resolution: 60 000
- Charge: 1

Tip To enter an elemental composition for a labeled compound, use brackets to identify the type and number of labeled atoms for each element.

For example, to enter the elemental composition of omeprazole where only one of the carbon atoms has been replaced with carbon-13, type C16 [13]C H19 N3 O3 S.

4. Refine the settings for the intensity threshold, resolution, and charge, as appropriate and in any order:
   - In the Int. Threshold [%] box, type the relative intensity threshold.

     The application removes isotopic peaks below this relative intensity threshold from the Mass Shift versus Intensity [%] table.
   - In the Resolution box, type the resolution for the scans.

     Note The scan header in the raw data file lists the resolution of each scan, and the instrument method that is associated with the raw data file lists the resolution of each scan event.
   - In the Charge box, type or select the charge state of the ions.

     The application uses the charge state to display the theoretical mass spectrum in the graphical display.
5. Select the check boxes of the required peaks.

Copy an elemental composition from the Expected Compounds library

You can copy the elemental composition of a compound in the Expected Compounds library to the Clipboard, and then paste it to other places in the application where the input is an elemental composition.

❖ To copy an elemental composition from the Expected Compounds library

1. If the Isotope Ratio Editor dialog box is open, close it.
2. From the menu bar, choose **Libraries > Expected Compounds**.

   The Expected Compounds library opens.
3. Right-click anywhere on the page and choose **Cell Selection Mode**.
4. Click the elemental composition of interest.

   The table cell turns a lighter blue than the remaining cells in the table row.
5. Right-click the highlighted cell and choose **Copy**.

6. Open the Isotope Ratio Editor dialog box. See Open the Isotope Ratio Editor.
7. Right-click in the Elemental Composition box and choose **Paste**.

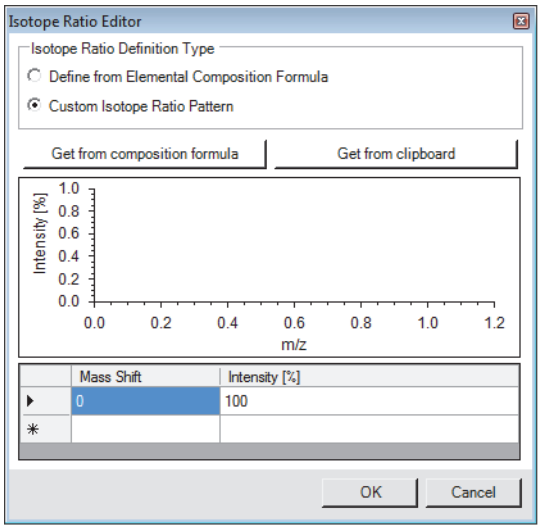
Set up a custom isotope pattern

❖ **To set up a custom isotope pattern**

1. Open the Isotope Ratio Editor dialog box. See Open the Isotope Ratio Editor.
2. Select the **Custom Isotope Ratio Pattern** option.

   Below the Isotope Ratio Definition Type area, the available parameters change.

   Figure 61. Custom Isotope Ratio Pattern view



3. To set up the custom isotope ratio pattern, do one of the following:
   - Type values in the Mass Shift and Intensity boxes.
   - Click **Get from Composition Formula**.

     The application uses the text in the hidden Elemental Composition box.
   - Click **Get from Clipboard**.

     The application uses the mass spectrum data that you copied to the Clipboard.

Export a mass spectrum from a raw file to the Clipboard

This topic describes how to export a mass spectrum from the FreeStyle 1.8 browser application to the Clipboard. For later versions of the FreeStyle application, refer to the FreeStyle Help system.

❖ To export a mass spectrum from a raw data file to the Clipboard

1. From the FreeStyle™ data-visualization application, do the following:
   a. Open the raw data file that contains the mass spectrum of interest and make the mass spectrum view or the spectrum list view the active view.
   b. In the Exports area of the Spectrum Workspace Options toolbar, click Exports to open the dropdown list. Then, select **Export Selection AS**.
   c. In the Copy to Clipboard/Export dialog box, select the **To CSV File** option and click **OK**.
   d. In the Export Data dialog box, select a folder, name the file, and click **Save**.

      The spreadsheet opens in a spreadsheet application.
2. In the spreadsheet application, select up to 20 rows of *m/z* and intensity values and copy them to the Clipboard. Do not select the spectrum header information.

Isotope Ratio Editor parameters

Table 25 describes the parameters in the Isotope Ratio Editor dialog box. For information on how to open the editor, see Open the Isotope Ratio Editor.

Table 25. Isotope Ratio Editor dialog box parameters (Sheet 1 of 3)

Parameter	Description
Isotope Ratio Definition Type	
These two options define the parameters that appear below the Isotope Ratio Definition Type area.	
Define from Elemental Composition Formula	Selecting this option makes the following features visible: • Elemental Composition box • Int. Threshold [%] box • Resolution box • Charge box

Table 25. Isotope Ratio Editor dialog box parameters (Sheet 2 of 3)

Parameter	Description
Custom Isotope Ratio Pattern	Selecting this option makes the following features visible: • Get from Composition Formula button • Get from Clipboard button • Bar graph of Intensity [%] versus the *m/z* ratio of the isotopic mass peaks • Data entry table where you define a custom isotope pattern in terms of the mass shift and intensity of each mass peak Use this option to create a custom isotope pattern.
Elemental composition view Selecting the Define from Elemental Composition Formula option makes the following parameters visible: Elemental Composition, Int. Threshold [%], Resolution, and Charge.	
Elemental Composition	Specifies the elemental composition of the compound of interest. When you type a composition in this box, the application automatically creates a table of mass shifts and intensities. Default: Empty (unless you have already specified the elemental composition in the Isotope Ratios box under General Settings for the Pattern node)
Int. Threshold [%]	Specifies the intensity threshold of the isotope pattern. Default: 0.10; range: 0–100
Resolution	Specifies the resolution of the isotope pattern. Default: 60 000; range: 2–1 000 000 000
Charge	Specifies the charge of the ion fragment. Default: 1; range: 1–100
Graph of Intensity [%] versus *m/z* value Displays a graph of the full isotope distribution in the mass shift and intensity table.	

Table 25. Isotope Ratio Editor dialog box parameters (Sheet 3 of 3)

Parameter	Description
Mass shift and intensity table	
Use this table to specify the required peaks in the isotope pattern. When you select the Define from Elemental Composition Formula option, the application automatically populates this table; you cannot edit the entries.	
Required (for an isotope pattern defined from a user-specified elemental composition)	Specifies whether the isotope is required. • When the check box is selected, the isotope is required. • When the check box is clear, the isotope is not required.
Mass Shift	Specifies the mass shift from the pattern base peak (A0).
Intensity [%]	Specifies the relative intensity [%] of the isotope to the pattern base peak.
Rows	Specify the values for the isotopes.
Custom isotope ratio pattern view	
Selecting the Custom Isotope Ratio Pattern option makes the following buttons visible: Get from Composition Formula and Get from Clipboard.	
Get from Composition Formula	Creates an isotope pattern for an elemental composition formula. The application reads the elemental composition that you entered in the Elemental Composition box before selecting the Custom Isotope Ratio Pattern option.
Get from Clipboard	Imports the isotope pattern from the Clipboard. You can export a custom pattern to the Clipboard from the spectrum list view in the FreeStyle application or from a third-party software application.
Graph of Intensity [%] versus *m/z* value	
Displays a graph of the full isotope distribution in the mass shift and intensity table.	
Mass shift and intensity table	
When you select the Custom Isotope Ratio Pattern option, you can edit the mass shift and intensity values for the isotope pattern.	

Create an isotope patterns list by using the Pattern List Editor

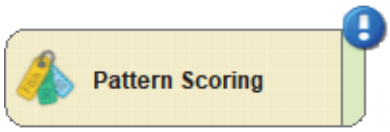
Use the Pattern List Editor to set up a table of isotope patterns.

❖ To create a list of isotope patterns for the Pattern Scoring node

1. Add the Pattern Scoring node to a processing workflow.

   For LC studies, the Group Compounds node automatically connects to the Pattern Scoring node.

   The blue exclamation mark in the upper-right corner of the node indicates that you need to define a parameter setting inside the node.

2. In the Workflow Tree area on the Workflows page, select the Pattern Scoring node.

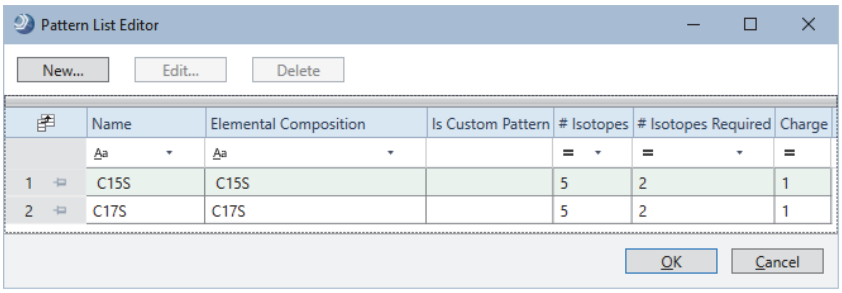
   The parameters pane for the Pattern Scoring node opens at the left.

3. In the Isotope Patterns box, type the elemental composition formulas for the defined isotope patterns that you want to compare. Separate each pattern with a semicolon and a space—for example, C15S; C17S.

4. Click the more icon, , to the right of the Isotope Patterns box.

   The Pattern List Editor opens. The table contains the elemental compositions that you entered.

   Figure 62. Pattern List Editor

5. Select the isotope pattern that you want to edit, and then click **Edit Pattern**.

   The Isotope Ratio Editor dialog box opens. To edit the pattern, see Set up individual isotope patterns by using the Isotope Ratio Editor.

6. For each pattern that you want to add, click **New**, and then set up the isotope pattern in the Isotope Ratio Editor.

After you add a pattern, it appears in the Patterns table of the Pattern List Editor dialog box. The Name and Elemental Composition columns display the elemental composition of the pattern. The text in the Name column is editable.

7. Click **OK** to close the Pattern List Editor dialog box.

   The isotope patterns appear in the Isotope Patterns box of the Pattern Scoring node.

Table 26 describes the commands and table columns in the Pattern List Editor dialog box.

Table 26. Pattern List Editor parameters

Parameter	Description
Commands	
New	Opens the Isotope Ratio Editor dialog box for setting up an isotope pattern.
Delete	Deletes the selected pattern.
Edit	Opens the Isotope Ratio Editor dialog box for editing the selected pattern.
Columns	
Name	By default, displays either the elemental composition for each isotope pattern that you create with a defined elemental composition or the text "*CustomPattern #*" for each isotope pattern that you create by setting up a custom isotope ratio pattern. You can edit the text in this column.
Elemental Composition	Displays the elemental composition for each isotope pattern that is based on a defined elemental composition.
Is Custom Pattern	Displays an X for each isotope pattern that is based on a custom isotope ratio pattern.
# Isotopes	Displays the number of isotopes in the defined pattern that are above the intensity threshold.
# Isotopes Required	Displays the number of isotopes required to calculate the SFit% score.
Charge	Displays the charge state used to simulate the isotope pattern.

Extract analog and PDA traces

For LC studies, you can extract analog and PDA traces from the raw data.

Note To extract UV traces and PDA traces in the same analysis, you must add two Create Analog Trace nodes to the processing workflow. Set up one node to extract UV traces and the other node to extract PDA traces.

For details, see these topics:

- Extract analog traces
- Extract PDA traces

Extract analog traces

For LC studies, you can extract analog traces from the raw data.

Analog traces include data from a UV-Vis detector, analog data from LC devices controlled by the Xcalibur data system or an equivalent Thermo Scientific application, and analog signals from devices connected to the analog channels on the communications panel of your mass spectrometer.

❖ To extract UV or analog traces from the raw data

1. Add the Create Analog Trace node to the processing workflow.

   The Input Files node automatically connects to the Create Analog Trace node.

2. In the Workflow Tree area on the Workflows page, select the **Create Analog Trace** node.

   Note For details about this node, see "Create Analog Trace node."

3. In the Parameters pane, under General Settings, select **UV** or **Analog** from the Trace Type list.

4. In the RT offset [min] box, type the offset time, in minutes, for the UV-Vis or Analog trace.

   If there is a time difference between when the sample enters the mass spectrometer and the UV-Vis or analog detector's flow cell, use the offset time to align the chromatographic traces. A value of 0 indicates that the UV-Vis or analog detector and the mass spectrometer simultaneously detected the sample.

5. In the Custom Label box, type text to identify the trace in the Specialized Traces table of the result file window.

Extract PDA traces

For LC studies, you can extract traces acquired by a photodiode array (PDA) detector from your raw data.

❖ To extract a PDA trace from the raw data

1. Add the Create Analog Trace node to the processing workflow.

   The Input Files node automatically connects to the Create Analog Trace node.

2. In the Workflow Tree area on the Workflows page, select the **Create Analog Trace** node.

   Note For details about this node, see "Create Analog Trace node."

3. In the Parameters pane, under General Settings, do the following in any order:

   - In the Trace Type list, select **PDA**.
   - In the RT offset [min] box, type the offset time, in minutes, for the PDA traces.

     If there is a time difference between when the sample enters the mass spectrometer and the PDA detector's flow cell, use the offset time to align the chromatographic traces. A value of 0 indicates that the PDA detector and mass spectrometer simultaneously detect the sample.

   - In the Custom Label box, type text to identify the trace in the Specialized Traces table on the result file page.

4. In the PDA Settings area, do any of the following:

   - To extract a plot of the average intensity of the scanned wavelength range versus time, select **True** for Total Scan.

     This trace is labeled as a Total Scan in the Specialized Traces table.

   - To extract a plot of the spectrum maximum of the scanned wavelength range versus time, select **True** for Spectrum Maximum.

     This trace is labeled as a Spectrum Maximum in the Specialized Traces table.

   - To extract a plot for a specified wavelength range, select **True** for Wavelength Range. Then, type the wavelength range in the Min. and Max. Wavelength boxes.

Edit existing studies

In the Compound Discoverer application, you process your raw data files (run analyses) within the study environment. The following topics describe how to edit an existing Compound Discoverer study:

- Study files
- Open an existing study
- Study page commands and tabs
- Edit the study description and the study factors
- Add input files to an existing study
- Remove input files or update their location
- Edit the sample type and study factor values
- Save the study file if you turned off the auto-save feature

For information about adding and editing study factors, see "Add or edit the study factors," in Chapter 3.

Study files

When you create a study with the New Study and Analysis wizard, the application creates a study file (.cdStudy) and a study folder. The study file contains a list of input files (Xcalibur RAW files) with their associated sample information and a list of analyses with their associated result files (.cdResult). The sample information includes the sample type of each input file and the relationship between the input files.

When you open an existing study, it opens as a tabbed document with a command bar and a set of tabbed pages: Study Definition, Input Files, Samples, and Analysis Results.

- The Study Definition page contains an editable list of the study factors. See "Edit the study description and the study factors."
- The Samples page contains editable lists of the sample type and study factor values for each input file. See "Edit the sample type and study factor values."

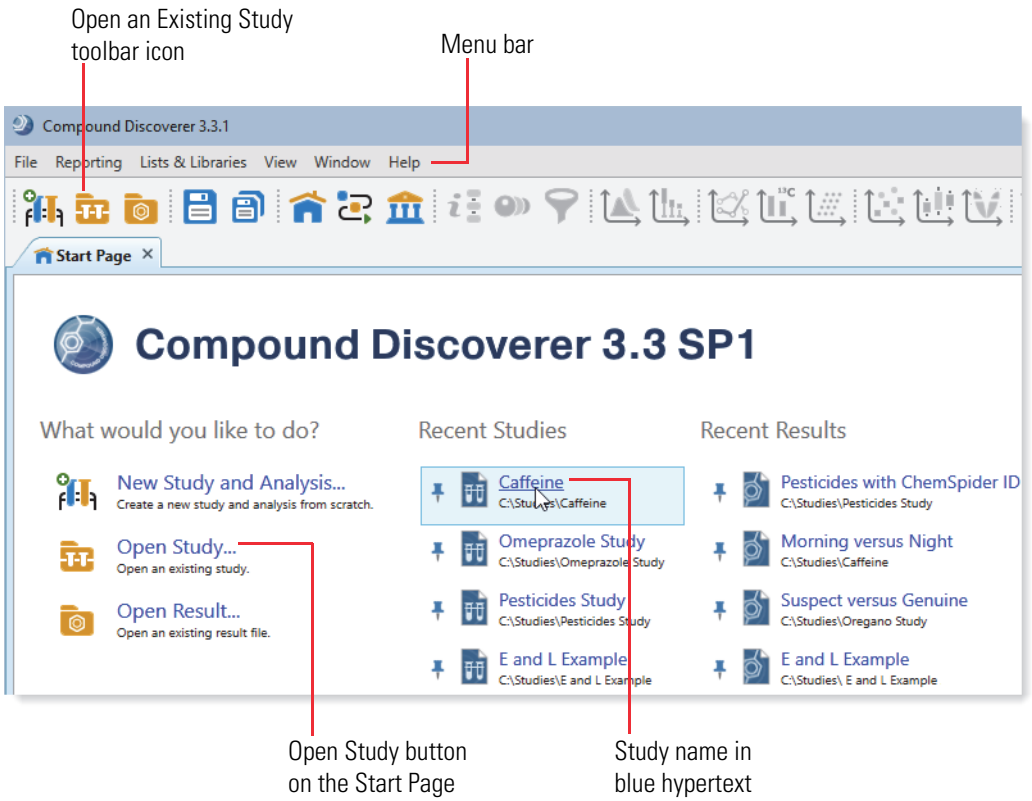
- The Input Files page tracks the location of the input files. These input files typically reside outside the study folder—for example, they might reside on your processing computer, on a shared server, or on the data system computer where they were acquired. If you delete or rename an input file from the specified folder location after you add it to a study, this warning symbol, , appears to the left of the ID column for the deleted file. Pointing to the warning symbol displays the expected location of the missing file and instructions for resolving the issue. See "Resolve the location of the input files in a study."
- The Analysis Results page tracks the result files generated by analyses run within the study. Result files reside within the study folder.

Open an existing study

You can open an existing study from the Start Page, the File menu, or the toolbar.

The Start Page lists the 20 most recent studies. The study name appears in blue hypertext. Pointing to the study name underlines it.

Figure 63. Application window and Start Page



❖ To open an existing study

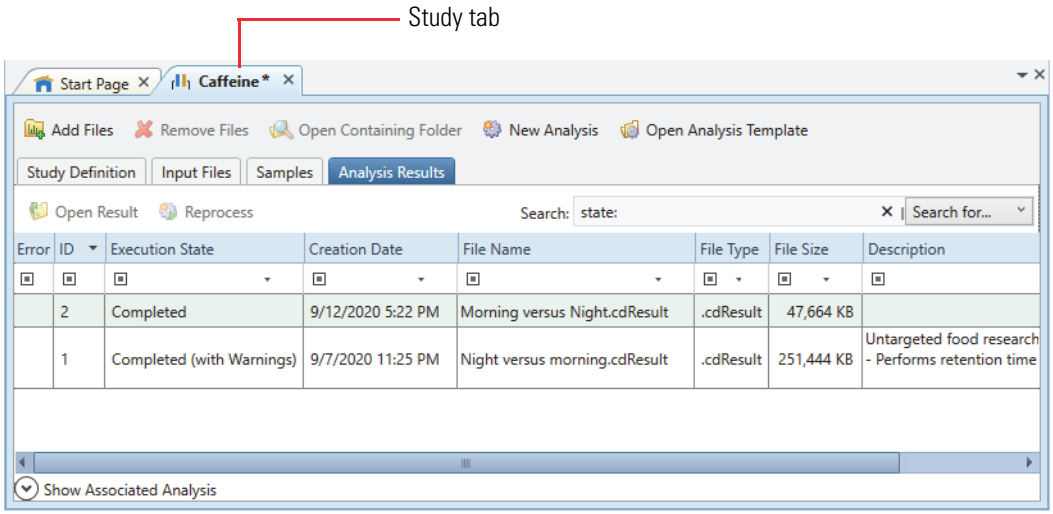
Do one of the following:

- From the Start Page, under What Would You Like to Do?, click **Open Study** to open the Open Study dialog box. Select a study file and click **Open**.
- From the Start Page, under Recent Studies, click the study name of interest.
- From the application menu bar, choose **File > Open Study** to open the Open Study dialog box. Then, select a study file and click **Open**.
- From the application toolbar, click the **Open an Existing Study** icon, , to open the Open Study dialog box. Select a study file and click **Open**.

The study opens to the Analysis Results page, which is the last page of four pages. The study tab includes an image of two racked test tubes, , on the left, the study name in the middle, and a close icon, , on the right.

Tip On the study tab, an asterisk to the right of the study name indicates unsaved changes.

Figure 64. Analysis Results page of a study



Study page commands and tabs

The study page includes a command bar and four tabbed pages.

Table 27. Study page parameters (Sheet 1 of 2)

Command or page	Description
Commands	
The Add Files, New Analysis, and Open Analysis Template commands are independent of the active page within the study. The Remove Files command is only active when a file is selected on the Input Files page or the Analysis Results page.	
Add Files	Opens the Open dialog box where you select the input files (Xcalibur RAW files) that you want to include in the study.
Remove Files	Executes one of two actions: • Removes the selected files on the Input Files page when it is the active page. • Removes the selected analysis results on the Analysis Results page when it is the active page.
Open Containing Folder	Opens the folder that contains the selected file. This command is only available for the Input Files and Analysis Results pages.
New Analysis	Opens the Analysis view and adds the Workflows tab to the tab set on the study page. The Workflows page is unpopulated. This command is unavailable when the Analysis view is open.
Open Analysis Template	Opens the Analysis Template dialog box where you select an analysis template. This command is unavailable when the Analysis view is open.
Tabbed pages	
Study Definition	Use to set up study factors and view the study name, file location, creation date, modification date, and description on this page.
Input Files	Use to track the status and resolve the location of input files, as this page lists the file ID, file name, file type, and sample information for each input file. Clicking Add Files opens the Input File Characterization dialog box and the Input Files page, if it is not already open.

Table 27. Study page parameters (Sheet 2 of 2)

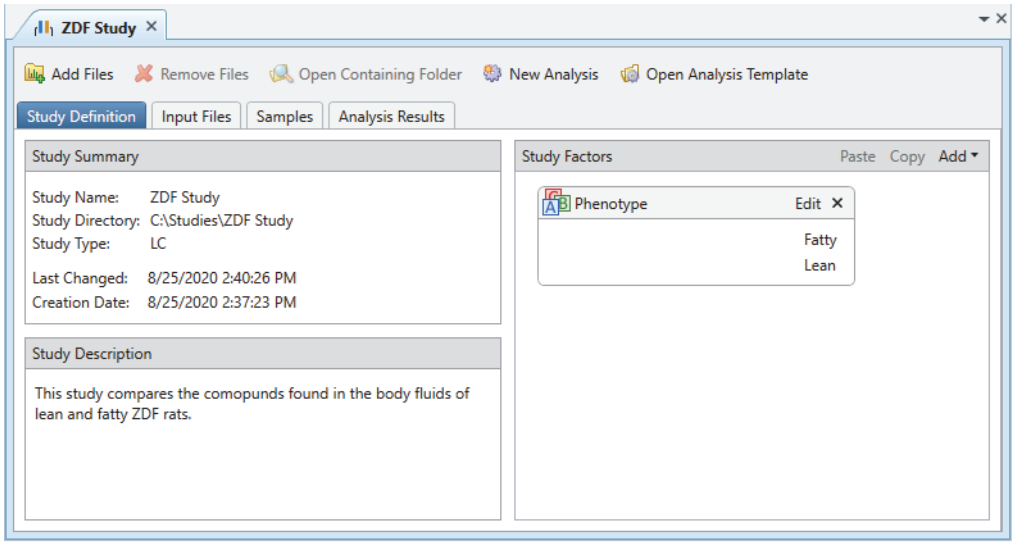
Command or page	Description
Samples	Use to select the sample type and study factors for each raw data file.
Analysis Results	Use to access the result files created within the study, review the analysis details, and reprocess an analysis.

Edit the study description and the study factors

Use the Study Definition page of a study to edit the existing study factors, to set up new study factors, and to edit or add a description of the study.

For information about adding and editing the study factors, see Add or edit the study factors in Chapter 3

Figure 65. Study definition page of a study



Note If you selected a study template with study factors when you created the study or added study factors by using the Input File Characterization page of the New Study and Analysis wizard, the Study Factors area contains the defined factors.

❖ To add or edit a description of the study

Type or edit the description in the Study Description area.

Table 28 describes the parameters on the Study Definition page of a study.

Table 28. Study Definition page parameters (Sheet 1 of 2)

Parameter	Description
Study Summary pane	
Study Name	Displays the study name.
Study Directory	Displays the file location where the study is stored.
Study Type	Displays the study type: GC or LC. After you create a study, you cannot change its study type.
Last Changed	Displays the date and time of the last saved change to the study.
Creation Date	Displays the creation date of the study file.
Study Description pane	
Use this pane to enter and store a description of the current study.	
Study Factors pane	
Use this pane to set up or edit the study factors.	
Menu commands	
Paste	Pastes the entries in the copied factors below the existing factors.
Copy	Copies the selected factors to the Clipboard.
Add > Biological Replicate Factor	Opens a blank biological replicate editor. You can use the biological replicate factor to create nested studies.
Add > Categorical Factor	Opens a blank categorical factor editor.
Add > Numeric Factor	Opens a blank numeric factor editor. The numeric factor editor only accepts numeric values.
Factor box	
Title bar	Displays the editable factor name.
Buttons and icons	
Apply	Saves the current entries in the factor editor.
Cancel	Closes the item or value entry box and removes any entries made during the current editing session. Does not remove previously saved entries.
X	Deletes the factor from the study.
Add	Adds an item to a categorical factor or a numeric value to a numeric factor.

Table 28. Study Definition page parameters (Sheet 2 of 2)

Parameter	Description
Delete	Deletes the selected item or value from the list in the respective Items or Values area.
Text entry boxes	
[new factor]	Type a factor name in this box.
Item box	Type the name of an item that you want to add to the Items list for a categorical factor in this box.
Value box	Type a numeric value that you want to add to the Values list for a numeric factor in this box.

Add input files to an existing study

Use the Add Files button on the study command bar to add input files to a study.

❖ **To add input files to an existing study**

1. Open the study. See "Open an existing study."
2. On the study command bar, click **Add Files**.
3. In the Add Files dialog box, select the files of interest and click **Open**.

   The Input File Characterization dialog box opens.
4. Select the sample types and study factor values for the new samples. See "Characterize the new input files."
5. Click **OK**.

   The Input Files page of the study opens.

Remove input files or update their location

Use the Input Files page to remove or update the location of the input files in an existing study. The input files for the Compound Discoverer application are Xcalibur RAW files acquired by a Thermo Scientific HRAM mass spectrometer.

Tip To add input files to an analysis, drag the files of interest from the Input Files page to the Analysis view. See "Set up a new analysis from within an existing study."

For details, see the following topics:

- Display the location of the input files for a study
- Remove input files from a study
- Resolve the location of the input files in a study
- Input Files page parameters

Display the location of the input files for a study

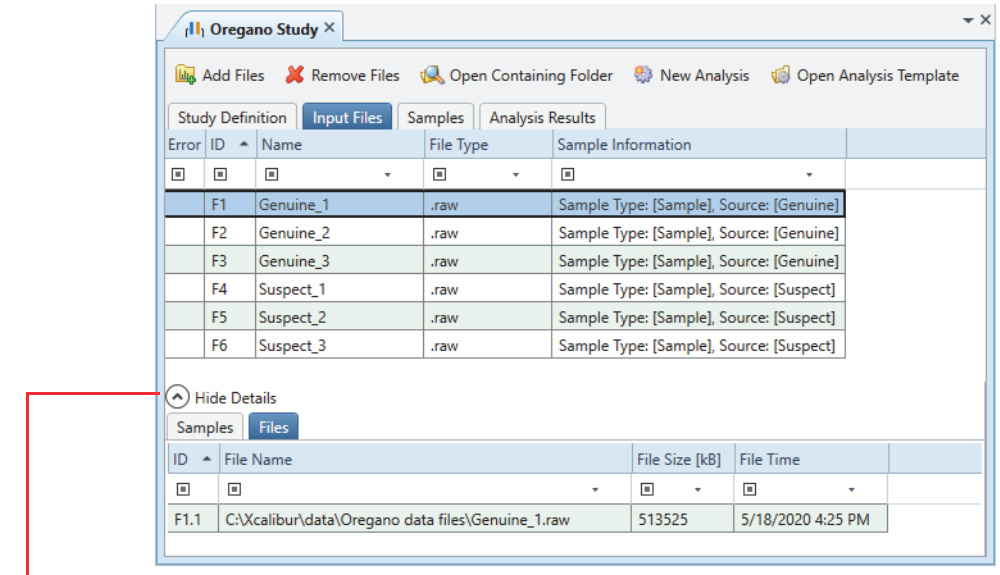
❖ **To display the file path for an input file**

1. On the Input Files page of a study, select the input file of interest.
2. Below the table, click **Show Details**.

   The Samples page opens below the input files table.
3. Click the **Files** tab.

   Figure 66 shows the hidden Files page that lists the full file name of the selected input file, including its directory location.

Figure 66. File path of selected input file



Show Details or Hide Details command

Remove input files from a study

Follow this procedure to remove input files from a study.

Note Removing input files from a study does not delete them from their directory location.

❖ To remove input files from a study

1. On the Input Files page, select the rows to remove and click **Remove Files** in the study command bar.

   Depending on whether you have run an analysis with the selected input files, one of the following confirmation boxes appears:

   - If you have not run an analysis, the Remove Input File confirmation box appears.
   - If you have run an analysis, the Remove Analysis Result Files confirmation box appears.

2. Do one of the following:

   - In the Remove Input File confirmation box, click **Yes** to remove the input files from the study.

   –or–

   - In the Remove Analysis Result Files message box, click **Remove Files** to remove the input files and their associated analyses from the study.

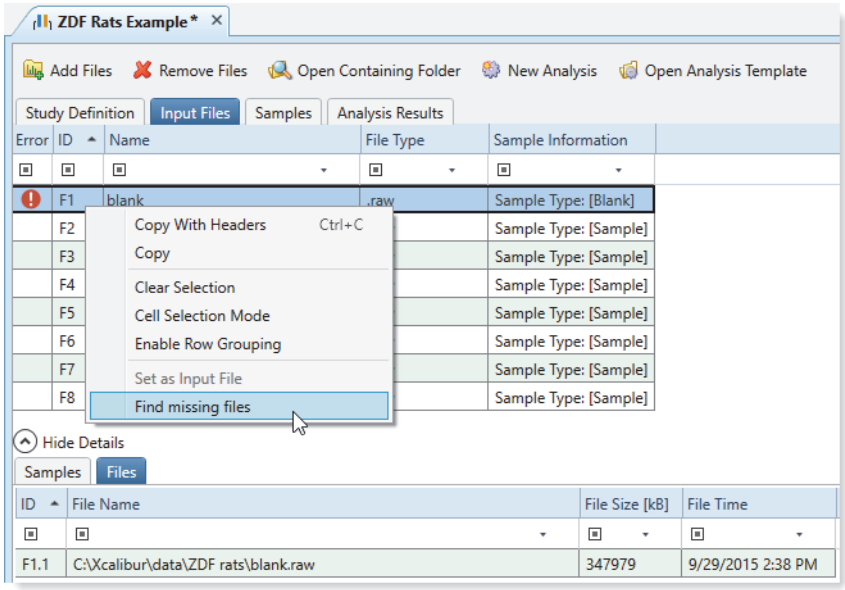
     When you remove an input file from the study, the analyses associated with the input file disappear from the Analysis Results page, but the result files (.cdResult) remain in the study folder.

Resolve the location of the input files in a study

Typically, the study file resides in the study folder and the raw data files that the study points to reside in a separate folder—for example, an Xcalibur\data*subfolder*.

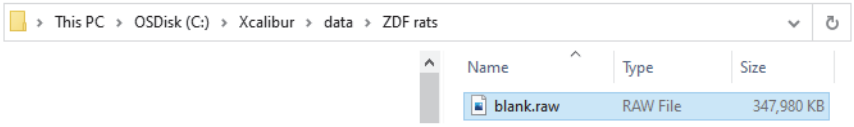
If the network or directory path changes between the study and the raw data files, an exclamation symbol () appears to the left of the file ID.

Figure 67. Exclamation symbol for missing input file, Find Missing Files command, and Files page of the Details section



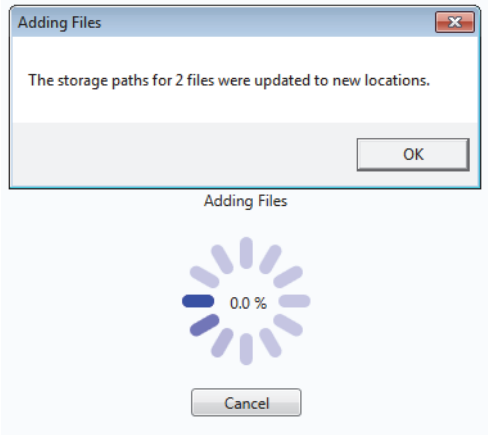
❖ To resolve the input files list when you move a study or the Xcalibur RAW files

1. On the Input Files page of a study, display the details for the missing files and check their original location.
2. If you know where the files are currently stored, add the files to the study by doing any of the following:
   - Open the Add Files browser by clicking the **Add Files** command in the Study page command bar. Then, select the files and click **Open**.
   - Right-click the row for the missing file and choose **Find Missing Files**. Then, in the Browse for Folder dialog box, browse to the holding folder, select the Xcalibur RAW files, and click **OK**.



The Adding Files confirmation box opens. The progress remains at 0.0% until you click OK.

Figure 68. Adding Files confirmation box with progress information



3. Click **OK** to continue.

   The Adding Duplicate Files message box opens. The progress again remains at 0.0% until you click OK.

4. Click **OK** to continue.

   The application restores the connection between the study and the raw data files.

Input Files page parameters

Table 29 describes the parameters on the Input Files page of a study.

Table 29. Input Files page parameters (Sheet 1 of 2)

Parameter or feature	Description
Show Details/Hide Details	Displays or hides the Samples and Files subpages.
Columns	
Error	Displays an exclamation mark, ❗, if the file is missing.
ID	Displays a unique ID in the following format: F#, where # is a unique integer. If you remove a file, and then add it again, the application updates the ID number.
Name	Displays the file name of the raw data file.
File Type	Displays the file type of the input file. The Compound Discoverer application supports Xcalibur RAW files (.raw).
Sample Information	Displays the sample type and any other selected study factors.
Hidden pages (Samples and Files)	
Samples page	
Sample	Displays a unique identifier for the input file.

Table 29. Input Files page parameters (Sheet 2 of 2)

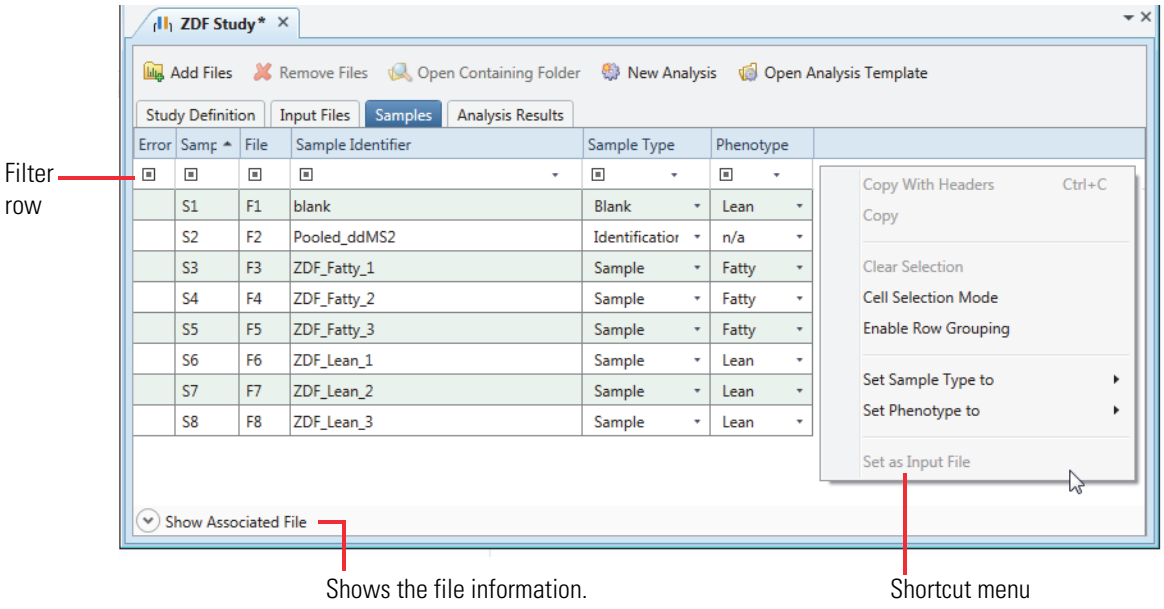
Parameter or feature	Description
Sample Identifier	Displays the file name of the raw data file.
Sample Type	Displays the sample type. See "Available sample types."
Study factor columns	Displays the study factor values. You can modify the study factor selections. Changing the factor values and sample types on the Input Files page also updates these items on the main Samples page.
Files page	
ID	Displays a unique ID (reserved for future implementation).
Name	Displays the file name and directory location of the raw data file.
Date Modified	Displays the acquisition date and time of the raw data file.
Size	Displays the size of the raw data file in bytes.
Shortcut menu for the Input Files page	
Set As Input File	Adds the selected input file to the Files for Analysis area in the Analysis view. Available when the Analysis view is open.
Find Missing Files	Opens the Browse for Folder dialog box. Browse to the folder where the file is stored and click **OK**. Then, click **OK** to close the confirmation message. Available when the Input Files table contains missing files.

Edit the sample type and study factor values

If you have not already characterized the samples in a study or you want to change their characteristics, use the Samples page of an existing study.

Tip To open the Samples page of a study, click the **Samples** tab.

Figure 69. Samples page and its shortcut menu



To select or modify the sample types and study factor values or view the file information on the Samples page, see the following topics as applicable:

- Edit the sample identifier on the Samples page
- Edit the sample types on the Samples page
- Edit the study factor values on the Samples page
- View the file information on the Samples page

Edit the sample identifier on the Samples page

To make it easier to identify each sample in a study, you can modify the text in the Sample Identifier column.

❖ To edit the text in the Sample Identifier column

1. Point to the sample cell.

   The Edit icon appears.

2. Click the **Edit** icon,  .
3. Place the cursor in the cell, and then type or paste the new text.

Edit the sample types on the Samples page

For information about sample types, see "Available sample types."

❖ **To edit the sample types of the input files in a study**

Tip To select a row, click a column that does not include a dropdown list.

Do any of the following:

- To select the sample type for a single sample, select **Sample**, **Control**, **Blank**, **Quality Control**, **Identification Only**, **Standard**, or **Labeled** from the Sample Type list.
- To assign the same sample type to a consecutive sample range, use the SHIFT key to select a range of samples. Then, right-click and choose **Set Sample Type To >** ***Sample Type***.
- To assign the same sample type to nonconsecutive samples, use the CTRL key to select the samples. Then, right-click and choose **Set Sample Type To >** ***Sample Type***.

Edit the study factor values on the Samples page

❖ **To edit the study factor values for the input files in a study**

Do any of the following:

- To select the factor values for a single sample, select the appropriate value from the list in each factor column.
- To select the same value for a consecutive sample range, drag the pointer across the rows of interest. Then right-click and choose **Set** ***Factor*** **To >** ***Value***.
- To select the same value for nonconsecutive samples, hold down the CTRL key and click the samples of interest. Then right-click and choose **Set** ***Factor*** **To >** ***Value***.

Tip To select a row, click a column that does not include a dropdown list.

View the file information on the Samples page

❖ **To view the file name and location for a selected sample**

Click **Show Associated File** at the bottom left of the Samples page.

The following details appear—the full file name and location, the file size in kilobytes, and the acquisition time of the Xcalibur RAW file.

Samples page parameters

Table 30 describes the parameters on the Samples page of a study.

Table 30. Samples page parameters

Parameter	Description
Show/Hide Associated File	Shows or hides the file information for a selected sample.
Columns	
Error	Displays an error symbol.
Sample	Displays a unique number for the sample (S#).
File	Displays a unique number for the input file (F#).
Sample Identifier	Displays the file name of the raw data file.
Sample Type	Specifies the sample type for each sample. For LC studies, the available selections are Sample, Control, Standard, Blank, Quality Control, Identification Only and Labeled. For information about the sample types, see "Available sample types."
Study factor columns	Specifies the study factor values for each sample. You can edit the study factor values.
Columns in hidden rows	
ID	Displays a unique file identifier.
File Name	Displays the file name and directory location of the Xcalibur RAW data file.
File Size	Displays the size of the Xcalibur RAW data file in bytes.
File Time	Displays the acquisition date and time of the Xcalibur RAW data file.
Shortcut menu commands For information about the Copy with Headers, Copy, Clear Selection, and Cell Selection Mode commands, see "Common operations for manipulating data tables."	
Set Sample Type To	Assigns the selected sample type to a sample range.
Set *Factor* To	Assigns the selected study factor value to a sample range.
Set As Input File	Adds the selected input file to the Files for Analysis area in the Analysis view. Available when the Analysis view is open.

Save the study file if you turned off the auto-save feature

By default, the application saves the study file after you submit an analysis and when you close the study file. However, you can change this behavior by turning off the auto-save feature.

IMPORTANT If you turn off the auto-save feature, the application prompts you to save your changes when you attempt to close a study file with unsaved changes. See "Turn off the auto-save feature for studies."

Unsaved changes include, for example, the last completed run on the Analysis Results page, new input files on the Input Files page, new study factors or study factor values on the Study Definition page, new sample assignments on the Samples page, and other study parameters.

❖ To save a study file

Do one of the following:

- Choose **File > Save All** from the menu bar. Or, click the **Save All Open Items** icon,  , in the toolbar.

–or–

- Click the study tab to make it the active page. Then, choose **File > Save** from the menu bar, or click the **Save the Currently Active Item** icon,  , in the toolbar.

6

Create and edit processing workflows

The application uses a node-based method to create processing workflows (processing methods) for the analysis of raw data files. You can create your own custom processing workflows (cdProcessingWF), use one of the many defined processing workflow templates provided with the application, or customize one of the existing processing workflow templates.

Note The parameter settings for the workflow nodes in the defined processing workflow templates are not necessarily the same as the default settings for the workflow nodes themselves. The parameter settings in the processing workflow templates provided with the application are optimized by the field of study (vertical market).

For details about editing and creating processing workflows, see these topics:

- Processing workflow templates
- Workflows page
- Edit an existing processing workflow
- Defined processing workflow templates for LC studies
- Create a completely new processing workflow for LC studies
- Connect the workflow nodes for an LC study
- Save a custom processing workflow as a template

Note For LC studies, the application provides more than 30 defined processing workflow templates organized by field of study.

Processing workflow templates

The Compound Discoverer application uses a node-based processing workflow (processing method) to analyze the MS data acquired with a high-resolution, accurate-mass LC/MS or GC/MS instrument.

In addition to analyzing the MS data, the application can display chromatograms from the following detectors:

- A photo-diode array (PDA) detector or an ultraviolet-visible (UV-Vis) detector that is controlled by a Thermo Scientific data system
- An analog detector that is connected to the mass spectrometer's analog input channels

Workflows page

Within an existing study, you use the Workflows page to select, create, and edit processing workflows. The Workflows page is a tabbed page that opens to the right of the tabbed study pages when you start a new analysis or reprocess an existing analysis. You cannot edit a processing workflow from outside a study.

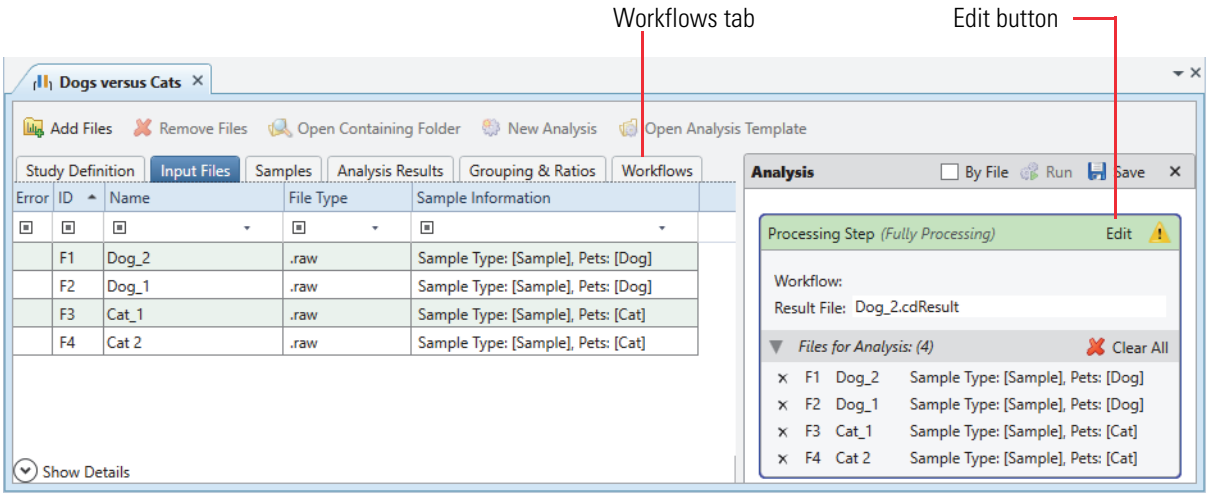
For details about the Workflows page, see the following topics:

- Open the Workflows page
- Workflows page command bar
- Workflows page shortcut menu

Open the Workflows page

Figure 70 shows the initial layout for a new study and analysis after you close the wizard.

Figure 70. Layout for the study and analysis pages after exiting the wizard



Closing a study erases the analysis settings, and reopening a study opens only the study pages.

❖ To open the Workflows page

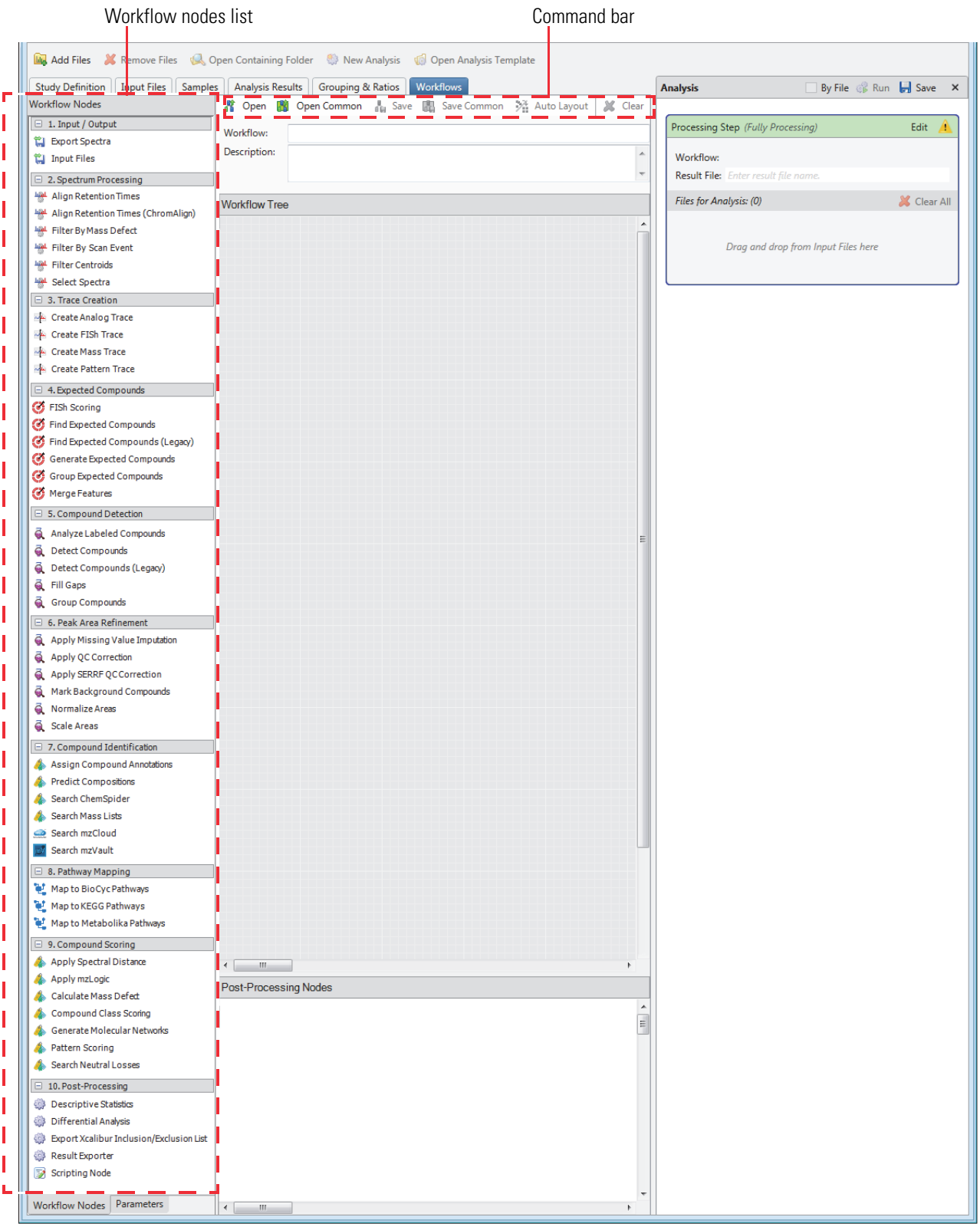
Do one of the following:

- Use the New Study and Analysis wizard to set up a new study and a new analysis. Then, click the **Workflows** tab in the set of tabbed pages or **Edit** in the Analysis view.
- Open an existing study, click **New Analysis** in the Study command bar, and then click the **Workflows** tab.
- From the Analysis Results page of a study, select an analysis, click **Reprocess**, and then click the **Workflows** tab.

The Workflow Tree and Workflow Nodes panes appear. For a new analysis, the Workflow Tree pane is empty. For an existing analysis or an analysis created by using the wizard, the Workflow Tree pane usually contains a processing workflow.

Figure 71 shows an empty analysis in the Analysis view at the right, an empty Workflow Tree pane in the middle, and the Workflow Nodes pane for an LC study at the left.

Figure 71. Workflows page without a selected processing workflow



Workflows page command bar

Table 31 describes the Workflows page commands.

Table 31. Workflows page commands

Command	Description
Open	Opens the Open Workflow dialog box for locating and opening a processing workflow.
Open Common	Opens the Open Workflow dialog box to the following folder where the application installs the three common processing workflow templates: C:\Users\Public\Public Documents\Thermo\Compound Discoverer 3.3\Common Templates
Save	Opens the Save Workflow dialog box for selecting a folder and entering a file name for the processing workflow in the Workflow Tree pane.
Save Common	Opens the Save Workflow dialog box to the folder where the application installs the common processing workflow templates. Saves the current processing workflow in the Workflow Tree pane to the Common Templates folder.
Auto Layout	Automatically formats the layout of the workflow nodes.
Clear	Clears the Workflow Tree pane.

Workflows page shortcut menu

Table 32 describes the commands in the shortcut menu for the Workflow Tree pane or a workflow node.

Table 32. Workflow Tree pane and workflow node shortcut menu commands (Sheet 1 of 2)

Command	Description
Cut	Removes the node from the workflow. Selecting any workflow node makes this command available.
Copy/Paste	Adds a copy of the selected node to the Workflow Tree pane. Selecting a workflow node that can appear more than once in a workflow makes this command available.
Auto Layout	Automatically formats the layout of the workflow nodes.

Table 32. Workflow Tree pane and workflow node shortcut menu commands (Sheet 2 of 2)

Command	Description
Hide Node Numbers	Turns the numbering on or off.
Reprocess	Sets the selected node for reprocessing or sets the selected node and its related nodes for reprocessing. Available for an analysis that you have set up for reprocessing [Workflow Tree (Reprocess)].

Edit an existing processing workflow

You can modify a processing workflow by adding and deleting workflow nodes and by changing the parameter settings in the workflow nodes.

The application automatically connects some of the workflow nodes as you add them to a processing workflow. But for some of the workflow nodes, you must make the appropriate connections. When a node is missing a connection, a Caution symbol appears in its upper-right corner.

Several workflow nodes require custom parameter selections. When a workflow node is missing a custom parameter selection, an exclamation mark appears in its upper-right corner.

For details, see these topics:

- Fix a workflow node that has a caution symbol
- Fix a workflow node that has an exclamation mark
- Add a workflow node to a processing workflow
- Delete a workflow node from a processing workflow
- Edit the parameter settings for a workflow node

Fix a workflow node that has a caution symbol

When the node is missing a connection, a Caution symbol,  , appears in its upper-right corner.

❖ To fix a workflow node that is labeled with a Caution symbol

1. To view the validation errors, point to the Caution symbol in the Analysis view.

   A missing connection begins with the following text:

   Missing connection for

2. Make the appropriate node connections.

   See Connect the workflow nodes for an LC study.

   If the node is also missing a required parameter selection or the selected item is not found in its corresponding list or library, an exclamation mark appears after you fix the missing connection. See "Fix a workflow node that has an exclamation mark."

Fix a workflow node that has an exclamation mark

To edit a processing workflow, you must open it from the Workflows page within a study.

An exclamation mark, , appears in the upper-right corner of a node when the node is missing a required parameter selection or the selected item is not found in its corresponding list or library. See "Troubleshoot common analysis errors."

❖ To fix a workflow node that is labeled with an exclamation mark

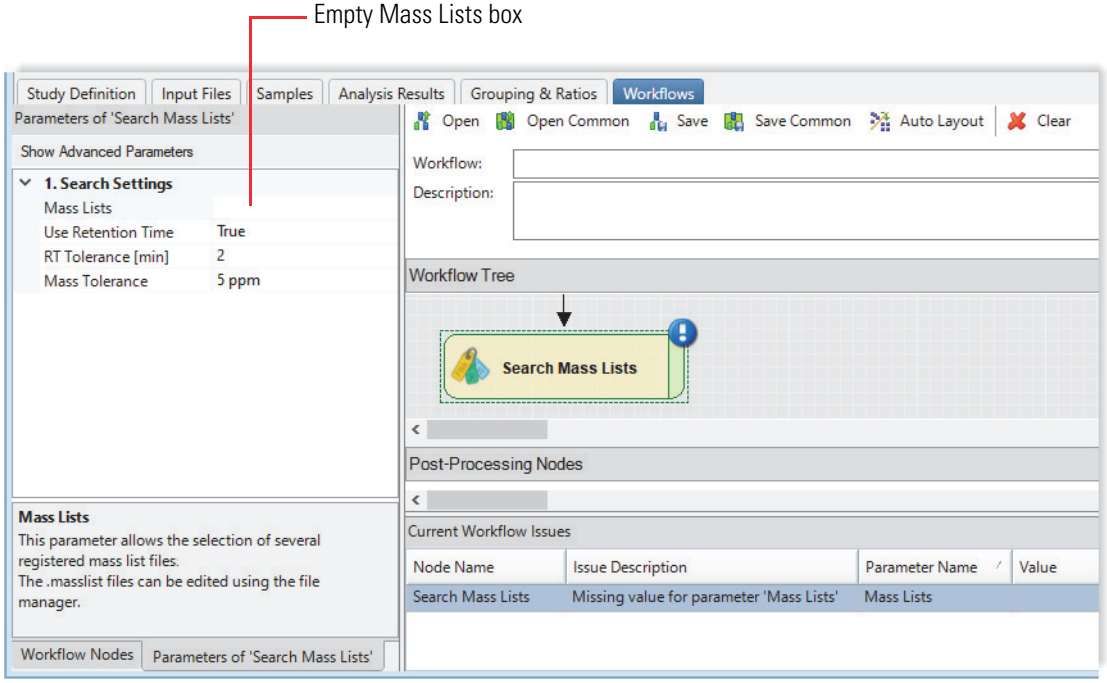
1. To view the validation errors, point to the Caution symbol in the Analysis view or review the issues described in the Current Workflow Issues pane below the Post-Processing Nodes pane.

   For a missing parameter selection, the issue description includes the following text:

   Missing value for parameter '*Node*'

2. To fix the workflow node error, select the node in the Workflow Tree pane.

Figure 72. Missing parameter value for the Search Mass Lists node



3. In the Parameters of '*Workflow Node*' pane to the left, make a selection for the missing parameter value.

Add a workflow node to a processing workflow

To edit a processing workflow, you must open it from the Workflows page within a study.

❖ **To add a node to the processing workflow**

1. Select the node in the Workflow Nodes pane and drag it to the Workflow Tree pane.

   Note A Caution symbol appears in the upper-right corner of a workflow node that is missing a connection. Because a missing connection takes priority over a missing parameter setting, if a workflow node is also missing a parameter setting, a blue circle with an exclamation mark appears after you fix the missing connection.

2. If necessary, make the appropriate node connections. See Connect the workflow nodes for an LC study.
3. To display the parameters for a workflow node, click the node in the Workflow Tree pane.

   The Parameters pane lists the parameters for the selected node.

4. Edit the parameter settings for the node.

Note For an LC study that includes a targeted analysis and an untargeted analysis, the processing workflow must include either the Detect Compounds (Legacy) node and the Find Expected Compounds (Legacy) node or the Detect Compounds node and the Find Expected Compounds node.

Delete a workflow node from a processing workflow

To edit a processing workflow, you must open it from the Workflows page within a study.

❖ **To delete a node from a processing workflow**

1. Right-click the node in the Workflow Tree pane and choose **Cut**.
2. Check whether any validation issues appear.
3. (Optional) To save the processing workflow for reuse, click **Save**. Then, rename the workflow if necessary, select an appropriate folder, and click **Save**.

   Tip If you use the processing workflow for the current analysis, you can reuse the processing workflow without saving it. After you successfully run the analysis, you can rerun it by selecting the completed analysis on the Analysis Results page of a study.

Edit the parameter settings for a workflow node

To edit a processing workflow, you must open it from the Workflows page within a study.

❖ **To edit the parameter settings for a workflow node**

1. In the Workflow Tree pane, select the node.

   The Parameters page opens with the parameters for the selected node.

2. Click **Show Advanced Parameters** below the Parameters page title bar.

   If the node contains hidden advanced parameters, the advanced parameters appear below the basic parameters.

   When you place the cursor in the box to the right of the parameter name, information about the parameter appears at the bottom of the Parameters page.

3. Enter the appropriate values or make the appropriate selection for each parameter.

   For more information about each parameter, see Chapter 7, "Workflow nodes."

Defined processing workflow templates for LC studies

These topics describe the provided templates and how the application processes data to find expected compounds for a targeted analysis or detect and identify unknown compounds for an untargeted analysis:

Targeted processing workflows for expected compounds

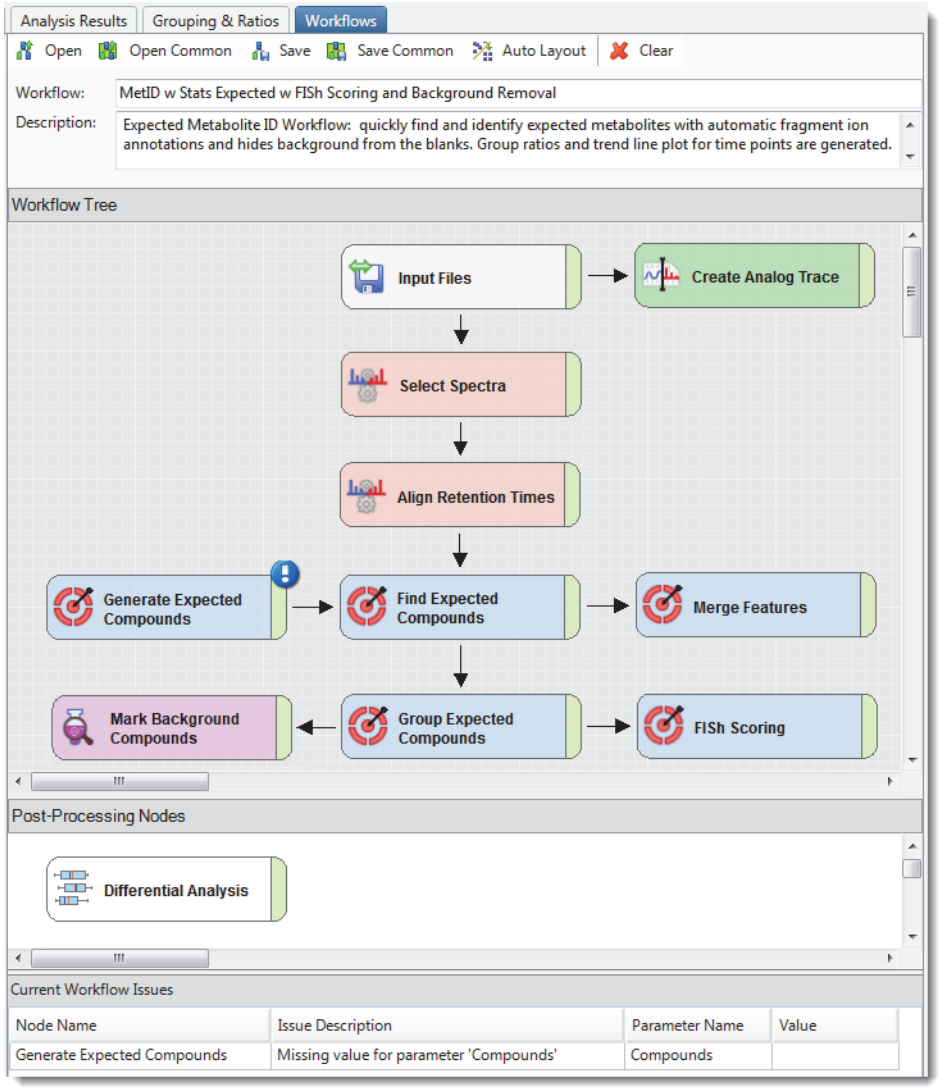
Use the Expected Compounds workflow nodes to run an analysis that targets known analytes—for example, the metabolites of a specific drug.

Figure 73 shows the workflow tree in the following processing workflow file:

MetID w Stats Expected w FISh Scoring and Background Removal.cdProcessingWF

This processing workflow uses the Generate Expected Compounds and Find Expected Compounds nodes to find expected parent[1] compounds and their dealkylation, dearylation, and transformation products. FISh Scoring is applied to explain the fragments in the fragmentation spectra based on in silico fragment prediction of the parent and dealkylation/dearylation products.

Figure 73. Processing workflow for a metabolism study



During this targeted analysis, the following processes occur:

1. The Input Files Node sends the file names and location of the input files to the connected nodes (typically the Select Spectra node, Create Analog Trace node, or both of these nodes).
2. The Select Spectra Node filters the MS scan data.

[1] A parent compound is the initial compound in a reaction or metabolic pathway.

IMPORTANT Because the Find Expected Compounds node requires full (MS1) scans, do not filter out all the full (MS1) scans for a targeted analysis.

Because the FISh Scoring node requires fragmentation scans to provide a confirmation score for the expected precursor ions, do not filter out the fragmentation scans when the processing workflow includes this node.

3. The Align Retention Times node chromatographically aligns features (chromatographic peaks with the same *m/z* × RT dimensions) across the input files in a sample set by using the specified alignment algorithm. The node finds features that are common across most samples. These are called landmark features. It then builds regression curves based on those landmark features.

   The Align Retention Times (ChromAlign) node builds correlation matrices based on spectral similarities. It then builds regression curves by using the optimal path in the correlation matrix. The node uses a reference file to build these matrices. The reference input file can be any input file assigned the Sample, Control, or Standard sample type.

   IMPORTANT The alignment algorithm looks for matching features (chromatographic peaks with the same *m/z* × RT dimensions) in the input files. The alignment algorithm can align input files that include polarity switching data; it cannot align input files that include only positive polarity scans with input files that include only negative polarity scans.

4. The Generate Expected Compounds node creates a list of expected compound ions by using the following user-specified parameter settings:

   - Parent compound or compounds
   - Number of dealkylation and dearylation steps
   - Number and type of transformation steps
   - List of possible adduct ions

   The Generate Expected Compounds node passes the following information to the Find Expected Compounds node for each expected compound:

   - Parent compound or compounds
   - Elemental composition of the expected neutral compound
   - Molecular weight of the expected neutral compound
   - Whether the expected compound is a product of a dealkylation step
   - Transformations required to produce the expected compound
   - Composition change between the parent and expected compound

It also passes the following information for each expected compound ion:

- Charge
- Theoretical *m/z* value

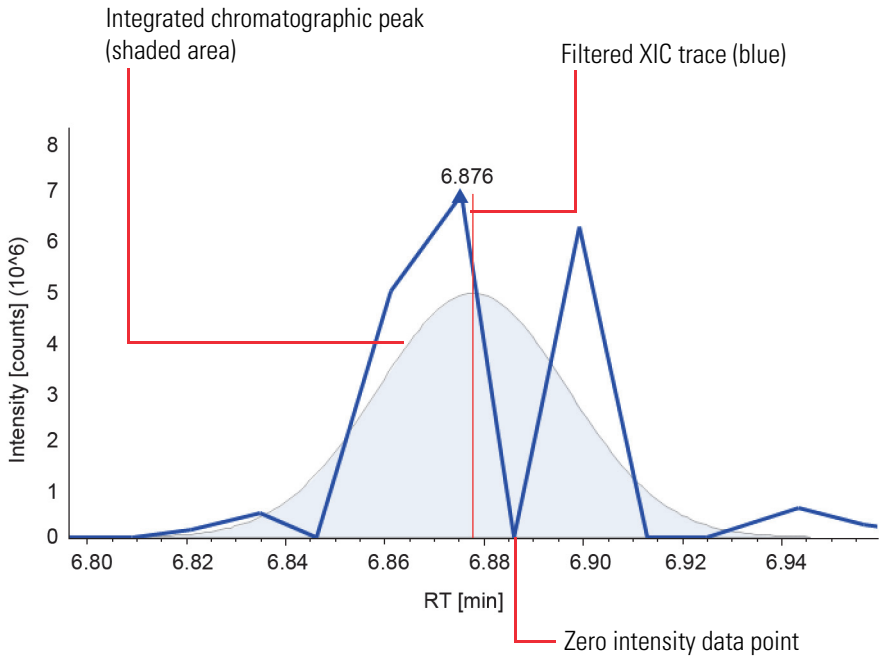
Note The Generate Expected Compounds node does not send information to a result table. It sends information to the Find Expected Compounds node, which requires input from at least one Generate Expected Compounds node. The Filter By Mass Defect node can also process the input from one or more Generate Expected Compounds nodes.

5. The Find Expected Compounds node performs the following steps by using the full (MS1) scan data from the Align Retention Times node and the information from the Generate Expected Compounds node (or multiple Generate Expected Compounds nodes):
   a. Creates a set of mass tolerance and intensity tolerance fit parameters for each expected compound ion (*m/z* value) by using the theoretical *m/z* value for the ion, the user-specified mass tolerance, the theoretical isotope pattern for the ion, and the user-specified intensity tolerance for the isotopic ions.
   b. For each expected compound ion, the Find Expected Compounds (Legacy) node does the following:
      i. Checks each full (MS1) scan that passes through the connected data processing node for centroids that match the mass and intensity tolerance rectangles. The pattern search (set of rectangles) looks for the base peak (most intense centroid) of the pattern first.

         In most cases, the base peak is the A0 centroid for the monoisotopic ion. But in some cases, for example, in compounds that contain two bromine atoms or four chlorine atoms, the isotopic peaks have a higher intensity than the monoisotopic peak.

      ii. Draws a filtered XIC trace by summing the centroids found for each data point. If a data point does not contain the user-specified number of matching isotopes and the theoretical intensity of the missing isotope was above the noise threshold, the node assigns a zero intensity value to the data point (see Figure 74).

Figure 74. Filtered XIC trace with a zero intensity data point



c. For each expected compound found, the Find Expected Compounds (Legacy) node creates a summed trace by summing the XIC traces of the associated expected compound ions.

d. Detects and integrates the chromatographic peaks in each XIC trace. Does not report chromatographic peaks with an apex peak height that is below the user-specified minimum (chromatographic) peak intensity. If the average peak width of the peaks in the processed retention time range is greater than the setting for the Average Peak Width parameter, the Find Expected Compounds node rejects all of the chromatographic peaks.

The Find Expected Compounds node passes the following information to the Expected Compounds per File table for each expected compound that it finds in an input file:

- RT (min)—Retention time of the chromatographic peak apex.

  Note If the node finds more than one adduct ion for an expected compound, the chromatogram is a summed trace.

- Best SFit [%]—Best spectral fit score between the measured and expected isotope patterns for the expected compound ions. When the node finds only one adduct ion, the best spectral score is equal to the score for the adduct ion that it found.
- Max # MI—Maximum number of matched isotopes for any of the adduct ions. When the node finds only one adduct ion, the maximum number of matched isotopes is equal to that of the adduct ion that it found.
- #Adducts—Number of adduct ions that it found.

- Area—Total area of the chromatographic peaks for the found adduct ions of the expected compound. Peak areas are reported in counts × seconds.
- Parent Area%—Relative area of the chromatographic peak for the expected compound as compared to the total area of all found peaks for the expected compound.

Note The parent area is the chromatographic peak area of the expected compound, rather than the area of the compound listed in the Parent Compound column. The compounds listed in the Parent Compound column are the library compounds that you selected in the Generate Expected Compounds node.

6. The Group Expected Compounds Node groups the chromatographic peaks by their molecular weight × retention time (MW × RT) dimensions across the input file set and creates the Expected Compounds table.[2]

   When you enable the peak ratings filter, the node filters out expected compounds that do not pass the peak quality threshold in the specified number of input files.

   You can select between two peak integration models:

   - Most Common Ion—Reports the chromatographic peak area of the most common adduct ion detected across the samples.
   - All Ions–Reports the summed areas of all the adduct ions detected in each sample.

   This node also selects the best hit ions for each compound across the input file set:

   - Selects the best ion and related MS1 scan for each compound as the one with the highest resolution and the highest intensity for the preferred ion. When you open a result file, the mass spectrum view displays the MS1 scan for the best ion across the input file set.
   - Selects the best fragmentation data by using the user-specified preferred precursor ion with the highest intensity that has data-dependent MS2 scans.

   Note You use the Preferred Ions parameter in the Group Expected Compounds node to specify the preferred ions.

7. When the input file set includes blank samples (Sample Type: Blank), the Mark Background Compounds node compares the peak areas of the compounds (same parent compound, molecular weight, and retention time) that are found in both the blank samples and the non-blank samples, and labels these compounds as Background Compounds if their peak areas do not meet the specified threshold.
8. When the spectrum data in the input files includes fragmentation scans (MS2, MS3, MSn), the FISh Scoring node compares the best fragmentation scan for an expected

[2] For result files generated in Compound Discoverer 2.0, the Group Expected Compounds node also added the Best Compounds column to the Expected Compounds per File table. The Workflow page of the Result Summary view displays the Best Compound criteria for updated result files.

compound across the input file set to the expected structures. The scoring process can add considerable processing time.

9. When the processing workflow includes both the Find Expected Compounds node and the Detect Compounds node, the Merge Features node consolidates the chromatographic peaks that these nodes find in the main Merged Features table. The consolidation is based on the *m/z* × RT dimensions of the features.

   Note The Merge Features node also creates the Merged Features table that is related to the Manual Peaks table. When you manually integrate a chromatographic peak for a specialized trace such as a UV trace, you can compare the selected peak in the Manual Peaks table to the peaks in the related Merged Features table. The application populates the related Merged Features table with the chromatographic peaks that fall within the retention time window specified in the Merge Features node—that is, the application populates the Merged Features table that is related to the Manual Peaks table with chromatographic peaks that have a similar retention time to the selected manual peak.

10. When the processing workflow includes any of the search nodes, the application searches the selected databases.

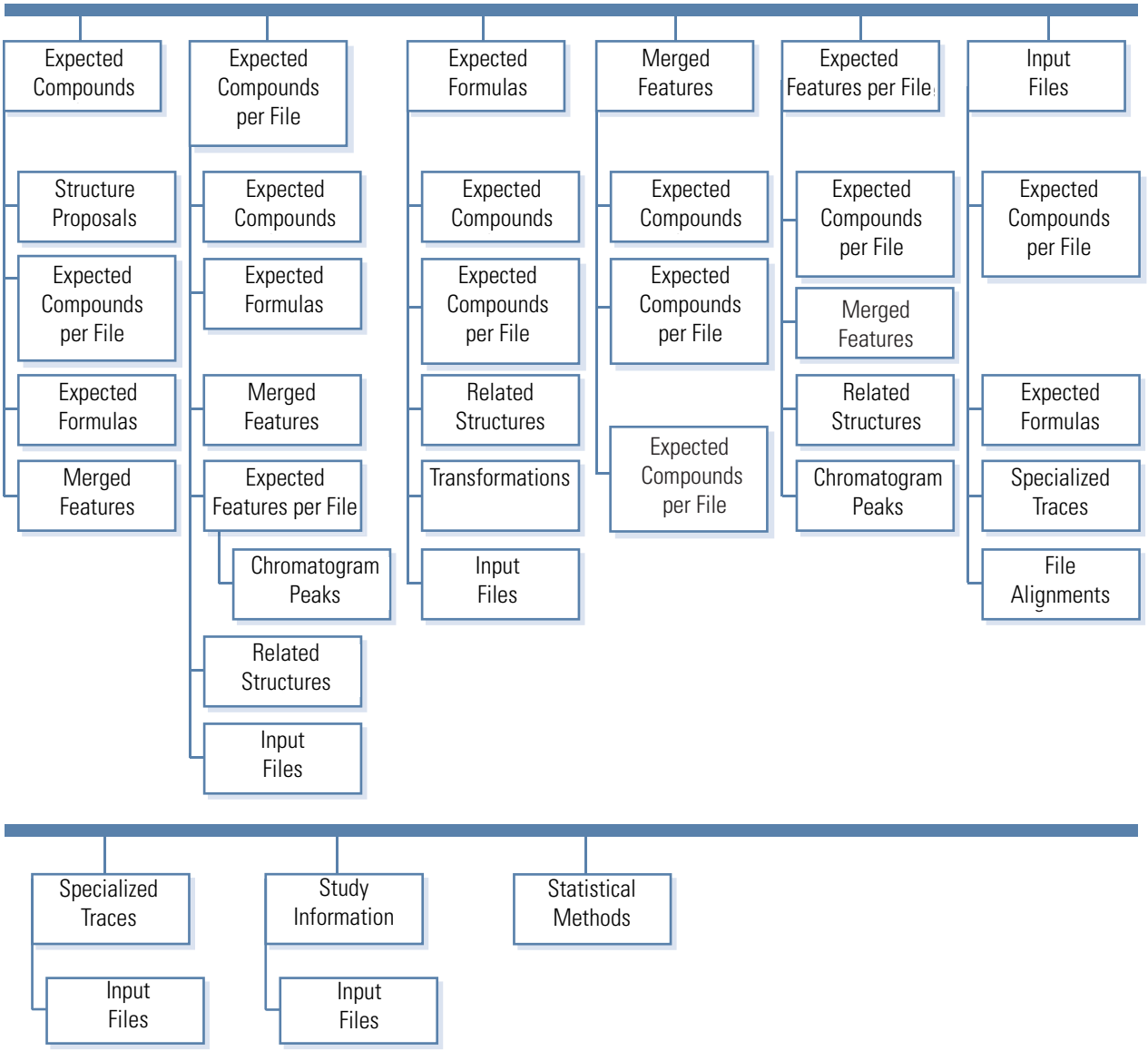
    Note You can connect the Group Expected Compounds node to any of the search nodes and any of the mapping nodes.

11. When the analysis includes group ratios, the Differential Analysis node runs the differential analysis.

After the analysis finishes, you can open the result file.

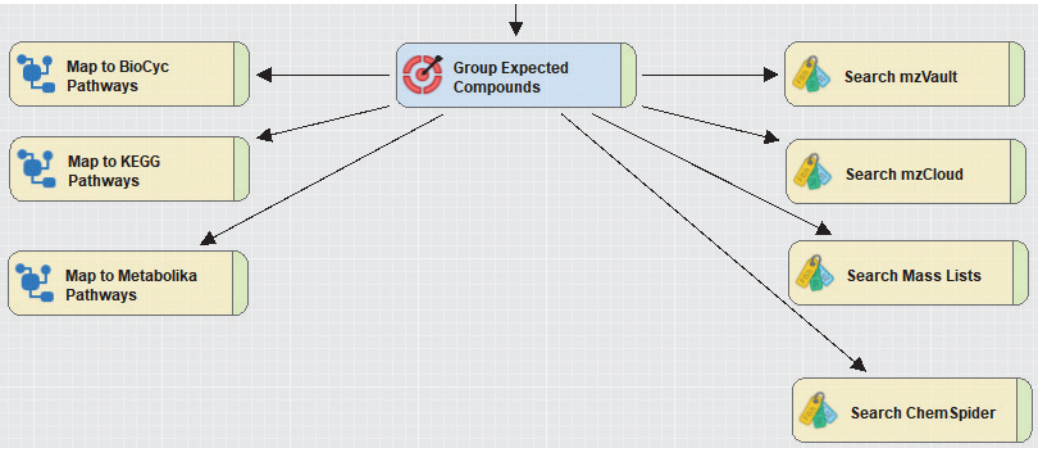
Figure 75 shows a schematic of the main and related result tables for the targeted workflow shown in Figure 73. The Structure Proposals table is empty until you populate it.

Figure 75. Result tables for a basic targeted workflow (with the Create Analog Traces and Merge Features nodes)



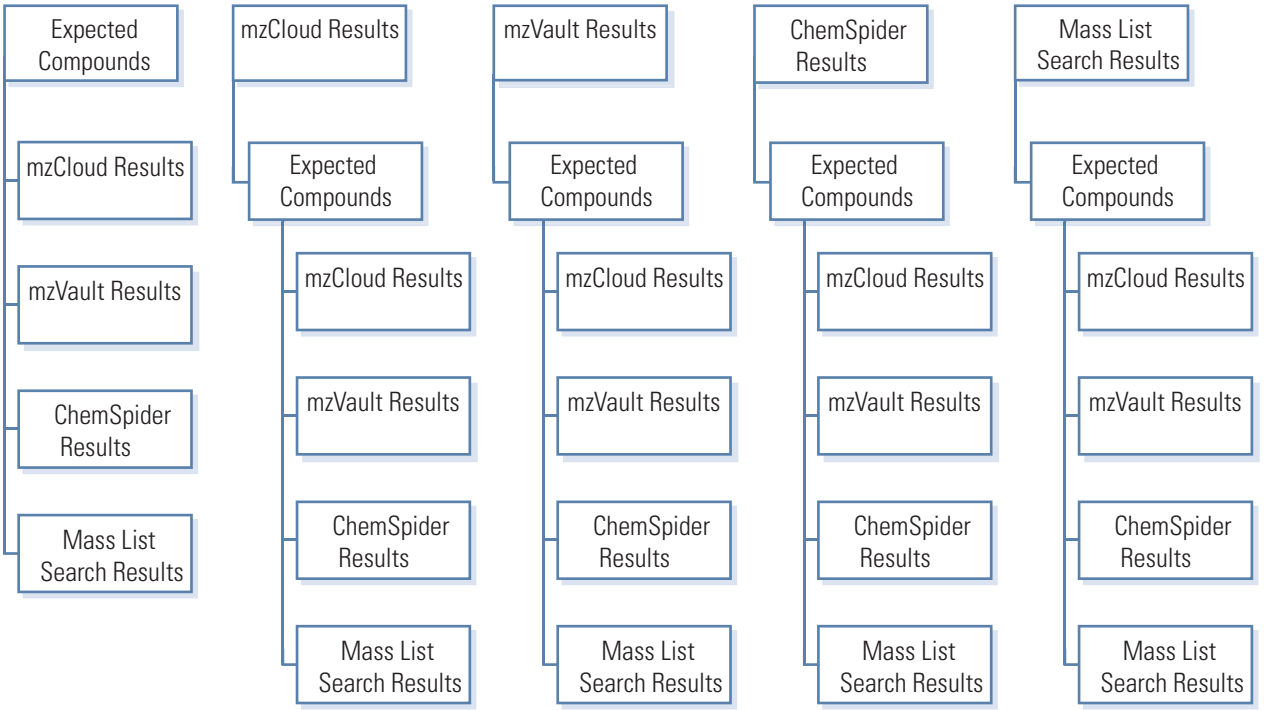
You can connect the Group Expected Compounds node to any of the search nodes and mapping nodes.

Figure 76. Group Expected Compounds node connected to the mapping nodes and the search nodes



Adding the search nodes to the processing workflow adds the main and related tables shown in Figure 77 to the result file.

Figure 77. Additional result tables generated by the search nodes



Adding the mapping nodes to the processing workflow adds the following result tables to the result file:

- Main: Metabolika Results, Metabolika Pathways, KEGG Pathways, BioCyc Pathways, and BioCyc Results
- Related result tables for specific expected compounds: Metabolika Results, Metabolika Pathways, KEGG Pathways, and BioCyc Pathways, and BioCyc Results
- Related result tables for specific Metabolika results: Expected Compounds and Metabolika Pathways
- Related result tables for specific Metabolika pathways: Expected Compounds and Metabolika Results
- Related result tables for specific KEGG pathways

You can connect the Group Expected Compounds node to the following peak refinement nodes: Mark Background Compounds and Scale Areas. You can add these nodes, and then reprocess the data set without reprocessing the entire workflow, as these nodes use only the data provided by the grouping node.

Untargeted processing workflows for identifying unknown compounds

Figure 78 shows the workflow tree for the metabolomics processing workflow that is provided with the application:

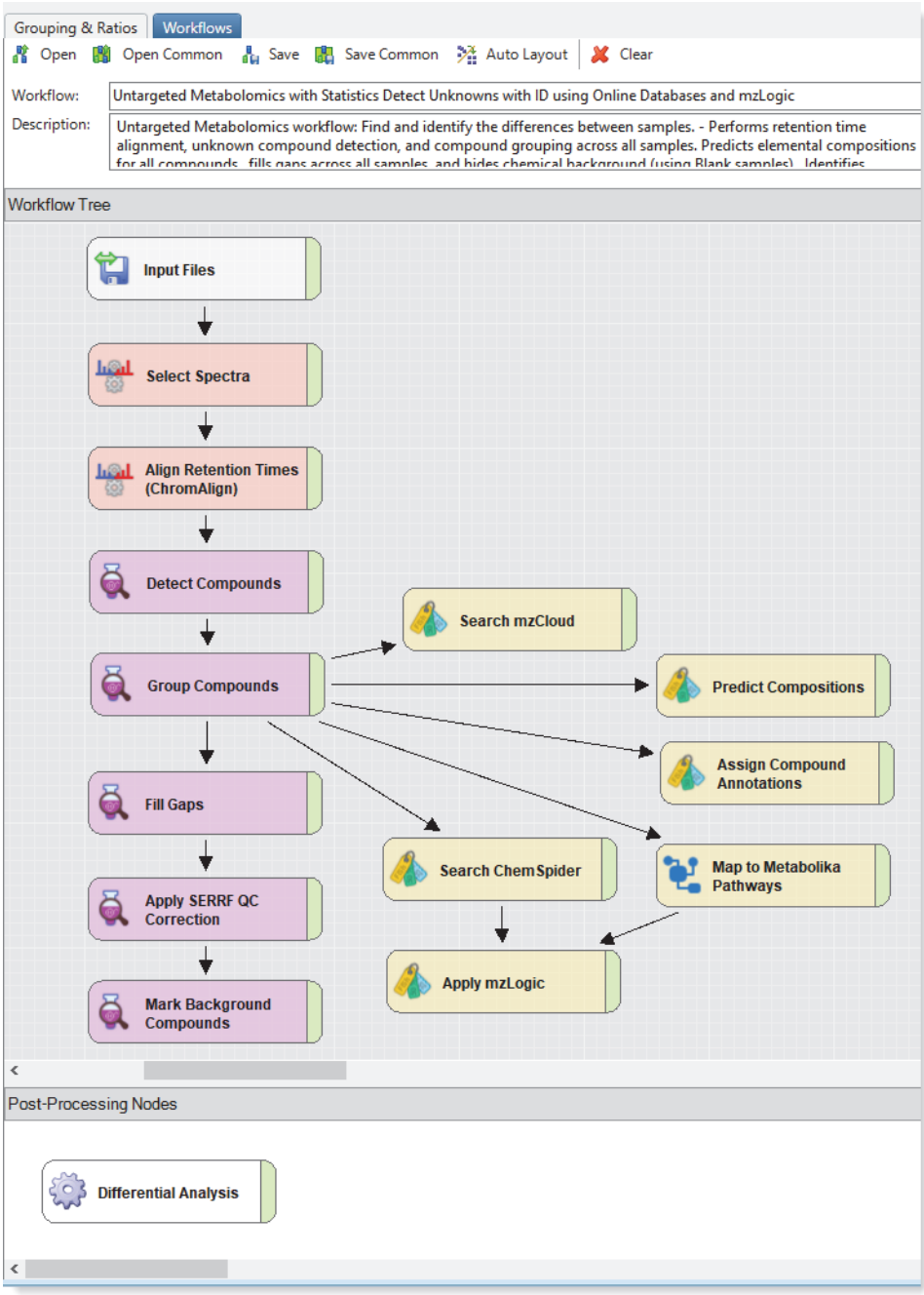
> Untargeted. Metabolomics with Statistics Detect Unknowns with ID using Online Databases and mzLogic.cdProcessingWF

This processing workflow uses the Detect Compounds node to find chromatographic peaks for unknown compounds (MW × RT) and the Predict Compositions node to determine the possible elemental compositions of the unknown compounds. It also determines the possible identity of the unknown compounds as follows:

- The Search ChemSpider node searches selected databases of MS1 scans by using the molecular weight or predicted formulas when available.
- The Search mzCloud node searches the mzCloud database of fragmentation scans by using the molecular weight or predicted formulas when available.
- The Map to Metabolika Pathways searches the pathways for the detected compounds. When the application finds a matching compound, it maps the pathway for ease of viewing.

The Assign Compound Annotations node assigns the following annotations to the detected compounds: Name, Formula, and Structure. The Apply mzLogic node combines mzCloud similarity searching (MS2 and MSn) with structure similarity matching to rank putative database results.

Figure 78. Processing workflow that finds and identifies unknown compounds



During this untargeted analysis, the following processes occur:

1. The Input Files node sends the file names and location of the input files to the Select Spectra node.
2. The Select Spectra node filters the MS scan data.

3. The Align Retention Times node chromatographically aligns the input files in a sample set.
4. The Detect Compounds (legacy) node does following:
   - Detects contiguous mass traces in the full (MS1) scans by using the parameter settings for the mass tolerance and intensity threshold.
   - Detects chromatographic peaks in the contiguous mass traces.
   - Groups isotopes.
   - Applies peak quality filters for isotopic features.
   - Groups adducts by using the user-specified ions and base ions lists.
   - Reports the unknown compounds (MW × RT) by occurrence in the Compounds per File table.

   IMPORTANT Make sure that the Preferred Ions list for the Group Compounds node includes the selections in the Base Ions list (advanced parameter) for the Detect Compounds node.
5. The Group Compounds node uses the specified mass and RT tolerances to group chromatographic peaks with the same MW × RT values in the Compounds table.

   You can select between two peak integration models:

   - Most Common Ion—Reports the chromatographic peak area of the most common adduct ion detected across the samples.
   - All Ions–Reports the summed areas of all the adduct ions detected in each sample.

   When you enable the peak ratings filter, the node filters out compounds that do not pass the peak quality threshold in the specified number of input files.

   It then sends the best fragmentation data across the input files to the Search mzCloud node and Predict Compositions node.

   This node also selects the best hit ions for each compound across the input file set:

   - Selects the best ion and related MS1 scan for each compound as the one with the highest resolution and the highest intensity for the preferred ion. When you open a result file, the mass spectrum view displays the MS1 scan for the best ion across the input file set.
   - Selects the best fragmentation data by using the user-specified preferred precursor ion with the highest intensity that has data-dependent MS2 scans.

   The Predict Compositions node and the search nodes use the best hit ions.

   Note You use the Preferred Ions parameter in the Group Compounds node to specify the preferred adducts.

6. The Search mzCloud node searches the mzCloud database for matching and similar fragmentation spectra.
7. The Predict Compositions node predicts the elemental compositions of the unknown compounds.
8. The Map to Metabolika Pathways node searches the Metabolika pathways for matching compounds.
9. The Search ChemSpider node searches the ChemSpider database for matching compounds.
10. The Fill Gaps node fills in missing peaks or peaks below the detection threshold (specified in the Detect Compounds node) for subsequent statistical analysis.

    IMPORTANT You can substitute the Fill Gaps node with the Apply Missing Value Imputation node. For details, see "Apply Missing Value Imputation node."

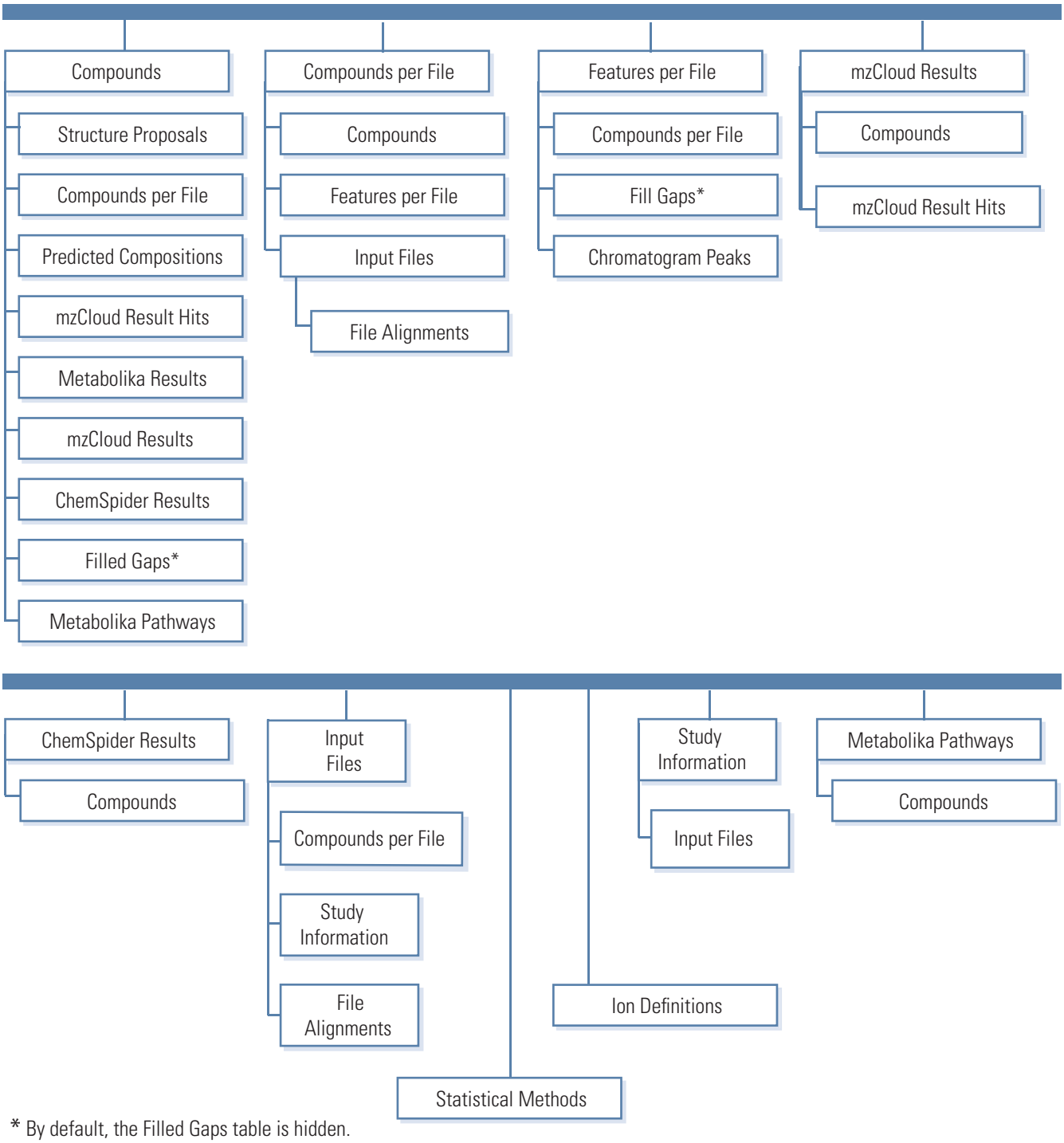
    Do not use the Apply Missing Value Imputation node when the processing workflow includes either of the QC correction nodes.

11. If the analysis includes QC samples, the Apply SERRF QC Correction node normalizes the chromatographic peak areas in the input files that you assigned the sample type of Sample.
12. The Mark Background Compounds node determines the background compounds in the blank samples (Sample Type: Blank) and labels these compounds as background compounds.
13. The Differential Analysis node runs a differential analysis on the defined sample ratios and calculates the p-values.
14. The Assign Compound Annotations node assigns and compares the annotations provided by the Predict Compositions, Search ChemSpider, Search mzCloud, and Search Mass Lists nodes.
15. The Apply mzLogic node runs a forward search and a reverse search using the mzCloud service. For compounds that have available MS2 scans, it scores all the structure candidates (or the specified maximum number of candidates) from the attached input nodes. Adds the following columns to the result tables: #Similarity Results (Compounds table) and mzLogic Score (search result tables).

For information about the result tables that this processing workflow generates, see Chapter 10, "Descriptive information for the result tables."

Figure 79 shows a schematic of the main and related tables for a basic untargeted workflow.

Figure 79. Result tables for an untargeted workflow



* By default, the Filled Gaps table is hidden.

Nomenclature for the provided processing workflow templates

When you open a defined processing workflow on the Workflows page of an analysis, descriptive text appears in the Description box. Read and understand the description before you use the workflow. The Description box does not enlarge to fit the text, so you must scroll down to read the complete description. Or, you can click the Description box, press CTRL+C copy the text to the Clipboard, and paste the text into Notepad.

The file names for the processing workflows include the following descriptive text:

- Expected—The workflow runs a targeted analysis with the Generate Expected Compounds and Find Expected Compounds nodes.

  IMPORTANT You must customize the targeted workflows by selecting the targeted compounds in the Generate Expected Compounds node. Before you can select the compounds for the node, you must add the compounds to the Expected Compounds library.

  In the defined processing workflows for targeted analyses, the Generate Expected Compounds node is set up to generate a mass list for the following adduct ions: [M+H]+1 and [M–H]–1. For best results, make the appropriate selections for your analysis from the Ions list in the Generate Expected Compounds node.

- Detect Unknowns, Unknown, or Untargeted—The workflow runs an untargeted analysis with the Detect Compounds node.

  Tip Mobile phase additives can have a significant effect on the base ions (adduct ions with the highest intensity) in the full scan data for an LC/MS experiment. To avoid misinterpreting the isotopic ion clusters, make sure that the Base Ions list in the Detect Compounds node includes the predominant adduct ions. For example, if the mobile phase contains a significant amount of ammonium acetate, consider adding the ammonium adduct, [M+NH4]+1, to the list.

  The processing workflows in the E and L folder include [M+NH4]+1 in the Base Ions list.

- Online Databases—The workflow searches the mzCloud and ChemSpider databases.

  Tip In the Search ChemSpider node, select the appropriate databases.

- Local Database—The workflow searches your local mzVault and mass list files. For metabolomics templates, the local databases include the local Metabolika pathways files.

  Tip In the Search mzVault and Search Mass Lists nodes, select the appropriate files. For LC studies, the application includes nine mzVault library files and nine mass lists.

  - mzVault libraries:
    - EpoxidizedSoybeanOil_Library_AN001586
    - mzCloud Offline for mzVault_Endogenous_2021B
    - mzCloud Offline for mzVault Autoprocessed_2021B
    - mzCloud_Offline for mzVault_Endogenous_2021B
    - mzCloud_Offline for mzVault_Endogenous-Autoprocessed_2021B
    - Bamba Lab 34 Lipid Mediators Library Stepped NCE 10 30 45
    - Bamba Lab 598 Polar Metabolites Stepped NCE 10 30 45
    - LipidBlast-VS68-Neg
    - LipidBlast-VS68-Pos
  - Mass lists
    - Arita Lab 6549 Flavonoid Structure Database
    - Chemical List PFASSTRUCT-2022-04-20
    - EFS HRAM Compound Database
    - Endogenous Metabolites Database 4400 Compounds
    - Extractables and Leachables HRAM Compound Database
    - LipidMaps Structure Database 2021-09-13
    - Natural Products Atlas_2020_06
    - PFAS NEG
    - PFAS NIST

- FISh Scoring—The workflow includes the FISh Scoring node, a structural confidence scoring and annotation tool for comparing the predicted fragments of expected compounds to the experimental fragmentation scans. This node adds a significant amount of processing time.
- Stats or Statistics—The workflow includes the Differential Analysis node. If you submit an analysis that does not include ratios, a warning message appears. If you do not want to run a differential analysis, you can ignore the warning and submit the run.

- Compound Class Scoring—The workflow includes the Compound Class Scoring node.

  IMPORTANT Before you can select the compounds classes for the node, you must add the fragment lists to the Compound Classes library.

- MMDF—The workflow includes the Filter By Mass Defect node.
- Background Removal—The targeted workflow includes the Mark Background Compounds node for filtering out expected compounds that are also found in the blank samples.

  Note All the untargeted workflows include the Mark Background Compounds node for filtering compounds detected in the blank samples.

- Pattern Scoring—The workflow includes the Pattern Scoring node.

Defined processing workflow templates

Tip To access these workflows from the Workflows page of an analysis, click **Open Common** from the command bar, open the Workflow Templates folder, open the folder for the applicable vertical market, and then select a template.

The following processing workflow templates are installed with the application:

- DegradantID folder
  - Degradants Related and Unknown ID w Database Searches
  - Degradants Unknown ID w Pattern Trace and Pattern Scoring
  - Degradants w Stats Related and Unknown ID w Database Searches
- EandL folder
  - E and L Expected w FISh Scoring
  - E and L Unknown ID with Online and Local Database Searches
  - E and L w Stats Unknown ID w Online and Local Database Searches
- Environmental folder
  - Environmental Expected w Transformation and FISh Scoring
  - Environmental Unknown ID w Online and Local Database Searches
  - Environmental w Stats Unknown ID w Online and Local Database Searches
- Food Research folder
  - Food Research Expected w FISh Scoring
  - Food Research Unknown ID w Online and Local Database Searches
  - Food Research w Stats Unknown ID w Online and Local Database Searches

- Forensics folder
  - Forensics Expected w FISh Scoring
  - Forensics Unknown ID w Compound Class Scoring and Database Searches
  - Forensics w Stats Unknown ID w Compound Class Scoring and Database Searches
- ImpurityID folder
  - Impurity ID Related and Unknown
  - Impurity ID w Stats Related and Unknown
- Lipidomics folder
  - Untargeted Lipidomics using Local Databases, LipidBlast in-silico library and LipidMaps database.cdProcessingWF
  - Untargeted Lipidomics using Online Databases, LipidBlast in-silico library and LipidMaps database.cdProcessingWF
- Metabolomics folder
  - Max ID - Detect Unknowns with ID Using Online Database Searches Single Sample
  - Untargeted Metabolomics Quick Detection Unknowns No ID
  - Untargeted Metabolomics using Online Databases, mzLogic, and Molecular Networks
  - Untargeted Metabolomics with Statistics Detect Unknowns with ID using Local Databases
  - Untargeted Metabolomics with Statistics Detect Unknowns with ID using Online Databases
  - Untargeted Metabolomics with Statistics Detect Unknowns with ID using Online Databases and mzLogic
- MetID folder
  - MetID Generate Inclusion List For Acquisition Pos Mode
  - MetID Generate Inclusion List For Acquisition Neg Mode
  - MetID Pattern Scoring with Background Removal
  - MetID w Stats Expected and Unknown w Background Removal
  - MetID w Stats Expected and Unknown w MMDF and Background Removal
  - MetID w Stats Expected w Background Removal
  - MetID w Stats Expected w FISh Scoring and Background Removal
- NaturalProduct
  - Natural Product Unknown ID w Online and Local Database Searches
  - Natural Product Unknown ID w Stats Online and Local Database Searches

- PFAS
  - PFAS Unknown ID w Database Searches and Molecular Networks.cdProcessingWF
- PolymerID
  - Unknown Polymer ID w Stats Online and Local Database Searches
  - Unknown Polymer ID with Online and Local Database Searches
- Stable Isotope Labeling folder
  - Stable Isotope Labeling w Metabolika Pathways and ID using Local Databases
  - Stable Isotope Labeling w Metabolika Pathways and ID using Online Databases

Create a completely new processing workflow for LC studies

A processing workflow is part of an analysis, and you can perform analyses only from inside a study. Therefore, to edit or create a processing workflow, you must open a study and start a new analysis or open an analysis template.

A processing workflow always begins with the Input Files node. All processing workflows that process MS data require the Select Spectra node. The only processing workflow that does not require the Select Spectra node is limited to processing the data from an analog detector.

❖ To create a completely new processing workflow from an empty Workflows page

1. Open the Workflows page. If the Workflows Tree area contains a processing workflow that you do not want to edit, click **Clear**.
2. Drag the required **Input Files** node from the Workflow nodes pane to the Workflow Tree pane.

   The Input Files node reads the information in the raw data files.
3. To process the spectral data, drag the **Select Spectra** node to the Workflow Tree pane.

   The Input Files node automatically connects to the Select Spectra node. The Select Spectra node reads and filters the MS scan data in the raw data files. The default parameter settings pass all the scan data to the next node.
4. To align multiple input files, drag the **Align Retention Times (ChromAlign)** node to the Workflow Tree pane. Then, connect the Select Spectra node to the alignment node.

   IMPORTANT The new Align Retention Times (ChromAlign) node is more rugged than the original alignment node. So for most analyses, use the Align Retention Times (ChromAlign) node instead of the Align Retention Times node. The original alignment node is available for comparing the results from previous data sets to new data sets of similar samples.

The alignment node chromatographically aligns the MS scan data in the input files. The Align Retention Times (ChromAlign) node

IMPORTANT For analyses with multiple input files, always add one of the alignment nodes to the processing workflow.

5. To find expected compounds, do the following:
   a. Check whether your Expected Compounds library contains the compounds of interest. To open the Expected Compounds library, choose **Lists & Libraries > Expected Compounds** from the application menu bar.
   b. Drag the **Find Expected Compounds** node to the Workflow Tree pane. Then, connect the alignment node to it.

      Note The Find Expected Compounds node accepts input from any of the Spectrum Processing nodes.

   c. Drag one or more **Generate Expected Compounds** nodes to the Workflow Tree pane.

      - To apply different transformation rules to multiple compounds, drag multiple Generate Expected Compounds nodes to the Workflow Tree pane, one for each set of rules.
      - To apply the same transformation rules to one or more compounds, drag a single Generate Expected Compounds node to the Workflow Tree pane.

      IMPORTANT The Generate Expected Compounds node generates a list of expected compounds by using one or more user-specified library compounds and a set of user-specified chemical reactions.

      The Compounds parameter is empty until you select the compounds of interest. If you submit an analysis to the job queue without selecting the compounds of interest, a Caution symbol appears.

   d. For each Generate Expected Compounds node, select the compounds of interest. See "Generate Expected Compounds node."
   e. Connect the Generate Expected Compounds node or nodes to the Find Expected Compounds node.
   f. Drag the **Group Expected Compounds** node to the Workflow Tree pane.

      The Find Expected Compounds node automatically connects to it.

   g. To add FISh scoring to the processing workflow for targeted compounds, drag the **FISh Scoring** node to the Workflow Tree pane.

      The Group Expected Compounds node automatically connects to it.

      Note FISh scoring adds a significant amount of processing time to an analysis.

h. Do one of the following:

- To detect unknown compounds in addition to the expected compounds, go to step 6.
- To merge the features found by the Expected Compounds node and detected by the Unknown Compounds node, go to step 12.

6. To detect unknown compounds, do the following:

   a. Drag the **Detect Compounds** node to the Workflow Tree pane. Then, connect the alignment node to the Detect Compounds node.

   b. Drag the **Group Compounds** node to the Workflow Tree pane.

      The Detect Compounds node automatically connects to it.

7. For statistical analyses, drag the **Fill Gaps** node to the Workflow Tree pane.

   The Group Compounds node automatically connects to it.

   Note If the processing workflow does not include the Apply SERRF QC Correction node, you can use the Apply Missing Value Imputation node instead of the Fill Gaps node. Because the Group Compounds node does not automatically connect to the Apply Missing Value Imputation node, you must manually connect the Group Compounds node to the Apply Missing Value Imputation node.

8. To correct for batch effects, connect the Fill Gaps node to the Apply QC Corrections node. Or, if the input files for the analysis are from more than one continuous batch, connect the Fill Gaps node to the Apply SERRF QC Correction node.

   If the analysis does not include quality control samples, the application ignores the QC correction node.

9. To identify unknown compounds, add identification nodes to the processing workflow. As you drag an identification node into the Workflow Tree pane, the Group Compounds node automatically connects to it.

   a. Drag the **Predict Compositions** node to the Workflow Tree pane.

      IMPORTANT For best results, always include the Predict Compositions node in a processing workflow for untargeted compounds. Without the Predict Compositions node, the workflow does not report the elemental compositions of the unknown compounds without a hit from the online search databases or the local Metabolika database.

   b. To assign a name, formula, and structure to the compounds in the Compounds table, drag the **Assign Compound Annotations** node to the Workflow Tree pane.

   c. (Optional) To search the online ChemSpider database, drag the **Search ChemSpider** node to the Workflow Tree pane.

d. (Optional) To search mass lists, drag the **Search Mass Lists** node to the Workflow Tree pane. In the Workflow Tree pane, select the **Search Mass Lists** node, and then, in the parameters pane, select the appropriate mass lists.

e. (Optional) To search the online mzCloud database, drag the **Search mzCloud** node to the Workflow Tree pane.

f. (Optional) To search your local mzVault database, drag the **Search mzVault** node to the Workflow Tree pane. In the Workflow Tree pane, select the **Search mzVault** node, and then, in the parameters pane, select libraries from the mzVault Library list.

10. To map detected compounds to a biochemical pathway, add pathway mapping nodes to the processing workflow. As you drag a pathway mapping node into the Workflow Tree pane, the Group Compounds node automatically connects to it.

    - To search the local Metabolika pathways, drag the **Map to Metabolika Pathways** node to the Workflow Tree pane.
    - To search the KEGG database, drag the **Map to KEGG Pathways** node to the Workflow Tree pane.
    - To search the BioCyc database, drag the **Map to BioCyc Pathways** node to the Workflow Tree pane.

11. To rank the hits from the Search ChemSpider node, Map to Metabolika Pathways node, Search Mass Lists node, and Map to BioCyc Pathways node, drag the Apply mzLogic node to the Workflow Tree pane.

    When present, the Search ChemSpider node, Map to Metabolika Pathways node, Search Mass Lists node, and Map to BioCyc Pathways node automatically connect to the Apply mzLogic node.

12. To compare the features found by the Find Expected Compounds and Detect Compounds nodes if applicable, drag the **Merge Features** node to the Workflow Tree pane.

    The Find Expected Compounds and Detect Compounds nodes automatically connect to the Merge Features node.

13. To add Trace Creation nodes to the processing workflow, do the following:

    - For each UV, PDA, or analog trace that you want to extract, drag a **Create Analog Trace** node from the Workflow Nodes pane to the Workflow Tree pane.

      The Input Files node automatically connects to the Create Analog Trace node.

    - For each pattern trace that you want to extract, drag a **Create Pattern Trace** node to the Workflow Tree pane. Then, connect the Align Retention Times (ChromAlign) node to each Create Pattern Trace node.
    - For each Fragment Ion Search (FISh) trace that you want to create, drag a **Create FISh Trace** node to the Workflow Tree pane. Then, connect the Align Retention Times (ChromAlign) node to each Create FISh Trace node.

- For each mass trace that you want to extract, drag a **Create Mass Trace** node to the Workflow Tree pane. Then, connect the Align Retention Times (ChromAlign) node to each Create Mass Trace node.

14. In the Post-Processing Nodes pane, do the following:
    - To add a differential analysis (volcano plot) to the workflow for the specified sample groups and ratios, drag the **Differential Analysis** node to the Post-Processing Nodes pane below the Workflow Tree pane.
    - To add the descriptive statistics columns to the Compounds and Expected Compounds tables in the result file, drag the **Descriptive Statistics** node to the Post-Processing Nodes pane below the Workflow Tree pane. The descriptive statistics columns provide information about the chromatographic peak areas (mean area, median area, minimum area, quartile areas, standard deviation and relative standard deviation of the areas) for each detected compound.

      Note In a result file, the descriptive statistics columns are hidden by default.

15. To export the MS scan data in the raw data files to a common data format, drag an **Export Spectra** node to the Workflow Tree pane. Then, connect one of these nodes to the Export Spectra node:
    - Select Spectra
    - Align Retention Times

    Note The Export Spectra node does not export analog data.

For details about each workflow node, see Chapter 7, "Workflow nodes."

Connect the workflow nodes for an LC study

For details about the workflow node connections, see these topics:

- Manually connect the workflow nodes
- Peak area refinement node connections
- Input and output nodes for the workflow nodes

Manually connect the workflow nodes

For an LC study, most but not all the processing workflow nodes automatically connect to the appropriate input and output nodes.

When you add any of the following nodes to a processing workflow, you must connect them manually:

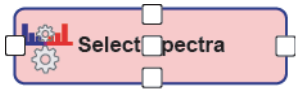
- Any of the spectrum processing nodes (except for the Select Spectra node)
- Any of the trace creation nodes (except for the Create Analog Trace node)
- Generate Expected Compounds node (connects to the Find Expected Compounds node)
- Input spectrum processing node to the Detect Compounds node
- Any of the peak area refinement nodes

For LC studies, you can use the following nodes multiple times in a processing workflow: the Generate Expected Compounds node, all the Trace Creation nodes, the Mark Background Compounds node, and all the Spectrum Processing nodes, except for the Align Retention Times node.

❖ To connect the workflow nodes

1. Point to the input node of interest.

   Five white boxes appear, with one box at the center of the node and the other boxes at the center of each side.



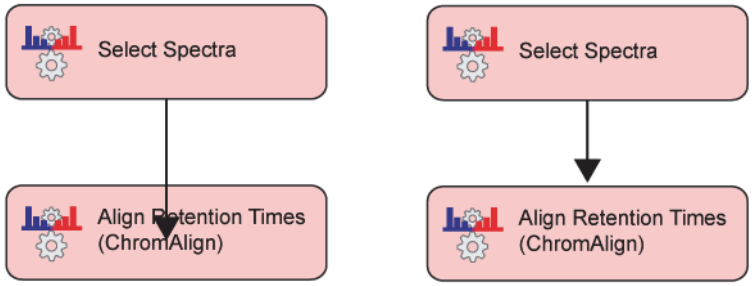
2. Click one of the white boxes and hold down the mouse button until a red border and an arrowhead appear.

3. Continue holding down the mouse button as you drag the arrowhead to the output node of interest.

Depending on the compatibility, one of the following occurs:

- If the selected input node is not compatible with the output node, a red border appears around the output node.
- If the selected input node is compatible with the output node, a green border appears around the output node. When you release the mouse button, a directional arrow connects the input node to the output node.

Figure 80. Connecting the Select Spectra node to the Align Retention Times node (LC study)



4. To automatically format the layout of the workflow nodes, click **Auto Layout** in the Workflows command bar.

Peak area refinement node connections

(For LC studies) This topic describes how to make the appropriate node connections for an untargeted processing workflow that includes the Fill Gaps node and any of the peak area refinement workflow nodes: Apply QC Correction, Mark Background Compounds, Normalize Areas, and Scale Areas.

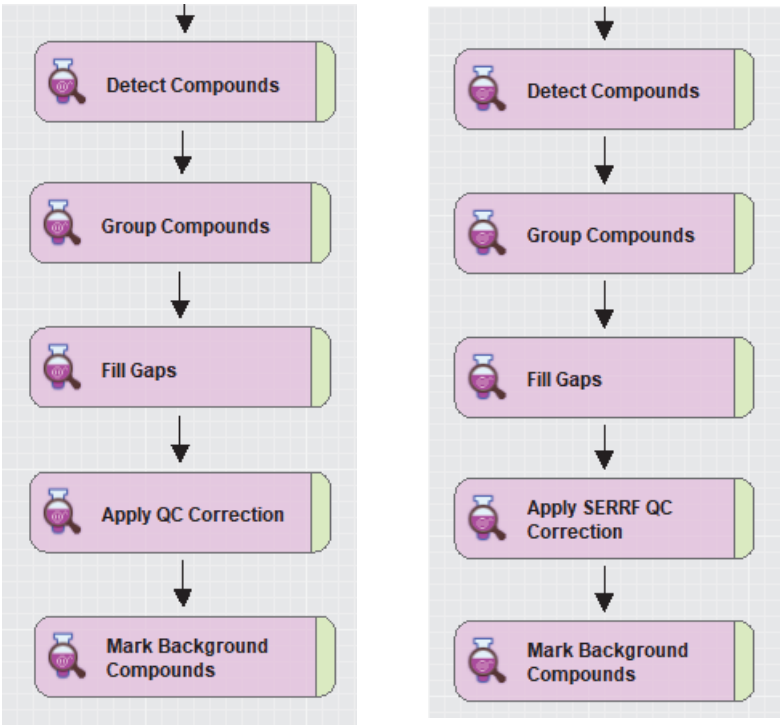
Note None of the provided processing workflow templates include the Normalize Areas node or the Scale Areas node. Thermo Fisher Scientific recommends using QC samples and the appropriate QC correction node to correct for batch errors.

The Fill Gaps node takes input only from the Group Compounds node, and the Group Compounds node automatically connects to it.

When you add any of the other peak area refinement nodes, you must make the appropriate connections.

The processing workflow templates provided with the application use the following peak refinement nodes in this connection order—Fill Gaps > Apply QC Correction or Apply SERRF QC Correction > Mark Background Compounds.

Figure 81. Suggested connection order for the peak area refinement nodes



If you add the Normalize Areas node to your processing workflow templates, the appropriate input and output connections depend on whether your blank samples are solvent blanks or matrix blanks:

- If the blanks are solvent blanks, connect the nodes in this order:

  Group Compounds > Fill Gaps > Apply SERRF QC Correction or Apply QC Correction > Mark Background > Normalize Areas

  IMPORTANT Do not use the Apply Missing Value Imputation node with either of the QC correction nodes. Use the Fill Gaps node instead.

  The Apply Missing Value Imputation node only imputes the missing peak area values—whereas, the Gap Filling node actually re-detects missing peaks by performing peak detection at a very low threshold.

  Because the Gap Filling node detects actual peaks, it provides more accurate results than the Apply Missing Value Imputation node. More of the gap-filled compounds will pass the RSD filter in the QC correction nodes and therefore have a QC correction applied to them.

- If the blanks are matrix blanks, connect the nodes in this order:

  Group Compounds > Fill Gaps > Apply SERRF QC Correction or Apply QC Correction> Normalize Areas > Mark Background.

If you add the Scaling Factor node, add it to the end of the processing workflow template.

Input and output nodes for the workflow nodes

Table 33 describes the node connections for the workflow nodes in an LC study.

Table 33. Input and output nodes for each workflow node in an LC study (Sheet 1 of 4)

Workflow node	Input nodes	Output nodes
1. Input/Output		
Export Spectra node	Select Spectra	Filter Centroids
Input Files (Begins every processing workflow)	None	• Select Spectra • Create Analog Trace
2. Spectrum Processing		
Align Retention Times node	Spectrum Processing	• Spectrum Processing • Trace Creation • Find Expected Compounds • Detect Compounds
Filter Centroids node	• Spectrum Processing	• Spectrum Processing • Trace Creation • Find Expected Compounds • Detect Compounds
Filter By Mass Defect node	• Spectrum Processing • Generate Expected Compounds	• Spectrum Processing • Trace Creation • Find Expected Compounds • Detect Compounds
Filter By Scan Event node	Spectrum Processing	• Spectrum Processing • Trace Creation • Find Expected Compounds • Detect Compounds
Select Spectra node	Input Files	• Spectrum Processing • Trace Creation • Find Expected Compounds • Detect Compounds
3. Trace creation		
Create Analog Trace node (LC studies)	Input Files	None
Create Mass Trace node (LC studies)	Spectrum Processing	None
Create FISh Trace node (LC studies)	Spectrum Processing	None
Create Pattern Trace node (LC studies)	Spectrum Processing	None
4. Expected Compounds		
FISh Scoring node (LC studies)	Group Expected Compounds	None

Table 33. Input and output nodes for each workflow node in an LC study (Sheet 2 of 4)

Workflow node	Input nodes	Output nodes
Find Expected Compounds node	• Generate Expected Compounds • Spectrum Processing	• Group Expected Compounds • Merge Features
Find Expected Compounds (Legacy) node	• Generate Expected Compounds • Spectrum Processing	• Group Expected Compounds • Merge Features
Generate Expected Compounds node	None	• Find Expected Compounds • Filter By Mass Defect
Group Expected Compounds node	Find Expected Compounds	• FISh Scoring • Mark Background Compounds
Merge Features node	• Find Expected Compounds • Detect Compounds	None
5. Compound Detection		
Analyze Labeled Compounds node	Assign Compound Annotations	None
Detect Compounds node	Spectrum Processing	• Group Compounds • Merge Features
Detect Compounds (Legacy) node	Spectrum Processing	• Group Compounds • Merge Features
Fill Gaps node	Group Compounds	Any of the peak area refinements nodes (except the Apply Missing Value Imputation node)
Group Compounds node	Detect Compounds	• Compound Identification • Pathway Mapping • Fill Gaps • Mark Background Compounds
6. Peak Area Refinement		
IMPORTANT For information about connecting the peak area refinement nodes in the correct input–output order, see "Peak area refinement node connections."		
Apply Missing Value Imputation node	One of these: • Group Compounds • Normalize Areas • Scale Areas • Apply QC Correction **IMPORTANT** Do not use the Apply Missing Value Imputation node with the QC correction nodes.	One of the other peak area refinement nodes. The most common output nodes are either one of the QC correction nodes or the Mark Background Compounds node. None of the provided processing workflow templates for LC studies include the Apply Missing Value Imputation node.

Table 33. Input and output nodes for each workflow node in an LC study (Sheet 3 of 4)

Workflow node	Input nodes	Output nodes
Apply QC Correction node	Fill Gaps	Normalize Areas or Scale Areas (Connecting the Apply QC Correction node to the Normalize Areas node or the Scale Areas node is not recommended.)
Apply SERRF QC Correction node	Fill Gaps	Normalize Areas or Scale Areas (Connecting the Apply SERRF QC Correction node to the Normalize Areas node or the Scale Areas node is not recommended.)
Mark Background Compounds node	One of these: • Group Expected Compounds • Group Compounds • Peak refinement node	Typically the last node in the processing workflow
Normalize Areas node	See "Peak area refinement node connections."	–
Scale Areas node	• Group Compounds • Fill Gaps • Mark Background Compounds • Apply QC Correction • Apply SERRF QC Correction	None
	Tip To use the Scales Areas node, the study must include assigned values for a numeric study factor.	
7. Compound Identification		
Assign Compound Annotations node	Group Compounds	None
Predict Compositions node	Group Compounds	None
Search ChemSpider node	• Group Expected Compounds • Group Compounds	None
Search Mass Lists node	• Group Expected Compounds • Group Compounds	None
Search mzCloud node	• Group Expected Compounds • Group Compounds	None
Search mzVault node	• Group Expected Compounds • Group Compounds	None

Table 33. Input and output nodes for each workflow node in an LC study (Sheet 4 of 4)

Workflow node	Input nodes	Output nodes
8. Pathway Mapping		
All	• Group Expected Compounds • Group Compounds	None
9. Compound Scoring		
Apply Spectral Distance node	• Search Mass Lists • Search ChemSpider • Map to KEGG Pathways • Map to Metabolika Pathways • Map to BioCyc Pathways	None
Apply mzLogic node	• Search Mass Lists • Search ChemSpider • Map to Metabolika Pathways • Map to BioCyc Pathways	None
Calculate Mass Defect node	Group Compounds	None
Compound Class Scoring node	Group Compounds	None
Generate Molecular Networks node	Assign Compound Annotations	None
Pattern Scoring node	Group Compounds	None
Search Neutral Mass Losses node	Group Compounds	None
10. Post-Processing (white nodes)		
Descriptive Statistics node	None	None
Differential Analysis node	None	None
Export Xcalibur Inclusion or Exclusion List node	None	None
Result Exporter	None	None
Scripting Node	None	None

Save a custom processing workflow as a template

You can run an analysis without saving the processing workflow in the Workflow Tree pane; however, you might want to save the processing workflow to a template for reuse. When you save the processing workflow as a template, the application does not automatically store it in the study folder. You can save a processing template to the Common Templates folder or a folder of your choice.

Note When you run an analysis, the application automatically saves the processing workflow to the result file. Selecting a result file on the Analysis Results page of a study and clicking **Reprocess** opens the processing workflow saved with the result file.

❖ To save a custom processing workflow as a template

1. Do one of the following:
   - To save the template in the Common Templates folder, click **Save Common**.

     The Save Workflow dialog box opens to the Common Templates folder.
   - To save the template, click **Save**.

     The Save Workflow dialog box opens to the last opened folder.
2. Select the folder where you want to store the template, name the template, and click **Save**.

   If the processing workflow is valid, the application saves the template with the file name extension.cdProcessingWF. If the processing workflow contains an error, an error message box opens.
3. If the Exporting Template Workflow Failed message box opens, read the list of errors, close the message box, fix the errors, and click **Save**.

Use the Workflows page (in any study) to create or edit processing workflows. The Workflows page is a tabbed page to the right of the Grouping & Ratios page and is available only when the Analysis view is open.

7

Workflow nodes

A processing workflow consists of a set of connected workflow nodes, and each workflow node has a set of associated parameters. To create and edit processing workflows, see Chapter 6, "Create and edit processing workflows."

Note For information about the workflow nodes for GC studies, refer to the *Compound Discoverer User Guide for GC Studies* or the Help system.

In the Compound Discoverer 3.3.x application, Thermo Fisher Scientific has improved the functionality of the Detect Compounds and Find Expected Compounds nodes, which now require fewer if any custom parameter settings.

To support legacy processing workflows, the Workflow Nodes pane still includes the Detect Compounds (Legacy) and the Find Expected Compounds (Legacy) nodes.

The Align Retention Times (ChromAlign) and Result Exporter nodes were added in the Compound Discoverer 3.3.0 application.

The processing workflow templates use the improved Detect Compounds and Find Expected Compounds nodes and the new Align Retention Times (ChromAlign) node.

In the Workflow Nodes pane on the Workflows page, the workflow nodes are organized into functional groups. For information about the workflow nodes, see the following topics:

Input and Output nodes

For LC studies, the Input/Output area in the Workflow Nodes pane on the Workflows page of an analysis includes these nodes:

- Export Spectra node
- Input Files node

Note All processing workflows begin with the Input Files node.

Export Spectra node

Use the Export Spectra node to export all or a subset of the mass spectrum scans in an Xcalibur RAW file to an open-source format file. The Export Spectra node does not export the data from analog detectors.

Note You can add multiple Export Spectra nodes to a processing workflow.

The Export Spectra node requires input from one of the data processing nodes. The processing workflow shown in Figure 82 reads the input files, extracts the MS scans of interest, and exports the data to an open source format file. Running this processing workflow does not require an active software license.

Figure 82. Minimum processing workflow for the Export Spectra node

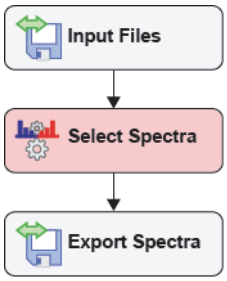


Table 34 describes the parameters for the Export Spectra node.

Table 34. Export Spectra node parameters (Sheet 1 of 2)

Parameter	Description
1. Output Data	
File Name	Specifies the file name of the exported file. If you leave this box empty, the node uses the result file name.
File Name Suffix	Specifies the suffix that the application appends to the file name of the exported file.

Table 34. Export Spectra node parameters (Sheet 2 of 2)

Parameter	Description
Export Format	Specifies the data format of the exported file. Selections: • Mascot Generic Format (*.mgf)—Generates an MGF file, which lists the MS scans by retention time. The scan data for each time point consists of two columns: mass and intensity. • mzDATA (*mzData)—Generates an XML-based file that third-party mass spectrometry software packages can read. • mzML (*mzML)—Generates an XML-based file that third-party mass spectrometry software packages can read.

Input Files node

Every processing workflow must begin with the Input Files node. This node has no parameters.

To view information about the input files for a result file, open its Input Files table.

Spectrum Processing nodes

The nodes under Spectrum Processing extract the mass spectral data from the input file set.

For an LC study, the following workflow nodes are available in the Spectrum Processing area of the Workflow Nodes pane:

- Align Retention Times node
- Align Retention Times (ChromAlign)
- Filter By Mass Defect node
- Filter By Scan Event node
- Filter Centroids node
- Select Spectra node

Align Retention Times node

For LC studies, use the Align Retention Times node for chromatographic alignment of multiple input files. The Align Retention Times node compensates for small differences in the retention times of the components in a sequence of sample runs.

IMPORTANT In the spectrum processing node that supplies spectra to the Alignment, do not apply a scan filter that excessively reduces the retention time window, as doing so might cause an alignment failure. The Align Retention Times node requires a minimum amount of representative scan data to chromatographically align the input files in an analysis.

Note The Align Retention Times node generates the File Alignments result table. When you open a result file from an analysis that included the Align Retention Times node, the Retention Time Correction view is available.

For details, see these topics:

- Retention Time Corrections view
- File Alignments table

Table 35 describes the parameters for the Align Retention Times node.

Table 35. Align Retention Times node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Alignment Model	Specifies the curve-fitting algorithm for chromatographically aligning the input files. Default: Adaptive Curve Selections: • Adaptive Curve—Calculates a flexible curve for the retention time shift for each retention time point for a compound. • Linear—Uses a linear function to fit all the retention time points for a compound.

Table 35. Align Retention Times node parameters (Sheet 2 of 2)

Parameter	Description
Alignment Fallback	Specifies the alternate model to apply when the Adaptive Curve regression model fails. Default: Use Linear Model Selections: • None—There is no alternative. Continue to use the Adaptive Curve model. • Don't Align—Do not chromatographically align the input files. • Use Linear Model—Use the Linear model instead of the Adaptive Curve model.
Maximum Shift [min]	Specifies the maximum retention time shift between the alignment features (chromatographic peaks with the same *m/z* × RT dimensions) in the input files. Default: 2 (± 2 minutes for each feature); range: 0.01–4.0
Shift Reference File	Specifies whether to shift the retention time of all the detected features to eliminate any negative retention time values in the input file set. Default: True Selections: • True: If the data set includes features with negative retention times, the algorithm shifts all of the features to avoid cropping. • False: Removes features with negative retention time values from the analysis (crops the feature from the feature list passed to the connected nodes).
Mass Tolerance	Specifies the mass tolerance to be used for feature matching. Default: 5.0 ppm; range: 0.1–50 ppm
Remove Outlier	Specifies whether the retention time algorithm ignores outlier landmark features. Default: True

Align Retention Times (ChromAlign)

Table 36 describes the parameter for the Align Retention Times node.

Table 36. Align Retention Times node parameter

Parameter	Description
1. General Settings	
Reference File	Specifies the input file that the analysis aligns all other input files to. When you leave this parameter setting empty, the application automatically uses the first QC file as the reference file. If the analysis does not include any QC files, the application automatically uses the first sample file. In the result file that the analysis generates, the Statistical Methods table lists the reference file.

Filter By Mass Defect node

For LC studies, use the Filter By Mass Defect node to keep or remove mass spectral peaks (centroids) in the full (MS1) scan data that fall within a set of specified mass tolerance and mass defect windows.

You can add multiple Filter By Mass Defect nodes to a processing workflow.

To specify the elemental compositions for the node, you can enter the elemental compositions in the Custom Compositions area of the node, or you can use the Generate Expected Compounds node to provide the compositions.

Tip For more information about mass defects, see "Mass defect types and visualization techniques."

Table 37 describes the parameters for the Filter By Mass Defect node.

Table 37. Filter By Mass Defect node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Filter Direction	Specifies whether the selected mass defect filter keeps or removes mass spectral peaks (centroids) from further processing. Default: Keep; Selections: Keep or Remove
Mass Defect Type	Specifies the mass defect type. Default: Standard Mass Defect Selections: Fractional Mass = exact mass – floor (exact mass) Standard Mass Defect = exact mass – nominal mass $\text{Relative Mass Defect} = \frac{1e6 \times (\text{exact mass} - \text{nominal mass})}{(\text{exact mass})}$ Kendrick Mass Defect = Kendrick mass – nominal Kendrick mass Where: Exact mass = Monoisotopic mass of the elemental composition Nominal mass = Integer mass Calculates the integer mass using the selected rounding function (floor, ceiling, or round) $\text{Kendrick Mass} = \text{exact mass} \times \frac{\text{nominal mass of Kendrick formula}}{\text{exact mass of Kendrick formula}}$
Kendrick Formula	When you select the Kendrick Mass Defect type, this user-specified elemental composition specifies the Kendrick formula.
Nominal Mass Rounding	Specifies how the node calculates nominal masses. Default: Floor Selections: • Floor rounds down. • Ceiling rounds up. • Round rounds to the nearest integer value.

Table 37. Filter By Mass Defect node parameters (Sheet 2 of 2)

Parameter	Description
2. Tolerances	
Using the calculated mass defect values calculated and the exact mass values calculated from the elemental composition input, these mass tolerance values define the rectangular mass defect filters.	
Mass Tolerance	The input from the data processing nodes is a table of *m/z* values and intensities for each full (MS1) scan. Specifies the mass tolerance for the ions that the filter removes or passes through to the next node. Default: 50 Da; Selection: 0 to 6000 Da
Mass Defect Tolerance	Specifies the mass defect tolerance for the ions that the filter removes or passes through to the next node. Default: 0.025 (Da or unit-less for the Relative Mass Defect selection) Range: 0–No limit
3. Custom Compositions	
Composition (5 entry boxes)	Specify the elemental compositions that the node uses to create the mass defect filters. Leave these boxes empty if you want to use one or more Generate Expected Compounds nodes to generate the list of elemental compositions.
Ions	Specifies the ion definitions to be used with the custom compositions. For each elemental composition, the node creates one mass defect filter for each ion definition—that is, if you select five ion definitions, the node creates five mass defect filters for each elemental composition. Select the ion definitions from the dropdown list. Use the Ion Definition Editor to create new ion definitions.

Filter By Scan Event node

For LC studies, use the Filter By Scan Event node to filter the mass spectra by scan events.

Table 38 describes the parameters for the Filter By Scan Event node.

Table 38. Filter By Scan Event node parameters (Sheet 1 of 3)

Parameter	Description
Filter Settings	
Mass Analyzer	Specifies the mass analyzer that the instrument used to acquire the scan. A Thermo Scientific hybrid mass spectrometer, such as the LTQ Orbitrap mass spectrometer, contains two mass analyzers and can acquire both ITMS (low-resolution) and FTMS (high-resolution) scans in one data file. Filter selection: Any, Is, Is Not; default: (Not Specified)—The application does not filter scan events by the mass analyzer that was used to acquire the data. Check box selections: • Ion Trap (ITMS) • Fourier Transform (FTMS)) • Time of Flight (TOFMS) • Single Quad (SQMS) • Triple Quad (TSMS) • Sector Field (SectorMS)
MS Order	Specifies the MS order (scan power that the instrument used) of the scans that you want the node to filter. Filter selection: Any, Is, Is Not; default: (Not Specified)—The node does not filter the scans by MS order. Check box selections: MS1–MS7 **Note** The Detect Compounds and Find Expected Compounds nodes search the full (MS1) scans for mass peaks. If you filter out the MS1 scans by selecting Is MS2 or higher for the MS Order, the result tables for these nodes are empty.

Table 38. Filter By Scan Event node parameters (Sheet 2 of 3)

Parameter	Description
Activation Type	Specifies the activation types that the instrument used to produce the product ion spectra. Filter selection: Any, Is, Is Not; default: (Not Specified)—The node does not filter the scans by activation type. Check box selections: • CID (Collision Induced Dissociation) • MPD (Multi Photon Dissociation) • ECD (Electron Capture Dissociation) • PQD (Pulsed Q Collision Induced Dissociation) • ETD (Electron Transfer Dissociation) • HCD (Higher Energy Collision Dissociation) • EThcD (ETD With Supplemental HCD) • UVPD (Ultra Violet Photo Dissociation) • Any Activation Type
Min. Collision Energy	Specifies the minimum Normalized Collision Energy™ for a higher-order scan to pass through the filter. Default: 0 (no filtering); Minimum value: 0; Maximum value: unchecked
Max. Collision Energy	Specifies the maximum Normalized Collision Energy for a higher-order scan to pass through the filter. Default: 1000; Minimum value: 0; Maximum value: 1000

Table 38. Filter By Scan Event node parameters (Sheet 3 of 3)

Parameter	Description
Scan Type	Specifies the scan type for the scan event that the instrument used to produce the product ion. Filter selection: Any, Is, Is Not; default: (Not Specified)—The node does not filter the scan events by scan type. Check box selections: • Full • Single Ion Monitoring (SIM) • Single Reaction Monitoring (SRM)
Polarity Mode	Specifies the polarity mode for the scan. Filter selection: Any, Is, Is Not Default: (Not Specified)—The node does not filter the scan events by polarity mode. Check box selections: • Positive • Negative

Filter Centroids node

Use the Filter Centroids node to remove mass spectral peaks (centroids) that are below a user-specified intensity threshold from the mass scans, below a user-specified signal-to-noise threshold for FTMS scans, or both.

Table 39 describes the parameters for the Filter Centroids node.

Table 39. Filter Centroids node parameters

Parameter	Description
1. General	
S/N Threshold (for FT-only)	Specifies the minimum signal-to-noise threshold for each centroid in an FTMS scan. The node excludes centroids from the analysis that are below this intensity value. The application uses the spectrum noise reported by an instrument. Default: 1.5
Minimum Intensity Threshold	Specifies the minimum intensity threshold for the mass spectral peaks (centroids). The node excludes centroids from the analysis that are below this intensity value. Default: 0 (no filtering)

Select Spectra node

The raw data file (Xcalibur RAW file) contains the mass spectral scans that the Thermo Scientific mass spectrometer acquired and, for LC/MS data, any optional data acquired by a PDA, UV-VIS, or analog detector during the acquisition run. The Select Spectra node can read and filter the mass spectral scan data. The Select Spectra node cannot read the optional data acquired by a PDA, UV-VIS, or analog detector.

The mass spectral scans are numbered 1, 2, 3, and so on in single integer increments from the beginning to the end of the acquisition run. Use the Select Spectra node to select the scans that you want the application to process. Limiting processing to the scans of interest decreases processing time and minimizes false positives. For example, if you know the retention time of the compounds of interest, exclude scans that fall outside a specific retention time window.

IMPORTANT For LC studies, the default parameter settings for the Select Spectra node are appropriate for most analyses. When using settings other than the defaults, follow these guidelines:

- Because the application uses the full (MS1) scans to measure the accurate mass and isotope patterns of the mass spectral peaks, do not filter out the full (MS1) scans when the processing workflow includes any of these nodes:
  - Find Expected Compounds
  - Find Expected Compounds (Legacy)
  - Detect Compounds
  - Detect Compounds (Legacy)
- The following nodes require a representative amount of data to function properly:
  - Align Retention Times
  - Align Retention Times (ChromAlign)
  - Find Expected Compounds
  - Find Expected Compounds (Legacy)

  If you excessively reduce the retention time window (for example, by using an RT or scan number range), the chromatographic alignment algorithm (for the alignment nodes) and the automatic peak width detection algorithm (for the find expected compounds nodes) might fail to produce satisfactory results.

Table 40 describes the parameters in the Select Spectra node.

Table 40. Select Spectra node parameters (Sheet 1 of 9)

Parameter	Description
1. Spectrum Properties Filter	
The only basic parameters in this group are the lower and upper RT limits.	
Note The retention time filter excludes scans outside the specified limits; however, the application does not check the validity of the retention time settings against the actual acquisition time for the raw data file. When both the lower and upper RT limits are set to 0 (default), the application does not use retention time to filter scans.	
Lower RT Limit	Excludes scans acquired before the user-specified retention time. Default: 0; Minimum value: 0; Maximum value: Unchecked

Table 40. Select Spectra node parameters (Sheet 2 of 9)

Parameter	Description
Upper RT Limit	With the exception of a setting of 0, excludes scans that were acquired after the user-specified retention time. Default: 0; Minimum value: 0; Maximum value: Unchecked
Note The scan number filter excludes scans outside the specified limits—however, the application does not check the validity of the scan number settings against the actual scan numbers in the raw data file. When both the first and last scan number are set to 0 (default), the application does not filter scans by scan number. When filtering by scan number, verify the scan number range in Thermo Scientific application where you can browse the mass spectra, such as FreeStyle.	
First Scan	Specifies the scan number of the first available scan that you want the node to process. When this parameter is set to 0, the node processes the first scan that passes through the other filters. When this parameter is set to a value that is greater than the last available scan number, the node filters out all of the scans. Default: 0 (no filtering) Minimum value: 0; Maximum value: Unchecked
Last Scan	Specifies the last available scan number that you want the node to process. When this parameter is set to 0 or a value that is greater than the last available scan number, the node processes the last scan that passes through the other filters. Default: 0 (no filtering); Minimum value: 0; Maximum value: Unchecked

Table 40. Select Spectra node parameters (Sheet 3 of 9)

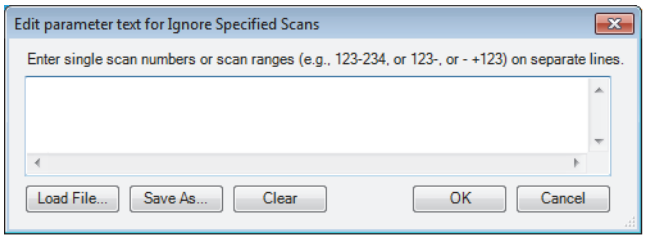
Parameter	Description
Ignore Specified Scans	Specifies the scan numbers that the analysis ignores. Placing the cursor in the Ignore Specified Scans box and clicking the More icon, ..., opens the Edit Parameter Text for Ignore Specified Scans dialog box. Use this dialog box to do any of the following: • Manually enter the scan numbers to ignore. • Load a text file that lists the scan numbers to ignore. • Create and save a list of scan numbers to ignore. 
Note The charge state filter excludes higher-order scans of precursor ions with a charge state that is outside the specified limits. The charge state filter does not affect the MS1 scans.	
Lowest Charge State	Excludes higher-order scans of precursor ions with a lower charge state than the specified charge state. Default: 0; Minimum: 0
Highest Charge State	Filters out scans from precursor ions with a higher charge state than the specified charge state. Default: 0 (specifies no upper limit)
Min. Precursor Mass	Specifies the minimum precursor mass for a higher-order scan. Default: 0 (no filtering); Minimum value: 0; Maximum value: Unchecked
Max. Precursor Mass	Specifies the maximum precursor mass for a higher-order scan. Default: 0 (no filtering); Minimum value: 0; Maximum value: Unchecked
Total Intensity Threshold	Excludes scans that fall below the specified total intensity threshold. The total intensity of a mass spectrum is the summed intensity of its mass spectrum peaks (centroids).

Table 40. Select Spectra node parameters (Sheet 4 of 9)

Parameter	Description
Minimum Peak Count	Specifies the minimum number of mass spectrum peaks (centroids) that must be in the spectrum for the scan to pass through the filter. Minimum value: 1; Maximum value: Unchecked
2. Scan Event Filters The only basic parameter in this group is Polarity Mode.	
Mass Analyzer	Specifies the mass analyzer that the instrument used to acquire the scan. An LTQ Orbitrap hybrid mass spectrometer can acquire both ITMS (low-resolution) and FTMS (high-resolution) scans in one data file. Filter selection: Any, Is, Is Not; default: (Not Specified)—The node does not filter scan events by the mass analyzer used to acquire the data. Check box selections: • Ion Trap (ITMS) • Fourier Transform (FTMS)) • Time of Flight (TOFMS) • Single Quad (SQMS) • Triple Quad (TSMS) • Sector Field (SectorMS)
MS Order	Specifies the MS order of the scans that you want the node to process. Filter selection: Any, Is, Is Not; default: Any—The application does not filter the scans by MS order. Check box selections: MS1–MS7
IMPORTANT The Detect Compounds and Find Expected Compounds nodes search the MS1 scans for mass peaks. If you filter out the MS1 scans by selecting Is MS2 or higher for the MS Order, the result tables for these nodes are empty.	

Table 40. Select Spectra node parameters (Sheet 5 of 9)

Parameter	Description
Activation Type	Specifies the activation type that the instrument used to produce the product ion spectra. Filter selection: Any, Is, Is Not; default: (Not Specified)—The node does not filter the scans by activation type. Check box selections (as displayed in the drop-down list): • CID (Collision Induced Dissociation) • MPD (Multi Photon Dissociation) • ECD (Electron Capture Dissociation) • PQD (Pulsed Q Collision Induced Dissociation) • ETD (Electron Transfer Dissociation) • HCD (Higher Energy Collision Dissociation) • EThcD (ETD With Supplemental HCD) • UVPD (Ultra Violet Photon Dissociation) • Any Activation Type
Min. Collision Energy	Specifies the minimum Normalized Collision Energy for a higher-order scan to pass through the filter. Default: 0 (no filtering) Minimum value: 0; Maximum value: Unchecked
Max. Collision Energy	Specifies the maximum Normalized Collision Energy for a higher-order scan to pass through the filter. Default: 1000; Minimum value: 0; Maximum value: 1000
Scan Type	Specifies the scan type for the scan event that the instrument used to produce the product ion. Filter selection: Any, Is, Is Not; default: Any—The application does not filter the scan events by scan type. Check box selections: • Full • Selected Ion Monitoring (SIM) • Selected Reaction Monitoring (SRM)

Table 40. Select Spectra node parameters (Sheet 6 of 9)

Parameter	Description
Polarity Mode	Specifies the polarity mode for the scan. Filter selection: Any, Is, Is Not Default: (Not Specified)—The node does not filter the scan events by polarity mode. Check box selections: • Positive • Negative
IMPORTANT When the input files for an analysis include mass range switching or CV switching and the processing workflow includes a compound detection node, use the MS1 Mass Range filter or the FAMS CV filter, respectively, to specify the mass range or CV value that you want to process. The compound detection nodes can process spectra for only one mass range and one CV value per input file.	
MS1 Mass Range	This filter applies only to MS1 scans. The format for this parameter setting is [50.0000-1000.0000], where the dash is a hyphen. MS1 scans must match the specified mass range to pass the filter. Default: Unspecified (Empty)
	IMPORTANT Enter the masses in the mass range to four decimal places, as the node checks the mass values to four decimal places.

Table 40. Select Spectra node parameters (Sheet 7 of 9)

Parameter	Description
FAIMS CV	When the compensation voltage (FAIMS CV value) is unspecified (empty), the analysis ignores CV values and all spectra pass the filter. When you specify a CV value, the analysis processes only the spectra for the specified CV value. Default: Unspecified (Empty)
	IMPORTANT The compound detection nodes require MS1 spectra from each input file in an analysis, but they can process spectra for only one CV value per input file. To prevent an analysis that includes a compound detection node from failing, do the following: • When any of the input files include spectra for more than one CV value (CV switching), specify the CV value that you want to process, and make sure that every file in the Files for Analysis list includes spectra for this CV value. • When the input files include only one CV value per file but not the same CV value for each file, do not specify the CV value.
3. Peak Filters	
S/N Threshold (FT-only)	Specifies the signal-to-noise threshold for mass peaks in an FTMS scan. Mass peaks below this threshold are filtered out. Default: 1.5
4. Replacements for Unrecognized Properties	
Unrecognized Charge Replacements	Specifies the charge state or states to process when the charge state of the precursor ion is indeterminate. Default: 1 In the Qual Browser window, an indeterminate charge state is specified with a question mark label (z=?) in a spectrum cell. In the FreeStyle application, ions with indeterminate charge states are labeled with a charge state of 0. Default: 1; Selections: All, 1, 2, 3, 4, 5, 6, 7, or 8

Table 40. Select Spectra node parameters (Sheet 8 of 9)

Parameter	Description
Unrecognized Mass Analyzer Replacements	Specifies the mass analyzer used to acquire the data when the application cannot retrieve this information from the input file. Default: ITMS Selections: • Ion Trap (ITMS) • Fourier Transform (FTMS) • Time of Flight (TOFMS) • Single Quad (SQMS) • Triple Quad (TSMS) • Sector Field (SectorMS)
Unrecognized MS Order Replacements	Specifies the MS order when the application cannot retrieve this information from the input file. Default: MS2; Selections: MS1–MS10
Unrecognized Activation Type Replacements	Specifies the activation type when the application cannot retrieve this information from the input file. Default: CID Selections (as displayed in the drop-down list): • CID (Collision Induced Dissociation) • MPD (Multi Photon Dissociation) • ECD (Electron Capture Dissociation) • PQD (Pulsed Q Collision Induced Dissociation) • ETD (Electron Transfer Dissociation) • HCD (High Energy Collision Dissociation) • EThcD (ETD With Supplemental HCD) • UVPD (Ultra Violet Photon Dissociation)
Unrecognized Polarity Replacement	Specifies the polarity mode when the application cannot retrieve this information from the input file. Default: (+); Selections: Positive (+) or Negative (–)
Unrecognized MS Resolution @ 200 Replacements	Specifies the resolution at *m/z* 200 for MS scans when the node cannot retrieve the resolution from the scan header. Default: 60 000
Unrecognized MSn Resolution @ 200 Replacements	Specifies the resolution at *m/z* 200 for MS/MS scans when the node cannot retrieve the resolution from the scan header. Default: 30 000

Table 40. Select Spectra node parameters (Sheet 9 of 9)

Parameter	Description
5. General Settings	
Precursor Selection	Specifies the MS order of the precursor scans for higher-order MS^n scans, such as MS^3, MS^4, and so on up to MS(n – 1). Default: Use MS(n – 1) Precursor Selections: Use MS1 Precursor or Use MS(n – 1) Precursor
Use Isotope Pattern in Precursor Reevaluation	Determines whether the node considers the isotope pattern in reevaluating precursors. Default: True Selections: • True—The node considers the isotope pattern in reevaluating precursors. • False—The node does not consider the isotope pattern in reevaluating precursors.
Provide Profile Spectra	When set to True, the node stores the profile data for the scans. When set to Automatic, the node checks whether any other nodes in the processing workflow require profile data. If the profile data is not required by any of the workflow nodes in the processing workflow, the node only stores the centroid data. Default: Automatic
Store Chromatograms	Specifies whether the analysis stores the total ion current (TIC) and base peak chromatograms in the result file. Default: False

Trace Creation nodes

For LC studies, these nodes create specialized chromatographic traces:

- Create Analog Trace node
- Create FISh Trace node
- Create Mass Trace node
- Create Pattern Trace node

Create Analog Trace node

For LC studies, use the Create Analog Trace node to view the chromatograms for these trace types: ultraviolet-visible (UV), photo-diode array (PDA), or analog. Your Thermo Scientific data system supports several brands of UV-Vis and PDA detectors. You can acquire UV traces from a UV-Vis or a PDA detector and PDA traces from a PDA detector. If your analog detector is not supported by a Thermo Scientific data system, you can acquire an analog trace by connecting the detector to one of the analog channels on the communications panel of your Thermo Scientific mass spectrometer.

You can access analog traces from the Specialized Traces table.

Note The Create Analog Trace node can also convert and display a pressure trace from an LC pump and a temperature trace from a column heater or autosampler with temperature control, when these instruments are controlled by the Xcalibur data system or equivalent Thermo Scientific application.

Table 41 describes the parameters for the Analog Traces node.

Table 41. Create Analog Trace node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Trace Type	Specifies whether the application extracts a UV, PDA, or analog trace from the raw data file. Default: UV; Selections: UV, PDA, or Analog
RT Offset [min]	Specifies the offset time, in minutes, between the UV, PDA, or analog detector and the mass spectrometer traces. A negative value shortens and a positive value lengthens the apparent retention time of the peaks detected by the UV, PDA, or analog detector. Default: 0; range: –10 to 10
Custom Label	Type text to identify the trace in the Specialized Traces table on the result file page.
2. PDA Settings	
Total Scan	Specifies whether the node extracts a total scan trace for the scanned wavelength range. Total scan traces display the average absorbance for each time point of all the wavelengths in the scan range. Default: False

Table 41. Create Analog Trace node parameters (Sheet 2 of 2)

Parameter	Description
Spectrum Maximum	Specifies whether the node extracts a spectrum maximum trace for the scanned wavelength range. Spectrum maximum traces display a plot of the maximum absorbance values in the scan range for each time point. Default: False
Note Use the Min. and Max. Wavelength boxes to specify a trace of average absorbance versus time. • To display the chromatogram for a specific scan wavelength, type the same wavelength number in the Min. and Max. Wavelength boxes. • To display a plot of the average absorbance values for a range of wavelengths, type the beginning wavelength number in the Min. Wavelength box and the ending wavelength number in the Max. Wavelength box.	
Wavelength Range	Specifies whether the node extracts the entire acquired scan or a wavelength range. Default: True—Uses a specified wavelength range.
Min. Wavelength	Specifies the beginning wavelength, in nanometers, of the trace that you want the node to extract. Default: 190; range: 190–800 nm
Max. Wavelength	Specifies the ending wavelength, in nanometers, of the trace that you want the node to extract. Default: 800; range: 190–800 nm

Create FISh Trace node

For LC studies, use the Create (Fragment Ion Search) FISh Trace node to create FISh traces. The Create FISh Trace node requires fragmentation scans and takes input from any of the data processing nodes. The output from the FISh trace node is a summed FISh trace that is accessible from the Specialized Traces Table, individual fragment traces that are accessible from the FISh Trace Fragments result table, or both.

Table 42 describes the parameters for the Create FISh Trace node.

Table 42. Create FISh Trace node parameters (Sheet 1 of 3)

Parameter	Description
1. Compound Selection	
Compound	Specifies the compound that the node uses to generate expected fragment ions. The selection list contains the compounds in the user-created Lists & Libraries > Expected Compounds library. See "Expected Compounds view." **IMPORTANT** To run an analysis that includes the Create FISh Trace node, you must select a compound from this list. To add compounds to the Expected Compounds library, see "Add and edit expected compounds with the Compound Editor."
2. Trace Settings	
Mass Tolerance	Specifies the mass tolerance that the node uses to create the FISh trace. Default: 2.5 mmu
Summed Trace	Specifies whether the node generates a summed trace of all the detected fragment ions. You can access the summed FISh trace from the Specialized Traces result table. Default: True
Individual Traces	Specifies whether the node generates individual traces for each generated fragment ion. You can access the individual traces from the FISh Trace Fragments result table. Default: True
Custom Label	Type text that you can use to identify the chromatogram in a report. This box accepts alphanumeric and special characters.

Table 42. Create FISh Trace node parameters (Sheet 2 of 3)

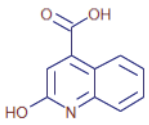
Parameter	Description
3. Scan Filter Settings	
Scan Polarity	Specifies the polarity of the scan. Default: + (Positive); Selections: Positive or Negative
Fragment Mode	Specifies the fragmentation mode of the fragmentation scans that you want the node to extract. Default: Data-Dependent; Selections: Data-Dependent or Data Independent Select Data-Dependent for data-dependent fragmentation (DDF) scans or Data Independent for all-ion fragmentation (AIF) scans.
4. Fragment Prediction Settings	
Use General Rules	Specifies whether the node uses the general fragmentation rules for fragment prediction.
Use Libraries	Specifies whether the node uses the fragmentation libraries for fragment prediction. Default: True
Max. Depth	Specifies the maximum number of steps in the fragmentation pathway. Range: 1 to 20
Aromatic Cleavage	Specifies whether the node includes a cleavage step in the fragmentation pathway for highly aromatic structures—that is, for aromatic structures where *n* in Huckel's rule is 2 or higher. $4n + 2$ = the number of electrons in the delocalized, conjugated p-orbital cloud For example, the following structure is aromatic with an *n* value of 2, and the number of electrons in its delocalized, conjugated p-orbital cloud is 10.  Default: True

Table 42. Create FISh Trace node parameters (Sheet 3 of 3)

Parameter	Description
Min. Fragment *m/z*	Specifies the minimum *m/z* value of a fragment ion to be generated by the prediction fragmentation pathway. Default: 50; range: 0 or higher
Max. Fragment *m/z*	Specifies the maximum *m/z* value of a fragment ion to be generated by the prediction fragmentation pathway. When the value is set to 0, the node ignores this parameter. Default: 0

Create Mass Trace node

Use the Create Mass Trace node to extract a mass chromatogram that you can access from the Specialized Traces Table of the result file. You can specify the type, the fragmentation order, and the polarity of the trace. For an XIC trace, you must specify the mass range.

Table 43 describes the parameters for the Create Mass Trace node.

Table 43. Create Mass Trace node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Trace Type	Specifies the chromatogram type to be generated. Default: BPC Selections: TIC (total ion chromatogram), BPC (base peak chromatogram), or XIC (extracted ion chromatogram)
MS Order	Specifies the MS order of the mass spectra that make up the chromatogram. Default: MS1; Selections: MS1–MS10
Polarity	Specifies the ionization polarity used to produce the mass spectra that make up the chromatogram. Default: + (Positive); Selections: + (Positive) or – (Negative)
Custom Label	Use this box to type text that you can use to identify the chromatogram. This text appears in the Custom Label column of the Specialized Traces result table. This box accepts alphanumeric and special characters.

Table 43. Create Mass Trace node parameters (Sheet 2 of 2)

Parameter	Description
2. XIC Settings	
Mass [Da]	Defines the mass-to-charge (*m/z*) value of the extracted ion chromatogram (XIC). Default: 0
Mass Tolerance (typed numeric value and selected units)	Specifies the mass tolerance for the spectral search. When you select Da or mmu (0.001 Da) in the units list, the mass tolerance is an absolute ± value for the mass specified in the Mass box. When you select ppm (parts per million) in the Units list, the mass tolerance is a relative range: Mass ± (Mass × *User-specified* ppm)/1e6 Default: 3 ppm Range: 0 to no upper limit; units: Da, mmu, ppm

Create Pattern Trace node

Use the Create Pattern Trace node to draw a chromatogram from the mass peaks that match a specific pattern within the filtered set of spectra. The pattern can be based on the elemental composition of a target compound or on a user-specified pattern. To view the pattern trace in the Chromatogram view for a result file, open the Specialized Traces Table and select the pattern trace.

Tip For more information about working with isotope patterns, see these topics:

- Set up individual isotope patterns by using the Isotope Ratio Editor
- Specialized Traces table

Table 44 describes the parameters for the Create Pattern Trace node.

Table 44. Create Pattern Trace node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Isotope Ratios	Displays either the elemental composition of the compound of interest or the following text: [custom pattern]. You use the Isotope Ratio Editor to set up the isotope pattern for the compound of interest. The application can automatically set up the isotope pattern for a non-isotopically labeled compound by using its elemental composition. For isotopically-labeled compounds, you must enter the expected mass shifts of the isotopic peaks as well as their relative intensity to the A0 isotope. **IMPORTANT** In the defined processing workflows, this parameter is set to C15S with the following three isotope selections: • Monoisotopic ion (100% intensity) • A2 ion with one sulfur-34 atom (peak with a +1.9958 Da mass shift and a 4.52% relative intensity) • A2 ion with two carbon-13 atoms (peak with a +2.00669 Da mass shift and a 1.27% relative intensity) When you create a new processing workflow, you must specify the isotope ratios of interest to run an analysis.
Mass Tolerance	Specifies the mass tolerance for the mass shifts between the mass spectral peaks in the pattern. Range: 0.0–1e6 ppm; default: 5 ppm You set up the pattern with the Isotope Ratio Editor.
Intensity Tolerance [%]	Specifies the relative intensity tolerance of the mass spectral peaks in the pattern. Range: 0.01–100.0 The A0 isotope is always the isotope with the lowest *m/z* value, but it is not necessarily the isotope with the highest intensity. For example, with more than one bromine atom, a bromine and a chlorine atom, or more than four chlorine atoms, the M + 2 (A2) isotope is the most intense isotope.

Table 44. Create Pattern Trace node parameters (Sheet 2 of 2)

Parameter	Description
MS Order	Specifies the MS order of the mass spectrum. Selections: MS1–MS10
Polarity	Specifies the polarity of the mass spectrum. Selections: Positive or Negative
Custom Label	Use this box to enter a description of the trace.

Expected Compounds nodes

These nodes extract information about the compounds that you expect to find in the input file set. The Find Expected Compounds and FISh Scoring nodes require structural information about the targeted compounds. You supply this information by adding it to the Expected Compounds library.

- FISh Scoring node
- Find Expected Compounds node
- Find Expected Compounds (Legacy) node
- Generate Expected Compounds node
- Group Expected Compounds node
- Merge Features node

FISh Scoring node

Use the FISh Scoring node to provide a confirmation score for compounds that the Find Expected Compounds node detects and to annotate the fragmentation spectra for these compounds. The FISh Scoring node requires data-dependent fragmentation (DDF) scans to calculate the FISh coverage scores for related structures.

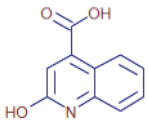
Note For information about how the node calculates the confirmation score, see "FISh scoring for proposed structures."

Table 45 describes the parameters for the FISh Scoring node.

Table 45. FISh Scoring node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Annotate Full Tree	Specifies whether the node annotates the full spectrum tree or only the MS2 scans in the Mass Spectrum view. For information about viewing the FISh annotations in the Mass Spectrum view, see "Mass Spectrum view." Default: True
Match Transformations	Specifies whether the node matches fragments with transformation shifts. Default: True
S/N Threshold	Specifies the signal-to-noise threshold for centroids. The node ignores centroids below this threshold in the fragmentation (MS/MS, MS^3, and so on) spectra. Default: 3
High Acc. Mass Tolerance	Specifies the mass tolerance for high-resolution mass spectra measured in the Orbitrap mass analyzer of a Thermo Scientific mass spectrometer. Default: 2.5 mmu; Minimum: 0.0; Maximum: Unchecked
Low Acc. Mass Tolerance	Specifies the mass tolerance for low-resolution mass spectra measured in the ion trap mass analyzer of a Thermo Scientific mass spectrometer. Default: 0.5 Da; Minimum: 0.0; Maximum: Unchecked
2. Fragment Prediction Settings	
Use General Rules	Specifies whether the node uses the general fragmentation rules. Default: True
Use Libraries	Specifies whether the node uses fragmentation libraries for fragment prediction. Default: True **Note** Using fragmentation libraries to predict fragments adds significant time to data processing; however, it also provides significantly more predicted fragments.

Table 45. FISh Scoring node parameters (Sheet 2 of 2)

Parameter	Description
Max. Depth	Specifies the maximum number of steps in the fragmentation pathway. Range: 1 to 20
Aromatic Cleavage	Specifies whether the node includes a cleavage step in the fragmentation pathway for highly aromatic structures—that is, for aromatic structures where *n* in Huckel's rule is 2 or higher. $4n + 2$ = the number of electrons in the delocalized, conjugated p-orbital cloud. For example, the following structure is aromatic with an *n* value of 2. The number of electrons in the delocalized, conjugated p-orbital cloud is 10.  Default: True
Min. Fragment *m/z*	Specifies the minimum *m/z* value of a fragment ion to be generated by the prediction fragmentation pathway. Default: 50

Find Expected Compounds node

Use the Find Expected Compounds node to search for compounds in the compound ions list provided by one or more Generate Expected Compounds nodes.

Using the input from one or more Generate Expected Compounds nodes, the Find Expected Compounds node looks for expected compounds in the MS1 scans filtered through the data processing nodes. The expected compounds are the parent compounds that the Generate Expected Compounds nodes provide to the Find Expected Compounds node, and the reaction products for these parent compounds. Each Generate Expected Compounds node predicts the reaction products by using the user-specified Dealkylation step and the user-specified transformation steps. The Dealkylation step can comprise multiple dealkylation and dearylation reactions.

The processing results for the Find Expected Compounds node appear in these tables: Expected Compounds Table, Expected Compounds per File Table, Expected Formulas Table, and Expected Features Table.

For more information about how the application finds expected compounds, see "Targeted processing workflows for expected compounds."

Table 46 describes the parameters for the Find Expected Compounds node.

Table 46. Find Expected Compounds node parameters (Sheet 1 of 3)

Parameter	Description
1. General Settings	
Mass Tolerance	Specifies the mass tolerance that the node uses to create each extracted ion chromatogram (XIC). Default: 5 ppm; range: 0.1 to 20 ppm
Intensity Tolerance [%]	Specifies the relative intensity tolerance that the node uses for isotope pattern comparison. Default: 30%; range: 0–100
Intensity Threshold [%]	Specifies the minimum intensity relative to the base peak for an isotopic peak in an isotope pattern simulation. The application does not search for isotopic peaks below the specified intensity threshold. Default: 0.1; range 0.01–10.0
Min. # Isotopes	Specifies the minimum number of isotopes (mass spectrum peaks in a centroided mass spectrum) that must match the theoretical isotope pattern of the expected elemental composition. Default: 2; range: 1 to no limit
Use Most Intense Isotope Only	Specifies whether the node reports the chromatographic peak area for the most intense isotope peak within an isotope pattern or for all the detected isotope peaks in the isotope pattern. When set to True, the analysis reports the area of the chromatographic peak for the most intense *m/z* value in the isotope pattern and reports this *m/z* value as the reference peak. The analysis result displays the XIC trace for the most intense isotope peak in the Chromatogram view. When set to false, the analysis reports the summed areas for all the isotope peaks in the isotope pattern. The analysis result displays the TIC for all the detected isotopes. Default: True

Table 46. Find Expected Compounds node parameters (Sheet 2 of 3)

Parameter	Description
Minimum Peak Intensity	Specifies the minimum apex intensity, in ion counts, of the detected chromatographic peak. The node discards chromatographic peaks below this intensity threshold. Default: 1000; Minimum: 0.0
Average Peak Width	Specifies the average chromatographic peak width (FWHM) in the filtered time range. Default: 0 (automatic peak width detection); range: unchecked When this value is set to 0, the node automatically determines the average peak width. **IMPORTANT** The node detects no chromatographic peaks in the following cases: • The filtered retention time is too small compared to the determined or user-specified average peak width value. For information about filtering the scan data, see "Select Spectra node." • The determined or user-specified average peak width value is too small compared to the scan rate of the instrument. For example, if the instrument acquires a full (MS1) scan every 0.01 minutes, do not enter an Average Peak Width value of less than 0.02 (2 × 0.01 minutes), as the peak detection algorithm requires a minimum of three data points to detect a chromatographic peak. For best results, keep the default setting of 0, which turns on automatic peak width detection. Enter a nonzero value only when the automatically detected peak width is not suitable or fails for your chromatographic method.
2. Peak Detection	
Chromatographic S/N Threshold	Filters out all chromatographic peaks below the specified threshold. Default: 1.5; range: 0.0 to unchecked

Table 46. Find Expected Compounds node parameters (Sheet 3 of 3)

Parameter	Description
Remove Baseline	Specifies whether the node applies a baseline correction to the XIC traces. When set to False, the node drops perpendicular tangent lines from the start and end points of each chromatographic peak and includes this additional area in the reported area for each compound. Default: False
Gap Ratio Threshold (advanced)	Does not store (ignores) chromatographic peaks from XIC traces that have a gap ratio exceeding the specified threshold. The gap ratio for an XIC trace is the number of missing data points (gaps) to the total number of data points for the XIC trace. Default: 0.35; range 0 to 1
Max. Peak Width [min] (advanced)	Specifies the maximum allowed peak width at half height in minutes for a chromatographic peak. Ignores chromatographic peaks that are wider than this limit. Default: 1 minute; minimum value: 0.05 minutes
Min. Relative Valley Depth (advanced)	Specifies the minimum valley depth between two chromatographic peaks to consider them resolved—that is, to report them as two separate peaks. The specified value is the minimum ratio of the height of the shorter peak to the valley height. Default: 0.1; range: 0.05 to 0.5
Min. #Scans per Peak (advanced)	Specifies the minimum number of scans required to define a chromatographic peak. Default: 5; range: 3 to 20

Find Expected Compounds (Legacy) node

Use the Find Expected Compounds node to search for compounds in the compound ions list provided by one or more Generate Expected Compounds nodes.

Using the input from one or more Generate Expected Compounds nodes, the Find Expected Compounds node looks for expected compounds in the MS1 scans filtered through the data processing nodes. The expected compounds are the parent compounds that the Generate Expected Compounds nodes provide to the Find Expected Compounds node, and the

reaction products for these parent compounds. Each Generate Expected Compounds node predicts the reaction products by using the user-specified Dealkylation step and the user-specified transformation steps. The Dealkylation step can comprise multiple dealkylation and dearylation reactions.

The processing results for the Find Expected Compounds node appear in these tables: Expected Compounds Table, Expected Compounds per File Table, Expected Formulas Table, and Expected Features Table.

For more information about how the application finds expected compounds, see "Targeted processing workflows for expected compounds."

Table 46 describes the parameters for the Find Expected Compounds node.

Table 47. Find Expected Compounds (Legacy) node parameters (Sheet 1 of 3)

Parameter	Description
1. General Settings	
Mass Tolerance	Specifies the mass tolerance that the node uses to create each extracted ion chromatogram (XIC). Default: 5 ppm; range: 0.1 to 20 ppm
Intensity Tolerance [%]	Specifies the relative intensity tolerance that the node uses for isotope pattern comparison. Default: 30%; range: 0–100
Intensity Threshold [%]	Specifies the minimum intensity relative to the base peak for an isotopic peak in an isotope pattern simulation. The application does not search for isotopic peaks below the specified intensity threshold. Default: 0.1; range 0.01–10.0
Min. # Isotopes	Specifies the minimum number of isotopes (mass spectrum peaks in a centroided mass spectrum) that must match the theoretical isotope pattern of the expected elemental composition. Default: 2; range: 1 to no limit

Table 47. Find Expected Compounds (Legacy) node parameters (Sheet 2 of 3)

Parameter	Description
Use Most Intense Isotope Only	Specifies whether the node reports the chromatographic peak area for the most intense isotope peak within an isotope pattern or for all the detected isotope peaks in the isotope pattern. When set to True, the analysis reports the area of the chromatographic peak for the most intense *m/z* value in the isotope pattern and reports this *m/z* value as the reference peak. The analysis result displays the XIC trace for the most intense isotope peak in the Chromatogram view. When set to false, the analysis reports the summed areas for all the isotope peaks in the isotope pattern. The analysis result displays the TIC for all the detected isotopes. Default: True
Minimum Peak Intensity	Specifies the minimum apex intensity, in counts, of the detected chromatographic peak. The node discards chromatographic peaks below this intensity threshold. Default: 1000; Minimum: 0.0

Table 47. Find Expected Compounds (Legacy) node parameters (Sheet 3 of 3)

Parameter	Description
Average Peak Width [min]	Specifies the average chromatographic peak width (FWHM) in the filtered time range. Default: 0 (automatic peak width detection); range: unchecked When this value is set to 0, the node automatically determines the average peak width. **IMPORTANT** The node detects no chromatographic peaks in the following cases: • The filtered retention time is too small compared to the determined or user-specified average peak width value. For information about filtering the scan data, see "Select Spectra node." • The determined or user-specified average peak width value is too small compared to the scan rate of the instrument. For example, if the instrument acquires a full (MS1) scan every 0.01 minutes, do not enter an Average Peak Width value of less than 0.02 (2 × 0.01 minutes), as the peak detection algorithm requires a minimum of three data points to detect a chromatographic peak. For best results, keep the default setting of 0, which turns on automatic peak width detection. Enter a nonzero value only when the automatically detected peak width is not suitable or fails for your chromatographic method.

Generate Expected Compounds node

Use the Generate Expected Compounds node to generate a list of *m/z* values for the ionized compounds that you expect to find in a sample. The list includes the parent compounds and their possible dealkylation, dearylation, and transformation products. The application generates the list by using the structures of the parent compounds, the user-specified transformation lists and number of combinatory steps, and the user-specified ionic species.

The default transformations library contains common Phase 1 and Phase 2 metabolic transformations. If the transformation list does not include the possible transformations for your compound, add them to the transformations library as described in "Add or edit transformations with the Transformation Editor."

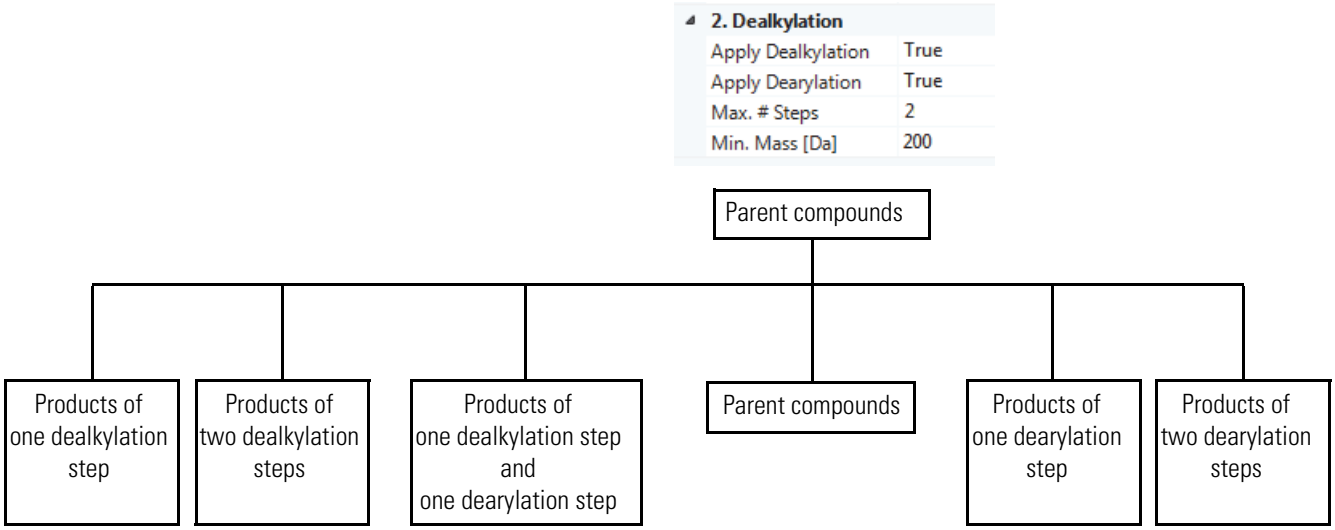
When you add transformations to the library, you can assign them to one of the following groups: Phase I, Phase II, or Others. The Generate Expected Compounds node treats transformations assigned to the Others group as Phase I transformations; that is, it applies Phase I and Others transformations before it applies Phase II transformations.

To predict the transformation products for the selected parent compounds, the Generate Expected Compounds node follows these rules:

1. When the user enables Dealkylation, apply the dealkylation steps first. If a subsequent transformation reverses the dealkylation step, reject the subsequent transformation. When the user enables both Dealkylation and Dearylation, apply both of these steps first, and then determine two separate reaction pathways for the remaining transformation steps.

   Consider all steps under Dealkylation together as one step. For example, consider the selections shown in Figure 83 as one step in the total set of reaction pathways and create separate reaction pathways. Apply the transformation steps on the parent compound and the reaction products from the dealkylation pathways.

   Figure 83. Dealkylation step example



2. When more than one reaction pathway produces the same elemental composition, use the pathway with the lowest number of transformation steps.
3. Reject transformations that remove elements that are not present. For example, do not apply an oxidative dechlorination step if the compound does not contain chlorine.

4. For Phase I and Others transformations, limit the maximum number of times to apply the transformation on a single compound to the lower of these two values:
   – Max Occurrence setting for the transformation in the Transformations library

     For example, for the oxidation transformation, the default value for Max Occurrence is 3.

Name	Arriving Group	Arriving Modification	ΔM [Da]	Phase	Max Occurrence
Aa	Aa	Aa	=	Aa	=
Oxidation	O	O	15.99491	Phase1	3

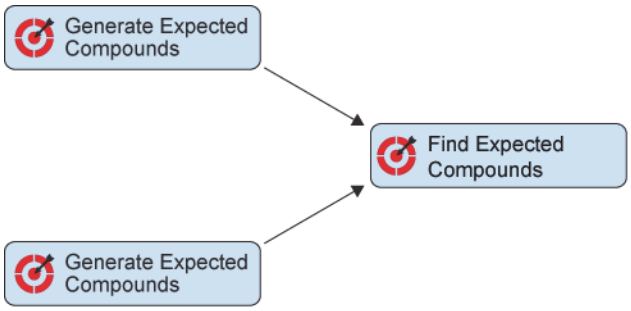
   – Maximum number of steps specified by the node's Max. # All Steps parameter minus any previously applied Dealkylation step.
5. For Phase II transformations, limit the maximum number of times to apply the transformation on a single compound to the lowest of these three values:
   – Max Occurrence setting for the transformation in the Transformations library
   – Maximum number of steps for all reactions (setting for node's Max. # All Steps parameter) minus any previously applied Dealkylation or Transformation step
   – Maximum number of steps for a Phase II transformation (setting for node's Max. # Phase II parameter)

You can connect one or more Generate Expected Compounds nodes to the Find Expected Compounds node and the Filter By Mass Defect node.

Table 48 describes the parameters for the Generate Expected Compounds node. The application cannot use the processing workflow until you select a compound from the Compound list.

If you want to generate expected compounds for more than one parent compound, do the following:

- To target multiple compounds with a different set of transformation rules for each compound, add multiple Generate Expected Compounds nodes to the processing workflow.



- To target multiple compounds with the same set of transformation rules, add one Generate Expected Compounds node to the processing workflow and select multiple compounds in the node's Compound list.

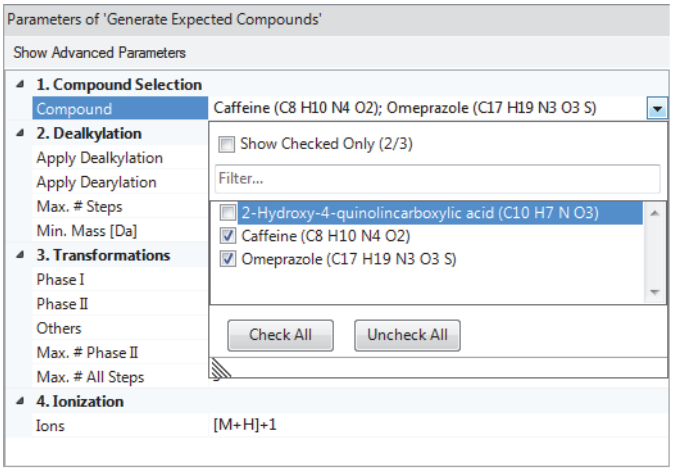


Table 48. Generate Expected Compounds node parameters (Sheet 1 of 3)

Parameter	Description
1. Compound Selection	
Compound	Specifies the parent compounds that the node uses to build a list of possible product compounds.
Show Checked Items Only	Displays only the selected compounds.
Check All	Selects all compounds in the list.
Uncheck All	Undoes all selections.
Note Before you can use the Generate Expected Compounds node to predict the transformation products of specific compounds, you must first add the compounds to the Expected Compounds library.	
2. Dealkylation	
Apply Dealkylation	When you select True, the node applies the dealkylation transformations for the specified compound before applying other transformations. Default: True
Apply Dearylation	When you select True, the node applies the dearylation transformations for the specified compound before applying other transformations. Default: False

Table 48. Generate Expected Compounds node parameters (Sheet 2 of 3)

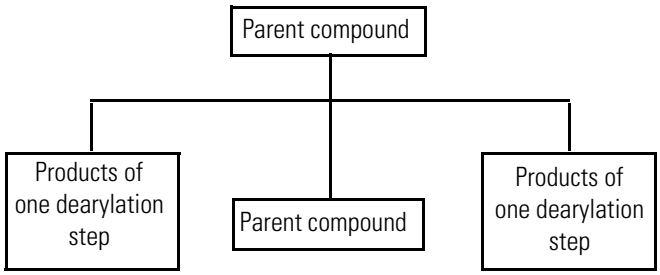
Parameter	Description
Max. # Steps	Specifies the maximum number of Dealkylation steps. For example, if you select True for Dealkylation, True for Dearylation, and 1 for the Max. # Steps, the node applies up to one dealkylation step and up to one dearylation step as the initial Dealkylation step in the set of reaction pathways. For another example, see Figure 83 on page 262.  Default: 1; Selection: 1–10
Min. Mass [Da]	Specifies the minimum mass of the dealkylation product. Default: 200
3. Transformations	
Phase I	Specifies the set of possible Phase 1 transformations. Default: All check boxes are clear.
Phase II	Specifies the set of possible Phase II transformations. Default: All check boxes are clear.
Others	Specifies other possible transformations. The node treats Others transformations as Phase I transformations.
Max. # Phase II	Specifies the maximum number of Phase II steps to be applied. Default: 1; range: 1–10

Table 48. Generate Expected Compounds node parameters (Sheet 3 of 3)

Parameter	Description
Max. # All Steps	Specifies the maximum number of all steps to be applied. All steps that occur as a result of the selections in the Dealkylation area equal one step in the maximum number of all steps—that is, after the node applies the steps in the Dealkylation area, the remaining number of possible steps is equal to the Max. # All Steps – 1. Default: 3; range: 1–10
4. Ionization	
Ions	Specifies the possible ionic species. Default: [M+H]+1 (protonated species for the positive mode) **Note** The ion definitions library that the application provides contains the common ionic species associated with the positive and negative modes for the electrospray ionization-mass spectrometry (ESI-MS) technique. If the Ions list does not include the possible ionic species for your analysis, add the ion definition to the Ion Definition library as described in "Ion Definitions view."

Group Expected Compounds node

Use the Group Expected Compounds node to combine similar components (chromatographic peaks with the same MW × RT dimensions) that the Find Expected Compounds node finds across the input file set. This node combines chromatographic peaks by using their chemical formula (resulting from the dealkylations and dearylations and transformations of a parent compound) and retention time. This node also selects the best representative MS1 scan and fragmentation tree, which other nodes, such as Predict Compositions, Search mzCloud, Search mzVault, and so on use for identification.

Table 49 describes the parameters for the Group Expected Compounds node.

Table 49. Group Expected Compounds node parameters (Sheet 1 of 3)

Parameter	Description
1. General Settings	
RT Tolerance [min]	Specifies the retention time tolerance, in minutes, that the node uses to group mass peaks generated from the same parent compound through the same reaction pathway. Default: 0.1; range: 0 to 1.0

Table 49. Group Expected Compounds node parameters (Sheet 2 of 3)

Parameter	Description
Align Peaks	Specifies whether the node aligns the chromatographic peaks for a specific compound across all the input files. Default: False
Preferred Ions	Select the preferred ions (adducts) from the list. The application uses the list to select the best fragmentation data for each compound to submit to an mzCloud or mzVault search. Selection: The selection list includes all the ion definitions in the Ion Definitions list under Lists & Libraries.
Area Integration	Specifies which ions the node uses to determine the chromatographic peak areas. For the Most Common Ion selection, the node uses the chromatographic peak area of the most common adduct ion detected across the input file set. For the All Ions selection, the node sums the areas of all the adduct ions detected in a particular input file. Default: Most Common Ion; selections: Most Common Ion and All Ions
2. Peak Rating Contributions These parameter settings determine how the node calculates the peak rating values for chromatographic peaks. See "Chromatographic peak rating filter." The maximum value for each contributing parameter is unlimited. The contribution of each individual parameter is as follows: (Contribution value for the individual parameter/Divided by the sum of all the contribution values)×10.	
Area Contribution	Specifies the chromatographic peak area contribution to the peak rating. Default: 3
CV Contribution	Specifies the contribution of the coefficient of variation for the peak areas across replicate samples to the peak rating. If an analysis includes no replicates, the node sets the CV contribution to 0 during processing. Default: 10

Table 49. Group Expected Compounds node parameters (Sheet 3 of 3)

Parameter	Description
FWHM to Base Contribution	Specifies the FWHM (full width at half the maximum peak height) to base contribution to the peak rating. Default: 5
Jaggedness Contribution	Specifies the jaggedness contribution to the peak rating. Default: 5
Modality Contribution	Specifies the modality contribution to the peak rating. Default: 5
Zig-Zag Index Contribution	Specifies the zig-zag index contribution to the peak rating. Default: 5
3. Peak Rating Filter The node does not store chromatographic peaks that have a peak rating below the threshold value in the specified number of files. When either or both of the peak rating parameters are set to 0, this filter is not enabled. By default, this filter is not enabled.	
Peak Rating Threshold	Specifies the minimum peak rating for the chromatographic peaks. The node ignores this parameter setting unless you specify a nonzero value for the number of files. Default: 0; range: 0 to 10
Number of Files	Specifies the minimum number of files across the input set where the chromatographic peak for a compound must meet the peak rating threshold to be stored in the result file. The optimum value depends on the number of files in the data set and the probability of similar compounds in these files. When there is a very low probability that the samples contain the same compounds, set this value to 0. For replicate samples that probably contain the same compounds, set this value to the number of replicates or one less than the number of replicates. The node ignores this value unless you specify a nonzero peak rating threshold. Default: 0

Merge Features node

Use the Merge Features node to do the following:

- Combine the expected compounds found by the Find Expected Compounds node and the unknown compounds found by the Detect Compounds node by using their chromatographic retention time and *m/z* values.
- Create the Merged Features table that includes four status columns: Ion Conflict Status, Detect Compounds, Find Expected Compounds, and Custom Explanations.
- Link the manual peaks table to the related Compounds table.

Table 50 describes the parameters for the Merge Features node.

Table 50. Merge Features node parameters

Parameter	Description
1. General Settings	
Mass Tolerance	Specifies the mass tolerance for chromatographic peak grouping. Default: 5 ppm; range: 0.1–20 ppm
RT Tolerance [min]	Specifies the retention time tolerance, in minutes, for chromatographic peak grouping. Default: 0.05; range: 0.0–1.0

Compound Detection nodes

Use these nodes to detect unknown compounds:

- Analyze Labeled Compounds node
- Detect Compounds (Legacy) node
- Detect Compounds node
- Fill Gaps node
- Group Compounds node

Analyze Labeled Compounds node

Use the Analyze Labeled Compounds node to detect labeled compounds and their labeling rates. For more information about reviewing the results for stable isotope labeling experiments, see "Isotopologues Distribution Chart view."

Table 51. Analyze Labeled Compounds node (Sheet 1 of 2)

Parameter	Description
1. Label Settings	
Label Element	Specifies the labeled element and its isotope in this format: [*mass number*]*element symbol* Where *element symbol* is the symbol in the periodic table
Max. Exchange	Specifies the maximum number of exchangeable atoms for any of the compounds. If the number of exchangeable atoms for a compound is below this number, the application uses the lower number. If set to zero, the compound's elemental composition determines the maximum number of exchangeable atoms. Default: 25
Source Efficiency [%]	Specifies the isotopic purity of the labeled compound introduced into the biological system. Most commercially available stable isotope labeled compounds have an isotopic purity of 98 to 99%. Keeping the setting at 100% is appropriate for these compounds. Default: 100
2. Pattern Analysis	
Mass Tolerance [ppm]	Specifies the mass tolerance for the isotope search and XIC trace generation. Default: 5 ppm
Intensity Tolerance [%]	Specifies the relative intensity tolerance for isotope pattern matching. Default: 30
Intensity Threshold [%]	Specifies the isotope intensity threshold, relative to the pattern's base peak, for the theoretical isotope pattern. Default: 0.1

Table 51. Analyze Labeled Compounds node (Sheet 2 of 2)

Parameter	Description
S/N Threshold	Specifies the signal-to-noise threshold for isotope pattern matching. Default: 3
3. General Settings	
Mark Irregular Exchange	Adds the Irregular Exchange status to the following result table columns: Labeling Status column of the Compounds Table and the Status column of the Compounds per File Table. The Irregular Exchange status applies to compounds where the exchange rate for the mid-mass isotopologues is less than 5% of the exchange rate for the isotopologues. Default: True
Exclude Blanks	Specifies whether to exclude blank samples (Sample Type: Blank) from the main Compounds table. Default: True
Hide Unprocessed	Specifies whether to hide compounds with unassigned formulas in the Compounds table. The node does not process compounds without formulas. Default: True

Detect Compounds (Legacy) node

Use the Detect Compounds node to detect unknown compounds for studies where you want to compare new analyses with analyses performed in earlier versions of the Compound Discoverer application.

The processing results for the Detect Compounds node appear in the Compounds per File table and the Features per File table.

For information about an untargeted processing workflow, see "Untargeted processing workflows for identifying unknown compounds."

Table 52 describes the parameters for the Detect Compounds (Legacy) node.

Table 52. Detect Compounds (Legacy) node parameters (Sheet 1 of 4)

Parameter	Description
1. General Settings	
Mass Tolerance [ppm]	Specifies the mass tolerance for the XIC traces. Default: 5.0 ppm; range: 1–20.0 ppm
Intensity Tolerance [%]	Specifies the intensity tolerance for the isotope pattern search. Default: 30%; range: 0 to 100%
Min. Peak Intensity	Specifies the minimum base peak height to detect peaks in the XIC traces. The analysis does not report chromatographic peaks below this minimum peak intensity (peak height at the apex). The optimal minimum peak intensity setting depends upon the instrument (see Table 53). Default: 10 000
Ions	Specifies the adduct ions that might be in your samples. Default: $[M+H]^{+1}$, $[M+K]^{+1}$, $[M+Na]^{+1}$ Selection: The list includes the ion definitions in your Ion Definitions library.
Base Ions	Specifies the adduct ions that you expect to have the highest intensity in your samples. Default: $[M+H]^{+1}$ and $[M-H]^{-1}$
Note The processing workflows (in the Common Workflows > Workflow Templates > E and L, MetID, folder) specify the following base ions: • $[M+H]^{+1}$ • $[M+NH_4]^{+1}$ • $[M-H]^{-1}$. The selection of base ions includes the ammonium adduct because extractable and leachable compounds tend to be nonpolar compounds that require ammonium acetate as a mobile phase modifier for optimal chromatography.	
Min Element Counts	Specifies the minimum number of each possible element. The node uses these values for the isotope pattern search. Default: C H

Table 52. Detect Compounds (Legacy) node parameters (Sheet 2 of 4)

Parameter	Description
Max Element Counts	Specifies the maximum number of each possible element. The node uses these values for the isotope pattern search. Default: C90 H190 Br3 Cl4 K2 N10 Na2 O15 P2 S5
Min. #Scans per Peak	Specifies the minimum number of scans (data points) required to define a chromatographic peak. Default: 5; range: 3 to 20
Use Most Intense Isotope Only	Specifies whether the node reports the chromatographic peak area for the most intense isotope peak within an isotope pattern or for all the detected isotope peaks in the isotope pattern. When set to True, the analysis reports the area of the chromatographic peak for the most intense *m/z* value in the isotope pattern and reports this *m/z* value as the reference peak. The analysis result displays the XIC trace for the most intense isotope peak in the Chromatogram view. When set to false, the analysis reports the summed areas for all the isotope peaks in the isotope pattern. The Chromatograms view in the analysis result displays the TIC for all the detected isotopes. Default: True
2. Trace Detection (advanced parameters)	
Max. Number of Gaps to Correct	Specifies the maximum number of contiguous missing values in the XIC trace for the compound. You can set the maximum number of allowed contiguous missing values from 0 to 3. When the XIC trace includes more than the maximum number of allowed contiguous missing values (gaps), the node does not store the trace in the analysis result. Default: 2; range: 0 to 3
Min. Number of Adjacent Non-Zeroes	Specifies the minimum number of non-zero values adjacent to a gap before the node fixes the gap. Default: 2; range: 1 to 3
3. Peak Detection (advanced parameters)	
Filter Peaks	Specify whether you want to turn on the chromatographic peak filtering parameters. Default: True

Table 52. Detect Compounds (Legacy) node parameters (Sheet 3 of 4)

Parameter	Description
Max. Peak Width [min]	When Filter Peaks is set to True, specifies the maximum peak width at half height, in minutes, for detected chromatographic peaks. Default: 0.3; range: 0.05 to no upper limit
Remove Singlets	If set to True, does not report a component if the chromatographic peak for the component contains only A0 centroids. Default: True
4. Isotope Pattern Detection (advanced parameters)	
Min. #Isotopes	Specifies the minimum number of isotopes in the isotope pattern are required in the mass spectrum scans that define the chromatographic peak. Default: 2
Use Peak Quality for Isotope Grouping	Specifies whether the node filters out low-quality chromatographic peaks before it groups the XIC traces for ions in an isotope pattern. When set to True, the node uses a two-stage approach for isotope grouping. In the first stage, the node groups only high-quality peaks that pass the peak quality thresholds. In the second stage, the node groups the remaining chromatographic peaks. When set to False, the node does not consider the peak quality thresholds for isotope grouping. Default: False
Filter out Features with Bad Peaks Only	Specifies whether to remove a feature when all the chromatographic peaks for the feature across the input file set are low-quality chromatographic peaks that do not pass the peak quality thresholds. Default: True
See "Chromatographic peak rating filter."	
Zig-Zag Index Threshold	Specifies the zig-zag index threshold for the chromatographic peaks. Default: 0.2; range 0 to 1

Table 52. Detect Compounds (Legacy) node parameters (Sheet 4 of 4)

Parameter	Description
Jaggedness Threshold	Specifies the jaggedness threshold for the chromatographic peaks. Default: 0.4; range 0 to 1
Modality Threshold	Specifies the modality threshold for the chromatographic peaks. Default: 0.9; range 0 to 1
Min. Spectral Distance Score	Specifies the minimum spectral distance score for grouping features together as part of one isotope pattern. Increasing this score filters out compounds with low-scoring isotope patterns, potentially decreasing the number of detected compounds. Default: 0; range: 0 to 100%
Remove Potentially False Positive Isotopes	Specifies whether to filter out an isotope in a spectrum if there is a gap of four missing isotopes between this isotope and the isotopes to its left (on the *m/z* axis). For example, if the analysis detects only one A0 and one A5 isotope in the isotope pattern, and you specify that it must find a minimum of two isotopes to detect a compound, it does not detect the compound. Default: True
5. Skipped	
6. AcquireX Settings (advanced)	
Detect Persistent Background Ions	When set to True, this parameter generates a related Background Ions table for each input file. This parameter is not relevant for typical operation of the Compound Discoverer application. Its use is currently limited to the AcquireX™ data acquisition workflow. Default: False

Table 53 lists the recommended range for the minimum peak intensity parameter. The optimal setting depends on the sensitivity of the mass spectrometer.

Table 53. Recommended minimum peak intensity range

Mass spectrometer	Minimum peak intensity (chromatographic peak height)
Q Exactive, Q Exactive Plus, and Q Exactive HF	500 000 to 1 000 000
Orbitrap Fusion, Orbitrap Lumos, and Orbitrap ID-X	50 000 to 100 000

Table 53. Recommended minimum peak intensity range

Mass spectrometer	Minimum peak intensity (chromatographic peak height)
Exactive, Exactive Plus, Orbitrap Elite, and Orbitrap Velos Pro	100 000 to 500 000
LTQ Orbitrap XL and LTQ Orbitrap Velos	25 000 to 100 000

Detect Compounds node

The new Detect Compounds node includes peak quality thresholds for filtering out XIC traces with low-quality chromatographic peaks. Use this node for most untargeted analyses. Only use the Detect Compounds (Legacy) node when you want peak detection to mimic a legacy analysis.

Table 54. Detect Compounds node parameters (Sheet 1 of 5)

Parameter	Description
1. General Settings	
Mass Tolerance	Specifies the mass tolerance for the XIC traces. Default: 5.0 ppm; range: 1–20.0 ppm
Min. Peak Intensity	Specifies the minimum base peak height to detect peaks in the XIC traces. The analysis does not report chromatographic peaks below this minimum peak intensity (peak height at the apex). The optimal minimum peak intensity setting depends upon the instrument (see Table 53). Default: 10 000
Min. #Scans per Peak (advanced)	Specifies the minimum number of scans (data points) required to define a chromatographic peak. Default: 5; range: 3 to 20

Table 54. Detect Compounds node parameters (Sheet 2 of 5)

Parameter	Description
Use Most Intense Isotope Only	Specifies whether the node reports the chromatographic peak area for the most intense isotope peak within an isotope pattern or for all the detected isotope peaks in the isotope pattern. When set to True, the analysis reports the area of the chromatographic peak for the most intense *m/z* value in the isotope pattern and reports this *m/z* value as the reference peak. The analysis result displays the XIC trace for the most intense isotope peak in the Chromatogram view. When set to false, the analysis reports the summed areas for all the isotope peaks in the isotope pattern. The analysis result displays the TIC for all the detected isotopes. Default: True
2. Trace Detection (advanced parameters) A gap is a missing data point in the XIC trace for a compound. If the XIC trace for a compound contains more than the specified number of contiguous gaps, the node ignores the chromatographic peaks for this XIC trace.	
Max. Number of Gaps to Correct	Specifies the maximum number of contiguous missing values in the XIC trace for the compound. You can set the maximum number of allowed contiguous missing values from 0 to 3. When an XIC trace includes with more than the maximum number of allowed contiguous missing values (gaps), the node does not store the chromatographic peaks for this trace in the analysis result. Default: 2; range: 0 to 3
Min. Number of Adjacent Non-Zeroes	Specifies the minimum number of non-zero values adjacent to a gap before the node fixes the gap. Default: 2; range: 1 to 3
3. Peak Detection	
Chromatographic S/N Threshold	Filters out all chromatographic peaks below the specified threshold. Default: 1.5; range: 0.0 to unchecked
Remove Baselines	Specifies whether the node applies baseline correction to the XIC traces. Default: False

Table 54. Detect Compounds node parameters (Sheet 3 of 5)

Parameter	Description
Gap Ratio Threshold (advanced)	Does not store (ignores) chromatographic peaks from XIC traces that have a gap ratio exceeding the specified threshold. The gap ratio for an XIC trace is the number of missing data points (gaps) to the total number of data points for the XIC trace. Default: 0.35; range 0 to 1
Max. Peak Width [min] (advanced)	Specifies the maximum allowed peak width at half height in minutes for a chromatographic peak. Ignores chromatographic peaks that are wider than this limit. Default: 1 minute; minimum value: 0.05 minutes
Min. Relative Valley Depth (advanced)	Specifies the minimum valley depth between two chromatographic peaks to consider them resolved—that is, to report them as two separate peaks. The specified value is the minimum ratio of the height of the shorter peak to the height of the valley between the peaks. Default: 0.1; range: 0.05 to 0.5
4. Isotope Pattern Detection	
Group Isotopes For	Specifies whether the node also groups the isotopic ions for chlorine and bromine. For example, when you select Cl, the node groups the isotopic ions for 35CI and 37CI. The node automatically groups the various isotopic ions for the elements C, H, N, O, and S. Default: The check boxes for Cl and Br are selected.
Use Peak Quality for Isotope Grouping (advanced)	Specifies whether the node filters out low-quality chromatographic peaks before it groups the XIC traces for ions in an isotope pattern. When set to True, the node uses a two-stage approach for isotope grouping. In the first stage, the node groups only high-quality peaks that pass the peak quality thresholds. In the second stage, the node groups the remaining chromatographic peaks. When set to False, the node does not consider the peak quality thresholds for isotope grouping. Default: True

Table 54. Detect Compounds node parameters (Sheet 4 of 5)

Parameter	Description
Filter Out Features with Bad Peaks Only (advanced)	Specifies whether to remove a feature when all the chromatographic peaks for the feature across the input file set are low-quality chromatographic peaks that do not pass the peak quality thresholds. Default: True
See "Chromatographic peak rating filter."	
Zig-Zag Index Threshold	Specifies the zig-zag index threshold for the chromatographic peaks. Default: 0.2; range 0 to 1
Jaggedness Threshold	Specifies the jaggedness threshold for the chromatographic peaks. Default: 0.4; range 0 to 1
Modality Threshold	Specifies the modality threshold for the chromatographic peaks. Default: 0.9; range 0 to 1
Remove Potentially False Positive Isotopes (advanced)	When set to True, the node runs an additional check for false positive isotopes. Default: True
5. Compound Detection	
Ions	Specifies the adduct ions that might be in your samples. Default: $[M+H]^{+1}$, $[M+K]^{+1}$, $[M+Na]^{+1}$ Selection: The ion definitions in your Ion Definitions library
Base Ions (advanced)	Specifies the adduct ions that you expect to have the highest intensity in your samples. Default: $[M+H]^{+1}$ and $[M-H]^{-1}$

Note The processing workflows (in the Common Workflows > Workflow Templates > E and L, MetID, folder) specify the following base ions: $[M+H]^{+1}$, $[M+NH_4]^{+1}$, and $[M-H]^{-1}$.

The selection of base ions includes the ammonium adduct because extractable and leachable compounds tend to be nonpolar compounds that require ammonium acetate as a mobile phase modifier for optimal chromatography.

Table 54. Detect Compounds node parameters (Sheet 5 of 5)

Parameter	Description
Remove Singlets (advanced)	If set to True, does not report a component if the chromatographic peak for the component contains only A0 centroids. Default: True
6. AquireX Settings (advanced)	
Detect Persistent Background Ions	When set to True, the node detects and stores persistent background ions. Default: False

Fill Gaps node

Use the Fill Gaps node to find chromatographic peaks that were detected by the Detect Compounds node in one of the input files but were missing from other input files in the file set.

For information about adding the Fill Gaps node to a processing workflow, see "Peak area refinement node connections."

The Fill Gaps node adds the (hidden) Gap Status column to the Compounds Table and creates the related (hidden) Filled Gaps Table.

The Filled Gaps table describes how the node calculated the missing chromatographic peak areas. Clicking a row in the Filled Gaps table displays the gap-filled trace and the integrated peak area.

Table 55 describes the parameters for the Fill Gaps node.

Table 55. Fill Gaps node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Mass Tolerance	Specifies the mass tolerance that the node uses to search for matching mass peaks. Search range = expected mass ± mass tolerance/1e6 Default: 5 ppm; range: 0.1 to 20 ppm
S/N Threshold	Specifies the minimum signal-to-noise threshold for centroids. Default: 1.5; minimum: 1

Table 55. Fill Gaps node parameters (Sheet 2 of 2)

Parameter	Description
Use Real Peak Detection	Specifies whether the analysis fills gaps in the chromatogram by using a peak detection algorithm or only a peak simulation algorithm. True—The node uses the Parameterless Peak Detection (PPD) algorithm to fill the gaps with redetected low-intensity peaks. Using PPD can significantly increase the processing time. False—The node uses only a peak simulation algorithm to fill the gaps with simulated chromatographic peaks.
Apply Restrictive Gap Filling	Specifies whether the node uses a more restrictive retention time tolerance for filling individual gaps than the retention time tolerance that the Group Compound node uses for compound grouping. True—The node uses a more restrictive retention time tolerance to avoid grouping peaks for other compounds. Thermo Scientific recommends this setting. False—The node uses the retention time tolerance that you specified in the Group Compounds node, except when a gap is due to missing ions. For gaps due to missing ions, the node sets the RT tolerance to the expected FWHM of the missing peak, because the expected RT of the missing peak is known. **Note** This parameter is new in Compound Discoverer 3.3 SP1. In previous versions of the Compound Discoverer application, the Fill Gaps node automatically used a more restrictive time tolerance than the Group Compounds node to avoid grouping peaks for other compounds. The default RT Tolerance [min] for the Group Compounds node is 0.2 min, and the available range is 0 to 1.0 min. See "Group Compounds node."

Group Compounds node

Use the Group Compounds node to combine unknown compounds across the input file set by their molecular weight and retention time. This node also selects the best representative MS1scan and fragmentation tree, which the Predict Compositions node and search nodes use for identification.

Table 56 describes the parameters for the Group Compounds node.

Table 56. Group Compounds node parameters (Sheet 1 of 3)

Parameter	Description
1. Compound Consolidation	
Mass Tolerance	Specifies the mass tolerance that the node uses to search for matching mass peaks. Default: 5 ppm; range: 0.1 to 20 ppm
RT Tolerance [min]	Specifies the retention time tolerance, in minutes, that the node searches for mass peaks within the specified mass tolerance. Default: 0.05; range: 1.0
Align Peaks	Specifies whether the node aligns the chromatographic peaks for a compound across all the input files. Default: False
Preferred Ions	Select the preferred ions (adducts) from the list. The application uses the list to select the best fragmentation data for each compound to submit to an mzCloud or mzVault search. Selections: One or more of the ions in your Ion Definitions library Default: [M+H]+1 and [M–H]–1
Area Integration	Specifies what ions the node uses to determine the chromatographic peak areas. For the Most Common Ion selection, the node uses the chromatographic peak area of the most common adduct ion detected across the input file set. For the All Ions selection, the node sums the areas of all the adduct ions detected in a particular input file. Default: Most Common Ion; selections: Most Common Ion and All Ions

Table 56. Group Compounds node parameters (Sheet 2 of 3)

Parameter	Description
2. Peak Rating Contributions	
These parameter settings determine how the node calculates the peak rating values for chromatographic peaks. See "Chromatographic peak rating filter."	
The maximum value for each contributing parameter is unlimited.	
The contribution of each individual parameter is as follows:	
(Contribution value for the individual parameter/Divided by the sum of all the contribution values)×10.	
Area Contribution	Specifies the chromatographic peak area contribution to the peak rating. Default: 3
CV contribution	Specifies the contribution of the coefficient of variation for the peak areas across replicate samples to the peak rating. If an analysis includes no replicates, the node sets the CV contribution to 0 during processing. Default: 10
FWHM to Base Contribution	Specifies the FWHM to base contribution to the peak rating. Default: 5
Jaggedness Contribution	Specifies the jaggedness contribution to the peak rating. Default: 5
Modality Contribution	Specifies the modality contribution to the peak rating.
Zig-Zag Index Contribution	Specifies the zig-zag index contribution to the peak rating. Default: 5
3. Peak Rating Filter	
The node does not store chromatographic peaks that have a peak rating below the threshold value in the specified number of files.	
When either or both of the peak rating parameters are set to 0, this filter is not enabled.	
By default, this filter is not enabled.	
For more information about the peak rating filter, see "Chromatographic peak rating filter."	

Table 56. Group Compounds node parameters (Sheet 3 of 3)

Parameter	Description
Peak Rating Threshold	Specifies the minimum peak rating for the chromatographic peaks. The node ignores this parameter setting unless you specify a nonzero value for the number of files. Default: 0; range: 0 to 10
Number of Files	Specifies the minimum number of files across the input set where the chromatographic peak for a compound must meet the peak rating threshold to be stored in the result file. The optimum value depends on the number of files in the data set and the probability of similar compounds in these files. When there is a very low probability that the samples contain the same compounds, set this value to 0. For replicate samples that probably contain the same compounds, set this value to the number of replicates or one less than the number of replicates. The node ignores this value unless you specify a nonzero peak rating threshold. Default: 0

Peak Area Refinement nodes

These nodes modify the chromatographic peak areas for compounds or mark the background compounds:

- Apply Missing Value Imputation node
- Apply QC Correction node
- Apply SERRF QC Correction node
- Mark Background Compounds node
- Normalize Areas node
- Scale Areas node

Apply Missing Value Imputation node

For LC studies, try using the Missing Value Imputation node if the Fill Gaps node does not yield the expected results.

The Apply Missing Value Imputation node provides two methods for imputing missing chromatographic peak areas for compounds: Random Forest and Median + Small Value.

- The Random Forest imputation method consists of a self-trained machine learning system.
- The Median + Small Value imputation method is a mixed method:
  - (Partially missing values) For study groups where a compound is detected in at least one of the samples, but not all the samples, the node imputes an area value for each value by using the mean of the values that are present in the same study group.
  - (Full gap) If the compound is not present in any of the samples in a study group, the node imputes area values for the compound in each sample by dividing the smallest detected peak area for any compound in a sample by 2.

Table 57. Missing Value Imputation node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Imputation Method	Specifies the imputation method for missing chromatographic peaks across a set of input files. Selections: • (Default) Automatic Selection—The application automatically uses the Median + Small Value with Variability imputation method when the analysis includes three or more study groups and the deconvolution node detects 50 or more compounds. If these conditions are not met, the application uses the Random Forest imputation method. For information about defining the study groups, see "Set up the sample groups and ratios for a new analysis." • Median + Small Value with Variability • Random Forest Imputation
Fill Blanks with Min Value	Specifies whether the node fills the chromatographic peak for a compound with a minimum value in blank samples. When your processing workflow includes a QC correction node, select True for this parameter. The QC correction node requires area values for each detected compound across all the input files, including the blanks (samples with the Blank sample type assignment). Default: False
2. Random Forest Settings These parameters apply only to the Random Forest Imputation method.	

Table 57. Missing Value Imputation node parameters (Sheet 2 of 2)

Parameter	Description
Number of Trees	Specifies the number of decision trees. Default: 100; range: 20 to 1000
Max Number of Iterations	Specifies the maximum number of iterations. Default: 10; range: 2 to 50

Apply QC Correction node

When acquiring raw data files for a large sample set, you can use pooled quality control (QC) samples to compensate for time-dependent batch effects.

When the processing workflow includes the Apply QC Correction node and the input file set includes QC samples, an analysis uses the QC samples to create a linear regression or cubic spline curve of area versus acquisition time for each detected compound. For more information, see Using quality control samples to compensate for batch effects.

The Apply QC Correction node adds the QC columns and the Norm. Area column to the compounds table (Compounds table). You can view the correction curves in the Compound Area Corrections view and the QC corrected areas for the compounds in the Normalized Area column. For more information, see "Compound Area Corrections view."

Table 58 describes the parameters for the Apply QC Correction node.

Table 58. Apply QC Correction node parameters (Sheet 1 of 3)

Parameter	Description
1. General Settings	
The analysis uses the QC samples to create a regression curve for each detected compound. Unless all three of the following conditions are met, the analysis does not create a regression curve for a particular compound or does not correct the areas in the non-QC samples: • It detects the compound in the specified minimum percentage of QC samples. • The relative standard deviation of the detected peak areas for the compound in the QC samples does not exceed the specified threshold. • The number of samples acquired between the QC samples does not exceed the specified number. If the analysis does not create a regression curve for a compound, it does not perform a batch normalization of the peak areas for the compound in the non-QC samples (Sample type: Sample, Control, or Standard).	

Table 58. Apply QC Correction node parameters (Sheet 2 of 3)

Parameter	Description
Regression Model	Specifies the regression model as Linear or Cubic Spline. Default: Linear
The Min. QC Coverage Max. [%], QC Area RSD [%], and Max. Corrected QC Area RSD [%] parameters act as display filters for the compounds table. When the compounds table includes compounds that the analysis was unable to normalize, a filter icon appears on the table's tab. Pointing to the tab displays the number of compounds displayed, the total number of compounds detected, and the number of compounds filtered out.	
Min. QC Coverage [%]	Specifies the minimum percentage of the QC samples where the analysis must detect a particular compound before it creates a regression curve for the compound. If the coverage falls below this value, the analysis does NOT perform a batch normalization of the peak areas for the compound in the non-QC samples. Default: 50%; range: 25 to 100%
Max. QC Area RSD [%]	Specifies the maximum relative standard deviation (RSD%) for the areas for a particular compound across the QC samples. If the RSD% exceeds this maximum percentage, the analysis does not create a regression curve for the compound, calculate the normalized areas for the compound, or report normalized areas in the compounds table. Default: 30%; range: 10 to 50%
Max. Corrected QC Area RSD (%)	Specifies the maximum allowed relative standard deviation for a particular compound area within the QC samples after correction. If the RSD% exceeds this maximum percentage, the analysis does not create a regression curve for the compound, calculate the normalized areas for the compound, or report normalized areas in the compounds table. Default: 25; range: 5 to 50%

Table 58. Apply QC Correction node parameters (Sheet 3 of 3)

Parameter	Description
Max. #Files Between QC Files	The application checks the acquisition time stamp for each input file in an analysis and orders the samples within an analysis set by acquisition time. Specifies the maximum number of non-QC samples that you can acquire between the QC samples. If the application detects more non-QC samples between the QC samples than the maximum allowable number, it does not correct the chromatographic peak areas in the non-QC samples—that is, it does not perform a batch normalization on these samples. Default: 15; range: 1 to unchecked value

Apply SERRF QC Correction node

For LC studies, use the Apply SERRF QC Correction node if you are processing input files from batches acquired on noncontiguous days. SERRF stands for systematic error removal with random forests.

The Apply SERRF QC Correction node takes input from the Group Compounds node or the Fill Gaps node. It creates the QC correction columns in the Compounds table and the Batch column in the Input Files table.

For information about how the Apply SERRF QC Correction node creates the time-based normalization curve for the chromatographic peak areas, see "Batch normalization for multiple sequence runs (LC studies)."

Table 59. Apply SERRF QC Correction node parameter descriptions

Parameter	Description
1. General Settings	
Min. QC Coverage [%]	Specifies the minimum percentage of the QC samples where the analysis must detect a particular compound before it creates a regression curve for the compound. If the coverage falls below this value, the analysis does NOT perform a batch normalization of the peak areas for the compound in the non-QC samples. Default: 50%; range: 25 to 100%

Table 59. Apply SERRF QC Correction node parameter descriptions

Parameter	Description
Max. QC Area RSD [%]	Specifies the maximum relative standard deviation (RSD%) for the areas for a particular compound across the QC samples. If the RSD% exceeds this maximum percentage, the analysis does not create a regression curve for the compound, calculate the normalized areas for the compound, or report normalized areas in the compounds table. Default: 30%; range: 10 to 50%
Max. Corrected QC Area RSD [%]	Specifies the maximum allowed relative standard deviation for a particular compound area within the QC samples after correction. If the RSD% exceeds this maximum percentage, the analysis does not create a regression curve for the compound, calculate the normalized areas for the compound, or report normalized areas in the compounds table. Default: 25; range: 5 to 50
Max. #Files Between QC Files	The application checks the acquisition time stamp for each input file in an analysis and orders the samples within an analysis set by acquisition time. Specifies the maximum number of non-QC samples that you can acquire between the QC samples. If the application detects more non-QC samples between the QC samples than the maximum allowable number, it does not correct the chromatographic peak areas in the non-QC samples—that is, it does not perform a batch normalization on these samples. Default: 15; range: 1 to unchecked value
# Batches	Specifies the maximum number of batches used to acquire the set of input files for the analysis. The node does not exceed this number when it determines the number of batches for the input file set. Default: 2; range 1 to 50
Interpolate Gap-filled QC Areas	When set to True, the node discards the gap-filled areas for the QC samples and instead uses the mean of the non-gap-filled areas for these compounds. Default: False

Table 59. Apply SERRF QC Correction node parameter descriptions

Parameter	Description
Correct Blank Files	Specifies whether the correction process adjusts the chromatographic peak area values for samples with the Blank sample type assignment. Typically, there are two types of blank samples—solvent blanks and matrix blanks. True: The node adjusts the chromatographic peak area values for blank samples. False: The node does not adjust the chromatographic peak area values for blank samples. **IMPORTANT** When using a QC correction node, the processing workflow must include the Fill Gaps node.
2. Random Forest Settings	
#Trees	Specifies the number of decision trees that the Random Forest algorithm uses. Default: 200; minimum: 10

Mark Background Compounds node

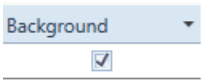
Use the Mark Background Compounds node to flag compounds that are also found in the sample blanks (Sample Type—Set to Blank). For information about editing the assigned sample types, see "Edit the sample type and study factor values."

IMPORTANT As you drag the Fill Gaps and the Normalize Areas nodes into the Workflow Tree pane, the application automatically connects the Group Compounds node to the Fill Gaps node, and the Fill Gaps node to the Normalize Areas node. The application does not connect the Mark Background Compounds node to other nodes, so you must manually make the appropriate connections.

For more information about the node connections, see "Peak area refinement node connections."

Table 60 describes the parameters for the Mark Background Compounds node.

Table 60. Mark Background Compounds node parameters

Parameter	Description
1. General Settings	
Max. Sample/Blank	Below this ratio threshold, the node labels the expected compound as a background compound in the compounds table. If the input file set includes more than one blank sample, the node uses the largest peak area for the compound in the blank input files as the peak area of the blank. $\frac{\text{Peak Area}_{\text{Sample}}}{\text{Peak Area}_{\text{Blank}}} < \text{Specified value}$ Default: 5 When this setting is 0, the node ignores this parameter.
Max. Blank/Sample	Below this ratio threshold, the node labels the compound as a background compound in the compounds table. If the input file set includes more than one blank sample, the node uses the largest peak area for the compound in the blank input files as the peak area of the blank. $\frac{\text{Peak Area}_{\text{Blank}}}{\text{Peak Area}_{\text{Sample}}} < \text{Specified value}$ If the compound is found in a blank sample but not in a non-blank sample, (ratio *X*/0), the node marks the compound as a background compound. Default: 0 (The node does not use this parameter to mark background compounds.)
Hide Background	When the Hide Background parameter is set to True, the tab for the compounds table includes a filter icon (), and the compounds that fall below the threshold are hidden. Clicking the filter icon displays the filtered compounds. When the Hide Background parameter is set to False, the background compounds appear in the result table. The Background column is a hidden column in the compounds table. When a compound is flagged as a background compound, its Background check box is selected.  Default: True

Normalize Areas node

Use the Normalize Areas node to normalize the chromatographic peak areas for each compound across the input file set.

Thermo Fisher Scientific does not recommend using this node. To compensate for batch effects, add quality control samples to the batch and a QC correction workflow node to the processing workflow.

When the Normalize Areas node is part of a processing workflow, the Use Normalized Areas check box is available in the Descriptive Statistics view and the Principal Component Analysis view. The Normalize Areas node adds the Norm. Area column to the compounds table.

IMPORTANT When both the Normalize Areas and Mark Background Compounds nodes are part of a processing workflow, do the following:

- If the analysis includes solvent blanks (Blank sample type), connect the Mark Background Compounds node to the Normalize Areas node.
- If the analysis includes matrix blanks (Blank sample type), connect the Normalize Areas node to the Mark Background Compounds node.

Table 61 describes the parameters for the Normalize Areas node.

Table 61. Normalize Areas node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Normalization Type	Specifies the algorithm for normalizing the peak areas for each compound across the input files. Selections: • Constant Sum • Constant Mean • Constant Median • Median Absolute Deviation (MAD) **Tip** For best results, select **Constant Mean** for input file sets that include matrix blanks.

Table 61. Normalize Areas node parameters (Sheet 2 of 2)

Parameter	Description
Exclude Blanks	Specifies whether to exclude Blank sample types from normalization. Default: True
	Tip For best results, follow these guidelines: • Select **True** for solvent blanks to exclude them from the normalization process. If you do not exclude the solvent blanks from the normalization process, the Fill Gaps node adds small "noise" peaks to the solvent blanks for each detected compound in the input file set. The Normalize Areas node magnifies these small peaks, causing the sample-to-blank ratio to fall below the user-specified value in the Mark Background Compounds node. The Mark Background Compounds node then hides most of the detected compounds across the input file set (marks them as background compounds). • Select **False** for matrix blanks, such as plasma and urine, as these blanks typically contain a large number of compounds that you might want to hide.

Scale Areas node

Use the Scale Areas node to scale the chromatographic peak areas on the basis of the numeric study factor values that you assigned to each sample file.

Table 62 describes the parameters for the Scale Areas node. If your processing workflow includes both of the grouping nodes, and you want to scale the output from both of these nodes, you must connect each grouping node to a separate Scale Areas node.

Figure 84. Connections to Scale Areas node

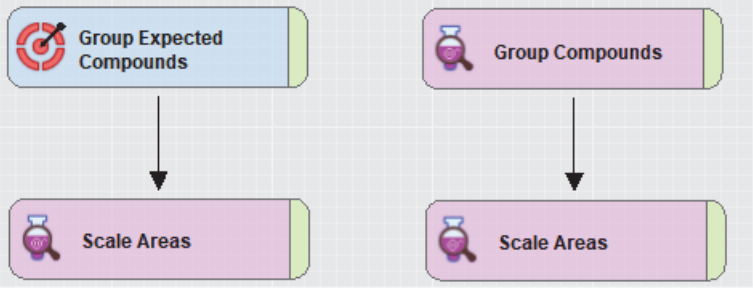


Table 62. Scale Areas node parameters

Parameter	Description
1. General Settings	
Study Factor Name	Specifies the study factor to use as the scaling factor for the chromatographic peak areas when you select Scaling Factor in the Normalization Type list. Multiplies the peak area for a compound by the value for the selected numerical study factor. Selections: Defined numerical study factors; default: Empty
Exclude Blanks	Specifies whether to exclude blank samples (where the sample type is set to Blank) from the scaling process. Default: True **Tip** For best results, follow these guidelines: • Select **True** for solvent blanks to exclude them from the scaling process. • Select **False** for matrix blanks, such as plasma and urine, as these blanks typically contain a large number of compounds that you might want to scale.

Compound Identification nodes

Use these nodes to identify unknown compounds:

- Assign Compound Annotations node (LC studies)
- Predict Compositions node
- Search ChemSpider node
- Search Mass Lists node
- Search mzCloud node
- Search mzVault node

Assign Compound Annotations node (LC studies)

Use the Assign Compound Annotations node to select the preferred data sources for the following annotations: name, formula, and structure. The application attempts to assign the annotations provided by the first data source. If the first source does not provide the annotation, the application uses the second data source, and so on until it goes through all the specified sources. If the processing workflow does not include the Assign Compound Annotations node, the application does not populate the Name, Formula, or Structure columns of the Compounds table for an LC study.

Table 63 describes the parameters for the Assign Compound Annotations node.

Table 63. Assign Compound Annotation node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Mass Tolerance	Specifies the mass tolerance for validating the annotations. Default: 5 ppm; range: 0.1–20 ppm
2. Data Sources	
Available sources: mzCloud Search, mzVault Search, BioCyc Search, Mass List Match, Metabolika Search, ChemSpider Search, and Predicted Compositions	
Data Source #1	Specifies the primary source for the compound annotations. Default: mzCloud Search **Tip** If a stable isotope analysis misidentifies known compounds, consider reprocessing the analysis after selecting your custom mass list as the first data source.
Data Source #2	Specifies the secondary source for compound annotations if the primary source is unavailable. Default: Predicted Compositions
Data Source #3	Specifies the source for compound annotations if the primary and secondary sources are unavailable. Default: Mass List Search
Data Source #4	Specifies the source for compound annotations if all the previous sources are unavailable. Default: ChemSpider Search
Data Source #5–7	Use to specify additional annotation sources in the list. Default: Empty

Table 63. Assign Compound Annotation node parameters (Sheet 2 of 2)

Parameter	Description
3. Scoring Rules	
Use mzLogic	When set to True, uses the score from the Apply mzLogic node to select the best candidate. Default: True
Use Spectral Distance	When set to True, uses the SFit score from the Apply Spectral Distance node to select the best candidate. Uses the SFit Threshold and SFit Range values to limit the number of valid candidates. Default: True
SFit Threshold	Specifies the minimum SFit score for a candidate. Default: 20; range: 0 to 100
SFit Range	Specifies the maximum allowed difference between the SFit scores for the best and worst candidates. Default: 20; range: 0 to 100
4. Reprocessing	
Clear Names	When set to True, the node clears the assigned annotations (name, formula, and structure) for the detected compounds when you reprocess the analysis. When set to False, the node does not remove the assigned annotations when you reprocess the analysis. If you modify the identification workflow nodes, these nodes can overwrite the existing annotations. If you remove the identification nodes responsible for the initial annotations, these annotations remain in the final analysis result. This parameter is new in the Compound Discoverer 3.3 application. In previous versions, the application always cleared the assigned annotations when you partially reprocessed an analysis result. Default: False

Predict Compositions node

Use the Predict Compositions node to predict the chemical formulas of the unknown compounds. This node creates the Predicted Compositions Table and populates the Formula column of the Compounds table for LC studies when the processing workflow also includes the Assign Compound Annotations node.

Table 64 describes the parameters for the Predict Compositions node.

Table 64. Predict Compositions node parameters (Sheet 1 of 4)

Parameter	Description
1. Prediction Settings	
Mass Tolerance	Specifies the mass tolerance for the XIC traces. Default: 5.0 ppm; range: 1–20.0 ppm
Min. Element Counts	Specifies the minimum count for each element in the hypothetical compound. If an element is not listed, its minimum count is zero. Default: C H
Max. Element Counts	Specifies the maximum count for each element in the hypothetical compound. If an element is not listed, its maximum count is the same as its minimum count. Default: C90 H190 Br3 Cl4 K2 N10 O18 P3 S5

Table 64. Predict Compositions node parameters (Sheet 2 of 4)

Parameter	Description
Min. RDBE and Max. RDBE	Specifies a range of values for ring and double-bond equivalents. The RDBE value is a measure of the number of unsaturated bonds in a compound. The specified value limits the calculated formulas to only those that make sense chemically. The following formula determines the RDBE value for an elemental composition: $$D = 1 + \frac{\left[\sum_{i}^{i\max} Ni\,(Vi - 2)\right]}{2}$$ where: • D is the value for the RDB equivalents • $i$max is the total number of different elements in the composition • Ni is the number of atoms of element i • Vi is the valence of atom i
Min. H/C	Specifies the minimum hydrogen-to-carbon ratio. Default: 0.1 The value of 0 means no limit. The application does not accept negative values.
Max. H/C	Specifies the maximum hydrogen-to-carbon ratio. Default: 3.5 The value of 0 means no limit. The application does not accept negative values.

Table 64. Predict Compositions node parameters (Sheet 3 of 4)

Parameter	Description
Note For most compounds, the hydrogen-to-carbon ratio falls within the range from 0.5 to 2.0. • Long chain alkanes have an H/C ratio of approximately 2. • Polycyclic aromatics have an H/C ratio of approximately 0.5.	
Max. #Candidates	Specifies the maximum number of compositions to store for each compound in the result file. Default: 10; range: 1–50
Max # Internal Candidates	Specifies the maximum number of compositions to calculate for each detected component. Default: 200; range: 1 to unchecked
	Tip To optimize the processing time, the maximum number of internal candidates is limited to 200 by default and sorted by the mass error. Normally, this works well for masses below 500 Da. However, as a component's mass or the number of elements increases, the number of possible elemental compositions also increases. This increase means that the chance of rejecting the correct formula, when it has a higher mass error than the first 200 candidates, also increases. For samples with components that have a relatively large number of elements or a mass above 500 Da, consider increasing the limit to 500.
2. Pattern Matching	
Intensity Tolerance [%]	Specifies the intensity tolerance for the isotope pattern search. Default: 30%; range: 0 to 100%
Intensity Threshold [%]	Specifies the intensity threshold, relative to the base peak (most intense ion) in the isotope pattern, for the isotope pattern search. The analysis ignores isotopes below this threshold. Default: 0.1%; range: 0.1 to 10%
S/N Threshold	Specifies the signal-to-noise threshold for the isotope search. Isotopes with a theoretical intensity below the threshold are not required.
Min. Spectral Fit [%]	Specifies the minimum spectral fit for reporting a predicted composition in the Predicted Compositions result table. Default: 30%; range: 0 to 100%

Table 64. Predict Compositions node parameters (Sheet 4 of 4)

Parameter	Description
Min. Pattern Cov. [%]	Specifies the minimum percentage for the summed intensity of the matching isotope peaks in the measured MS1 spectrum relative to the summed intensity of the theoretical isotope pattern. $\frac{\sum I_m}{\sum I_t} \times 100 = \text{Min. Pattern Cov. [\%]}$ where: I_m = the matching isotope peaks I_t = the theoretical isotope peaks Default: 90%; range: 0 to 100%
Use Dynamic Recalibration	Specifies whether the application uses the dynamic recalibration algorithm to shift the theoretical pattern for the candidate formula by the difference in the observed *m/z* value of the leftmost (A0) isotopic peak in the measured spectrum. Use dynamic recalibration when there is a systematic error (due to calibration) in the measured spectrum. Default: True
3. Fragments Matching	
Use Fragments Matching	Specifies whether the application uses the fragment matching algorithm, which ranks the identified candidates (chemical formulas) by the number of matching centroids (with an *m/z* value that matches a subset of the elemental composition for a particular candidate) in the fragmentation scan for the precursor ion. Default: True
Mass Tolerance	Specifies the mass tolerance for matching the centroids in the fragmentation scans to the *m/z* values for the expected fragments. Default: 5 ppm; range: 0 to unchecked
S/N Threshold	Specifies the signal-to-noise threshold for the centroids in the fragmentation scans. The node ignores centroids with an intensity below this threshold. Default: 3; range: 0 to unchecked

Search ChemSpider node

Use the Search ChemSpider node to search mass spectral databases for matching compounds within a specified mass tolerance range or with a certain elemental composition. This node requires input from the Group Compounds node. It adds the #ChemSpider Results column to the Compounds Table and creates the ChemSpider Results Table.

When the processing workflow includes a ChemSpider search, the processing computer must have Internet access. To verify whether the processing computer can access the ChemSpider database, run the Communication test. See Chapter 17, "Test communication to the online databases."

Table 65 describes the parameters for the Search ChemSpider node.

Table 65. Search ChemSpider node parameters (Sheet 1 of 2)

Parameter	Description
1. Search Settings	
Database(s)	Specifies the databases for the ChemSpider search. For more information about the ChemSpider databases, go to the Resources page on the My Compound Discoverer website. Default: KEGG
Search Mode	Default: By Formula or Mass Selections: By Formula or Mass, By Formula Only, By Mass Only
Mass Tolerance	Specifies the mass tolerance that the node uses to search for matching mass peaks. Default: 5 ppm; range: 0.1 to 20 ppm or 0.0 to 0.1 Da
Max# of Results Per Compound	Specifies the maximum number of hits (matches) to return (store in the result file). Default: 100; range: 1 to 2000
Max # of Predicted Compositions to be Searched per Compound	Specifies the maximum number of predicted compositions to search for in the ChemSpider database. Default: 3; range: 1 to 100

Table 65. Search ChemSpider node parameters (Sheet 2 of 2)

Parameter	Description
Result Order (for Max# of Results per Compound)	Specifies the sort order in the ChemSpider Results table. Selections: • Order By Reference Count (DESC)—Sorts the search results by the number of references for each compound. • Order By Data Source Count (DESC)—Sorts the search results by the number of data sources. • Order By Mass Deviation (ASQ)—Sorts the search results by mass deviation from the expected mass. • Order By PubMed Count (DESC)—Sorts the search results by the number of PubMed references. • Order By RSC Count (DESC)—Sorts the search results by the number of RSC references. • Order By CSID (ASQ)—Sorts the search results by the ChemSpider ID.
2. Predicted Composition Annotation	
Check All Predicted Compositions	Specifies whether to add a flag to the Predicted Compositions table. When set to True, the Search ChemSpider node adds the In ChemSpider column to the Predicted Compositions table and marks the matched Predicted Compositions with an X. Default: False

Search Mass Lists node

Use the Search Mass Lists node to search mass lists for masses that match the detected compounds. This node adds the #Matched Masses to the Compounds Table and creates the Mass List Search Results Table.

Table 66 describes the parameters for the Mass List Search node.

Table 66. Search Mass List node parameters

Parameter	Description
1. Search Settings	
Mass Lists	Specifies the mass list files that the node searches for matching masses. The mass list must have the following columns—Mass, Retention Time, and Name. The mass list can also contain the following additional columns—Molecular Structure and Text Annotation. ❖ **To select input files for the mass list search** 1. In the Mass box, click the browse icon,  . The Select Input Files dialog box opens. 2. Select the check boxes for the files that you want to use for the mass list search. 3. Click **OK**.
Use Retention Time	Specifies whether to search for compounds by retention time in addition to mass. Default: True
RT Tolerance [min]	Specifies the retention time tolerance, in minutes, for the search. The node searches for matching peaks in a retention time window equal to the expected retention time plus or minus the specified RT tolerance. Default: 2; range: 0 to 10
Mass Tolerance	Specifies the mass tolerance that the node uses to search for matching compounds. Default: 5 ppm; range: 0.1 to 20 ppm or 0.0 to 0.1 Da

Table 67 describes the table columns in the Select Input Files dialog box.

Table 67. Select Input File(s) dialog box parameters

Table column	Description
Selected	Selecting the check box for a mass list adds the list to the search.
Filename	Displays the file name of the imported file.
Description	Editable text field. Clicking the table cell displays a text entry field for typing a name or a description of the mass list. Use this column to name and sort your mass lists.
File Size	Displays the file size of the imported file.
Uploaded	Displays the date (month/day/year) and time (hour/minute) when you added the file to the library in the following format: MM/DD/yyyy HH:mm
Updated	Displays the date and time when the file was updated.
Context	Displays the source of the mass list—for example, Import from CSV or Import from XML.
State	Specifies whether the mass list is available, corrupted, or missing. If you remove a mass list file from the ServerFiles folder and restart the computer, the state of the file changes to Missing. If you edit a mass list file in the ServerFiles Folder and restart the application, the state of the file changes to Corrupted.

Search mzCloud node

Use the Search mzCloud node to search the mzCloud database for matching fragmentation spectra. This node creates the mzCloud Results table and adds the #mzCloud Results, mzCloud Best Match, and mzCloud Best Match Confidence columns to the compounds table.

For LC studies, the Search mzCloud node requires input from the Group Compounds node or the Group Expected Compounds table.

Note In addition to running an automated search with an analysis, you can manually submit a fragmentation scan to the mzCloud database from the Mass Spectrum view for an active result file.

When the processing workflow includes an mzCloud search, the processing computer must have Internet access. To verify whether the processing computer can access the mzCloud database, run the Communication tests.

Table 68 describes the parameters for the Search mzCloud node.

Table 68. Search mzCloud node parameters (Sheet 1 of 5)

Parameter	Description
1. General Settings	
Compound Classes	Specifies the compound classes for the search. Select **All** or select specific classes. Default: All
Precursor Mass Tolerance	Specifies the tolerance for the precursor mass. Default: 10 ppm; range: 0–0.1 Da or 0–20 ppm
FT Fragment Mass Tolerance	Specifies the mass tolerance for high-resolution fragmentation scans performed in the Orbitrap analyzer (FTMS). Default: 10 ppm; range: 0–0.5 Da or 0–100 ppm
IT Fragment Mass Tolerance	Specifies the mass tolerance for low-resolution fragmentation scans performed in the ion trap analyzer (ITMS). Default: 0.4 Da; range: 0–0.1 Da or 0–20 ppm
Library	Specifies the mzCloud library for the search: Autoprocessed, Reference, or both. • Reference library—Contains only spectra that have been manually curated by mass spectrometry experts. • Autoprocessed library—Contains spectra curated with an automated process. As time permits, spectra in the Autoprocessed library are manually curated and transferred to the Reference library.
Post Processing	Specifies whether to search the library for filtered or recalibrated spectra. Selections: • Filtered—Removes extraneous mass peaks that do not match the theoretical mass spectrum. • Recalibrated (Default)—The mass peaks for the known ion fragments are recalibrated to match the theoretical mass spectrum by a series of manually supervised ion calibration steps.

Table 68. Search mzCloud node parameters (Sheet 2 of 5)

Parameter	Description
Max. # Results	Specifies the maximum number of hits for each compound, for each fragmentation spectrum in the spectrum tree for the compound, and for each search library to store in the result file. Displays the hits with the highest match score above the cutoff storage number in the result file. For example, if you specify 2 as the maximum number of results per compound and select two libraries to search, the search returns up to four results for a compound that has one fragmentation scan in its spectrum tree and up to eight results for a compound that has two fragmentation scans in its spectrum tree. Default: 10; range: 1 to 50
Annotate Matching Fragments	Specifies whether the processing workflow annotates the matching fragments with structures that you can review in the Spectrum view of the result page. Default: False
Search MSn Tree	Specifies whether the analysis submits the full MSn spectral tree for the database search. Default: False

Table 68. Search mzCloud node parameters (Sheet 3 of 5)

Parameter	Description
2. DDA Search	
Identity Search	Specifies the identity search algorithm. Selections: • HighChem DP—Alternative score using a modified dot product algorithm that includes a "hard penalty" function for spectra with a low number of fragment ions. • HighChem HighRes—Use for high-resolution data. Correlation algorithm that uses the geometric mean of a modified Spearman's rank order correlation to separately determine the intensity and *m/z* accuracy of the fragment ions. • NIST • Cosine—Dot product algorithm with fragment intensities weighted by 0.75 and no weighting on fragment *m/z* values. Default: HighChem HighRes
Match Activation Type	Specifies whether to only search for fragmentation spectra with the same activation type. Default: True
Match Activation Energy	Specifies whether to search for fragmentation spectra generated by the same ion activation energy within a tolerance or by any ion activation energy. Default: Match with Tolerance
Activation Energy Tolerance	Specifies the tolerance as an absolute value for the ion activation energy used to generate the fragmentation spectrum. For example, if the ion activation energy used to generate your spectrum was a normalized collision energy of 35% and you specify an ion activation energy tolerance of ±20, the search looks for spectra with an ion activation energy from 15 to 55. Default: 20; range: 0 to 200

Table 68. Search mzCloud node parameters (Sheet 4 of 5)

Parameter	Description
Apply Intensity Threshold	Specifies whether to apply an automatic intensity threshold that sets the threshold intensity by calculating the spectrum noise level. Default: True
Similarity Search	Specifies the similarity search algorithm. Selections: • None (Default)—Does not run a similarity search. • Confidence Forward— Uses the dot product of the forward search match and distribution of peaks, and the ratio of the most intensive matching peaks as part of the similarity score. A higher similarity score indicates the extent to which the unknown component resembles the library compound. • Confidence Reverse—Uses the dot product of the reverse search match and distribution of peaks, and the ratio of the most intensive matching peaks as part of the similarity score. A higher similarity score indicates the extent to which the library compound resembles the unknown component. • Similarity Forward—Searches for a match between the best fragmentation scan for a compound (across the input file set) and a fragmentation scan in the mzCloud database. Unlike the Identity Search, this search ignores the *m/z* value of the precursor ion. • Similarity Reverse—Searches for a match between the fragmentation scans in the mzCloud database and the best fragmentation scan for a compound (across the input file set).
Match Factor Threshold	Specifies the minimum match factor for reporting a spectrum match. Default: 60; range: 0 to 100%

Table 68. Search mzCloud node parameters (Sheet 5 of 5)

Parameter	Description
3. DIA Search	
Use DIA Scans for Search	Specifies whether to submit data independent scans to the mzCloud database for a spectral search. Default: False **Note** Keep the default setting of False for GC CI data.
Max. Isolation Width [Da]	Specifies the maximum MS2 isolation width. The isolation width for a scan is listed in its scan header. Default: 500 Da; minimum width: 10 Da
Match Activation Type	See Match Activation Type under DDA Search. Default: False
Match Activation Energy	See Match Activation Energy under DDA Search. Default: Any
Activation Energy Tolerance	See Activation Energy Tolerance under DDA Search. Default: 100
Apply Intensity Threshold	See Apply Intensity Threshold under DDA Search. Default: False
Match Factor Threshold	See Match Factor Threshold under DDA Search. Default: 20

Search mzVault node

Use the Search mzVault node to search a local mass spectra database for compounds of interest.

For LC studies, this node requires input from the Group Compounds node or the Group Expected Compounds node. And it can process compounds from both of these nodes in one processing workflow.

For GC studies, this node requires input from the GC CI Deconvolution node.

The node creates the mzVault Results table. See "mzVault Results table."

❖ **To use mzVault libraries created with the mzVault 1.1 or earlier application**

Change the following settings:

- For the Match Ion Activation Type, select **False**.
- For the Match Ion Activation Energy, select **Any**.
- For the Match Ionization Method, select **False**.

Table 69 describes the parameters for the Search mzVault node.

Table 69. Search mzVault node parameters (Sheet 1 of 4)

Parameter	Description
1. Search Settings	
mzVault Library	Specifies the mzVault libraries to search. You can select one or more of the mzVault libraries in your Spectral Libraries list. See "Spectral Libraries view."
Compound Classes	Specifies the compound classes for the search. Select **All** or select specific classes. Default: All
Match Ion Activation Type	Specifies whether to only search for library scans that match the ion activation type of the query spectrum. Default: True
Match Ion Activation Energy	Specifies whether to search for library scans generated by the same ion activation energy within a tolerance of the query spectrum or by any ion activation energy. Default: Match with Tolerance
Ion Activation Energy Tolerance	Specifies the tolerance as an absolute value for the ion activation energy used to generate the fragmentation spectrum. For example, if the ion activation energy used to generate your spectrum was a normalized collision energy of 35% and you specify an ion activation energy tolerance of ±20, the search looks for spectra with an ion activation energy from 15 to 55. Default: 20; range: 0 to 200
Match Ionization Method	Specifies whether to only search for library spectra from the same ionization method (for example, HESI, APCI, and so on) as the query spectrum. Default: True

Table 69. Search mzVault node parameters (Sheet 2 of 4)

Parameter	Description
Apply Intensity Threshold	Specifies whether to apply an automatic intensity threshold that sets the threshold intensity by calculating the spectrum noise level. Default: True
Remove Precursor Ion	When set to True, the search ignores (removes from consideration) mass peaks within 2.2 Da of the precursor ion's *m/z* value in the query spectrum—that is, the match score is not negatively affected if the library spectrum does not include a mass peak within 2.2 Da of the *m/z* value for the precursor ion. Default: True
Precursor Mass Tolerance	Specifies the tolerance for the precursor mass. Default: 10 ppm; range: 0 to 0.1 Da or 0 to 20 ppm
FT Fragment Mass Tolerance	Specifies the mass tolerance for high-resolution fragmentation scans performed in the Orbitrap analyzer (FTMS). Default: 10 ppm; range: 0 to 0.5 Da or 0 to 100 ppm
IT Fragment Mass Tolerance	Specifies the mass tolerance for low-resolution fragmentation scans performed in the ion trap analyzer (ITMS). Default: 0.4 Da; range: 0 to 0.1 Da or 0 to 20 ppm
Match Analyzer Type	Specifies whether to only search for library spectra from the same mass analyzer type as the query spectrum. Default: True

Table 69. Search mzVault node parameters (Sheet 3 of 4)

Parameter	Description
Search Algorithm	Specifies the identity search algorithm. Selections: • HighChem DP—Alternative score using a modified dot product algorithm that includes a "hard penalty" function for spectra with a low number of fragment ions. • HighChem HighRes—Use for high-resolution data. Correlation algorithm that uses the geometric mean of a modified Spearman's rank order correlation to separately determine the intensity and *m/z* accuracy of the fragment ions. • NIST Default: HighChem HighRes
Match Factor Threshold	Specifies the minimum match factor for reporting a spectrum match. Default: 50; range: 0 to 100%
Max. # Results	Specifies the maximum number of hits for each compound, for each fragmentation spectrum in the spectrum tree for the compound, and for each search library to store in the result file. Displays the hits with the highest match score above the cutoff storage number in the result file. For example, if you specify 2 as the maximum number of results per compound and select two libraries to search, the search returns up to four results for a compound that has one fragmentation scan in its spectrum tree and up to eight results for a compound that has two fragmentation scans in its spectrum tree. Default: 10

Table 69. Search mzVault node parameters (Sheet 4 of 4)

Parameter	Description
RT Tolerance [min]	Specifies the retention time tolerance for the library search. Default: 2; range: 0 to 10 minutes
Use Retention Time	Specifies whether to filter the database hits by their retention time. Filters out scans without retention time information. Default: False

Pathway Mapping nodes

Use these nodes to map detected compounds to a biochemical pathway:

- Map to BioCyc Pathways node
- Map to KEGG Pathways node
- Map to Metabolika Pathways node

Map to BioCyc Pathways node

Use the Map to BioCyc Pathways node to map the BioCyc pathways for each compound. The input to this node is a list of molecular weights, chemical formulas, or both. For LC studies, the Group Compounds node and the Group Expected Compounds node provide this input.

The Map to BioCyc Pathways node adds the following items to the result file:

- The BioCyc Pathways and BioCyc Results main tables
- The #BioCyc Pathways and BioCyc Pathways columns in the main compounds table
- The BioCyc Compound IDs, BioCyc Compound Names, and BioCyc Compound Formula columns in the related compounds table and the related BioCyc Pathways table.

Table 71 describes the parameters for the Map to BioCyc Pathways node.

Table 70. Map to BioCyc Pathways node parameters (Sheet 1 of 2)

Parameter	Description
1. Search Settings	
BioCyc Database/Organism to be Searched	Specifies the databases for the search.

Table 70. Map to BioCyc Pathways node parameters (Sheet 2 of 2)

Parameter	Description
Search Mode	Default: By Formula or Mass Selections: By Formula or Mass, By Formula Only, By Mass Only
2. By Mass Search Settings	
Mass Tolerance	Specifies the mass tolerance that the node uses to search for matching compounds. Default: 5 ppm; range: 0.1 to 20 ppm
3. By Formula Search Settings	
Max. # of Predicted Compositions to be Searched per Compound	Specifies the maximum number of predicted compositions to search for per compound. Default: 3; range: 1 to 100
4. Display Settings	
Maximum # of Pathways in "Pathways" Column	Specifies the maximum number (n) of pathways to display by name in the Pathways column of the Compounds result table. The Pathways column displays the names of the first $n - 1$ pathways that include the compound. The other pathways that include the compound are grouped in the Other category. Default: 20; range: 1 to 30

Map to KEGG Pathways node

The KEGG (Kyoto Encyclopedia of Genes and Genomes) pathway database contains connection diagrams of molecular interactions, reactions, and relations.

Use the Map to KEGG Pathways node to add explanations to the result file about the reaction pathways for each detected compound.

The node requires the following input— a list of molecular weights or chemical formulas. For LC studies, the KEGG node requires input from the Group Compounds node, the Group Expected Compounds node, or both of these nodes.

The Map to KEGG Pathways node adds the following items (output) to the result file:

- The KEGG Pathways table
- The KEGG Compound IDs, KEGG Compound Names, and KEGG Compound Formula columns in the related compounds table
- The #Pathways and Pathways columns in the main compounds table

When the processing workflow includes the Map to KEGG Pathways node, the processing computer must have Internet access. To verify whether the processing computer can access the KEGG Pathways database, run the communication test as described in Chapter 17, "Test communication to the online databases."

Table 71 describes the parameters for the Map to KEGG Pathways node.

Table 71. Map to KEGG Pathways node parameters

Parameter	Description
1. Search Settings	
Search Mode	Specifies the search mode. Default: By Formula or Mass Selections: By Formula or Mass, By Formula Only, By Mass Only
2. By Mass Search Settings	
Mass Tolerance	Specifies the mass tolerance that the node uses to search for matching compounds. Default: 5 ppm; range: 0.1 to 20 ppm
3. By Formula Search Settings	
Max. # of Predicted Compositions to be Searched per Compound	Specifies the maximum number of predicted compositions to search for per compound. Default: 3; range: 1.0
4. Display Settings	
Maximum # of Pathways in "Pathways" Column	Specifies the maximum number (n) of pathways to display by name in the Pathways column of the Compounds result table. The Pathways column displays the names of the first $n - 1$ pathways that include the compound. The other pathways that include the compound are grouped in the Other category. Default: 20; range: 1–30

Map to Metabolika Pathways node

To search your local database of Metabolika pathways for pathways that include matching structures for the unknown compounds in your data set (by formula, mass, or both), add the Metabolika Pathways node to the processing workflow and select the pathways to search.

Note 378 Metabolika pathway files are automatically installed with the application. You can edit these pathways or create your own pathways by using the Metabolika pathway editor. For details, see "Metabolika Pathways view."

Table 72 describes the parameters for the Map to Metabolika Pathways node.

Table 72. Map to Metabolika Pathways node parameters

Parameter	Description
1. Search Settings	
Metabolika Pathways	Specifies the Metabolika pathways to search. Default: All
Search Mode	Specifies whether to search by formula, mass, or both. Default: By Formula or Mass Selections: By Formula or Mass, By Formula Only, By Mass Only
2. By Mass Search Settings	
Mass Tolerance	Specifies the mass tolerance that the node uses to search for matching compounds. Default: 5 ppm; range: 0.1 to 20 ppm
3. By Formula Search Settings	
Max. # of Predicted Compositions to be Searched per Compound	Specifies the maximum number of predicted compositions to search for per compound. Default: 3; range: 1 to 100
4. Display Settings	
Maximum # of Pathways in "Pathways" Column	Specifies the maximum number (n) of pathways to display by name in the Pathways column of the Compounds result table. The Pathways column displays the names of the first $n - 1$ pathways that include the compound. The other pathways that include the compound are grouped in the Other category. Default: 20; range: 1 to 30

Compound Scoring nodes

Use the nodes under Compound Scoring to score the explanations for each detected compound.

The Calculate Mass Defect, Compound Class Scoring, Pattern Scoring, and Search Neutral Losses nodes require input from the Group Compounds node. The Generate Molecular Networks node requires input from the Assign Compound Annotations node, and the Apply mzLogic and Apply Spectral Distance nodes take input from the Search ChemSpider node.

See these topics:

- Apply Spectral Distance node
- Apply mzLogic node
- Calculate Mass Defect node
- Compound Class Scoring node
- Generate Molecular Networks node
- Pattern Scoring node
- Search Neutral Losses node

Apply Spectral Distance node

Use the Apply Spectral Distance node to calculate a spectral similarity score (SFit[%]) for the compound annotations. The SFit[%] column appears in the related "compound annotations" tables for the compound selected in the Compounds table. Depending on the processing workflow, the related "compound annotations" tables can include any of these tables: ChemSpider Results, Mass List Search Results, Metabolika Results, and BioCyc Results. In addition to providing an SFit score for you to review in the related "compound annotations" tables, the node sends the scores to the Assign Compound Annotation node.

Table 73 describes the parameters for the Apply Spectral Distance node.

Table 73. Apply Spectral Distance node parameters

Parameter	Description
1. General Settings	
Mass Tolerance	Specifies the mass tolerance that the node uses to search for matching mass peaks. Search range = expected mass ± mass tolerance/1e6 Default: 5 ppm; range: 0.1 to 20 ppm
Intensity Tolerance [%]	Specifies the relative intensity tolerance of the mass spectral peaks in the isotope pattern. Default: 30; range: 0 to 100%
Intensity Threshold [%]	Specifies the isotope intensity threshold, relative to the base peak of the isotope pattern, that the node uses for pattern simulation. The node does not add isotopes below this threshold to the simulated pattern. Default: 0.1
S/N Threshold	Specifies the signal-to-noise threshold for the isotope search. The node does not include isotopes that are expected to be below this threshold in the SFit score—that is, these isotopes are not required in the measured isotope pattern. Default: 3
Use Dynamic Recalibration	Specifies whether to shift the theoretical isotope pattern if the pattern base peak in the query spectrum is shifted. Default: True

Apply mzLogic node

Use the Apply mzLogic node to score explanations from the ChemSpider node, Search Mass List node, Map to BioCyc Pathways node, and Map to Metabolika Pathways node.

Table 74. Apply mzLogic node parameters

Parameter	Description
1. Search Settings	
Max # Compounds	Specifies the maximum number of compounds to display and score in the result table. Default: 0 (no maximum limit)
Max # mzCloud Similar Results to Consider per Compound	Specifies the maximum number of compounds to consider from an mzCloud similarity search. Increasing the number of compounds to consider increases the processing time. Range: 5 to 100
Match Factor Threshold	Specifies the minimum match score returned for a compound by an mzCloud similarity search. The analysis ignores compounds with match scores below this threshold. Default: 30
Advanced parameters	
FT Fragment Mass Tolerance	Specifies the mass tolerance for the mass peaks in high-resolution fragmentation spectra when searching the mzCloud spectral database. Default: 10 ppm; range: 0 to 0.5 Da or 0 to 100 ppm
IT Fragment Mass Tolerance	Specifies the mass tolerance for the mass peaks in low-resolution fragmentation spectra when searching the mzCloud spectral database. Default: 0.4 Da; range: 0 to 1 Da or 0 to 1500 ppm

Calculate Mass Defect node

Use this node to calculate the mass defect for each detected compound. You can specify up to four calculation methods and up to five Kendrick formulas. This node adds the Mass Defect column to the Compounds table for reviewing the result of the specified calculations.

Table 37 describes the parameters for the Filter By Mass Defect node.

Table 75. Filter By Mass Defect node parameters

Parameter	Description
1. Mass Defect	
Fractional Mass	Fractional Mass = exact mass – floor (exact mass)
Standard Mass Defect	Standard Mass Defect = exact mass – nominal mass
Relative Mass Defect	Relative Mass Defect = 1e6 × (exact mass – nominal mass)/exact mass
Kendrick Mass Defect	Kendrick Mass Defect = Kendrick mass –nominal Kendrick mass Kendrick mass – nominal Kendrick mass where: Kendrick mass = a × (b/c) a = exact mass of the elemental composition b = nominal mass of the Kendrick formula c = exact mass of the Kendrick formula
Nominal Mass Rounding	Specifies how the node calculates nominal masses. Default: Round Selections: • Floor rounds down. • Ceiling rounds up. • Round rounds to the nearest integer value.
2. Kendrick Formulas	
When you select Kendrick Mass Defect as the Mass Defect Type, this user-specified elemental composition specifies the Kendrick formula.	
Formula 1–5	Use to add Kendrick formulas.

Compound Class Scoring node

Use the Compound Class Scoring node to score detected compounds against a set of fragment ions commonly present in the fragmentation scans for a compound class. The node compares the ions (*m/z* values) detected in the fragmentation scans to the fragments in the selected compound class libraries.

In a processing workflow, connect the Group Compounds node to the Compound Class Scoring node.

The Compound Class Scoring node does the following:

- Annotates the centroids in the fragmentation scans for a compound with the matching fragment structures from the selected compound class libraries.
- Provides a Class Coverage score in the Mass Spectrum view legend.
- Adds the Class Coverage column with the percent coverage to the Compounds table.
- Creates the Compound Class Matches Table—a table related to the Compounds table.

When you add the Compound Class Scoring node to a processing workflow, you must select the compound class fragment lists.

For information about adding compound class fragment lists to the Compound Classes library, see "Compound Classes view."

Table 76 describes the parameters for the Compound Class Scoring node.

Table 76. Compound Class Scoring node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Compound Classes	Select the compound classes that you want to use for the fragment search. Compound classes contain a list of fragment structures and *m/z* values that the application compares to the fragmentation scans for each detected compound. For details, see "Compound Classes view."
S/N Threshold	Specifies the signal-to-noise threshold for the centroids in the fragmentation spectra. The application ignores centroids below the signal-to-noise threshold. The application attempts to match centroids with *m/z* values above the threshold to the fragment structures in the selected compound classes. Default: 50

Table 76. Compound Class Scoring node parameters (Sheet 2 of 2)

Parameter	Description
High Acc. Mass Tolerance	Specifies the mass tolerance for high-resolution mass spectra measured in the Orbitrap mass analyzer of a Thermo Scientific mass spectrometer. Default: 2.5 mmu; Minimum: 0.0; Maximum: Unchecked
Low Acc. Mass Tolerance	Specifies the mass tolerance for low-resolution mass spectra measured in the ion trap mass analyzer of a Thermo Scientific mass spectrometer. Default: 0.5 Da; Minimum: 0.0; Maximum: Unchecked
Use Full MS Tree	Specifies whether scoring is applied on the full spectrum tree or only the MS2 scans.
Allow DIA Scoring	Specifies whether the node uses DIA scans for scoring when there are no available data-dependent scans. If set to false, the node annotates DIA scans, but it does not use them for scoring. Default: True

Generate Molecular Networks node

Use the Generate Molecular Networks node to determine and visualize the similarity between various compounds in the Compounds table for LC studies.

Note For LC studies, the Assign Compound Annotations node connects to the Generate Molecular Networks node.

Table 77 describes the parameters for the Generate Molecular Networks node.

Table 77. Generate Molecular Networks node parameters (Sheet 1 of 4)

Parameter	Description
1. Spectral Similarity	
These parameters define how fragmentation spectra are compared to determine the similarity score between two compounds.	
Use Full MSn Tree	Specifies whether the node determines the spectral similarity from the full MSn tree or only from the MS2 spectra. Default: True (uses the full MSn tree)

Table 77. Generate Molecular Networks node parameters (Sheet 2 of 4)

Parameter	Description
Match Mass Shift	For fragments that are not a direct match by mass, specifies whether the shift to the fragment mass must match the mass shift between the two compounds. Default: True
Match Transformations	For fragments that are not a direct match by mass, specifies whether the shift to the fragment's mass must match the mass of the assigned transformation between the two compounds. Default: True
Variate Transformations	For fragments that are not a direct match by mass, specifies whether the masses of all the variations of the individual steps of the assigned transformation between the two compounds are used as the expected fragments shifts. Fragments shifted by these masses are considered as matching. Default: False
S/N Threshold	Specifies the signal-to-noise threshold for the centroids in the fragmentation spectra. The node ignores centroids below the signal-to-noise threshold—that is, the node attempts to match only centroids with *m/z* values above the threshold. Default: 3
Mass Tolerance	Specifies the mass tolerance to use for fragments matching. Default: 2.5 mmu
Min. Fragment m/z	Specifies the minimum *m/z* values of the centroids to consider. Default: 50
2. Transformations	
Phase I	Specifies the set of possible single-step Phase 1 transformations. Default: All check boxes are clear.
Phase II	Specifies the set of possible single-step Phase II transformations. Default: All check boxes are clear.
Others	Specifies other possible single-step transformations. The node treats Others transformations as Phase I transformations.

Table 77. Generate Molecular Networks node parameters (Sheet 3 of 4)

Parameter	Description
Max. # Phase II	Specifies the maximum number of Phase II steps to be applied. Default: 1; range: 1 to 10
Max. # All Steps	Specifies the maximum number of all steps to be applied. All steps that occur as a result of the selections in the Dealkylation area equal one step in the maximum number of all steps—that is, after the node applies the steps in the Dealkylation area, the remaining number of possible steps is equal to the Max. # All Steps – 1. Default: 3; range: 1 to 10
3. Applied View Filters These parameters filter out (hide) connections with lower confidence in the Similar Compounds table for a compound. This filtering has no effect on the stored data—that is, you can click the filter icon on the Similar Compounds tab to undo all of these filters.	
Require Transformation	When set to True, similar compounds without assigned transformations are hidden. Default: True
Require MSn	When set to True, similar compounds without a spectral similarity score are hidden.
Min. MSn Score	Specifies the minimum MSn Score value for a similar compound. If a similar compound has no fragmentation data, the application does not apply this filter.
Min. MSn Coverage	Specifies the minimum Forward or Reverse Coverage value for a connection. The connection is hidden only if both values are below this threshold. If a similar compound has no fragmentation data, the application does not apply this filter.
Min. # Fragments	Specifies the minimum Forward or Reverse Matches value for a connection. The connection is hidden only if both values are below this threshold. If a similar compound has no fragmentation data, the application does not apply this filter. Default: 3

Table 77. Generate Molecular Networks node parameters (Sheet 4 of 4)

Parameter	Description
4. Applied Thresholds	
These parameters define the filtering rules for storing connections. The application does not store connection that fall below these thresholds. The main purpose of these filters is to reduces the amount of stored data by removing low confidence connections.	
Require Transformation	If set to True, removes connections without assigned transformations. Default: False
Require MSn	If set to True, removes connections without a spectral similarity score. Default: False
Min MSn Score	Specifies the minimum MSn Score value for a stored connection. If the connection has no fragmentation data, the application does not apply this filter and stores the connection if it passes the other filters. Default: 20; range 0 to 100
Min MSn Coverage	Specifies the minimum Forward or Reverse Coverage value for storing a connection. The application removes the connection only if both values are below this threshold. If the connection has no fragmentation data, the application does not apply this filter and stores the connection if it passes the other filters. Default 20; range 0 to 100
Min. # Fragments	Specifies the minimum number of matched fragments for storing a connection; that is, if both of these match scores are below the user-specified threshold, the application does not store the connection. If the connection has no fragmentation data, the application does not apply this filter and stores the connection if it passes the other filters. Default: 0

Pattern Scoring node

Use the Pattern Scoring node to provide a spectrum fit score (SFit%) for each detected compound in the Compounds table (LC studies). The Pattern Scoring node compares the measured isotope pattern for each detected compound to a defined isotope pattern—that is, it compares the mass shifts and intensities of the centroids in the isotope pattern for the detected compound to set of defined mass shifts and relative intensities. Use the Pattern List Editor dialog box to store defined isotope patterns for your analyses.

The Pattern Scoring node adds the Pattern Matches column to the compounds table and creates the related Matched Patterns Table.

Table 78 describes the parameters for the Pattern Scoring node.

Table 78. Pattern Scoring node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Isotope Patterns	Specifies the isotope patterns to be used for scoring. For information about setting up the isotope patterns, see Set up individual isotope patterns by using the Isotope Ratio Editor and Create an isotope patterns list by using the Pattern List Editor.
Mass Tolerance	Specifies the mass tolerance for calculated elemental compositions and pattern matching. Default: 5 ppm; range: 0.0 to no limit
Intensity Tolerance [%]	Specifies the relative intensity tolerance of the mass spectral peaks in the isotope pattern. Default: 30; range: 0.01 to 100.0
S/N Threshold	Specifies the signal-to-noise threshold for the search. The application ignores isotopes with a theoretical intensity value below this threshold.
Min. Spectral Fit [%]	Specifies the minimum required spectral fit value as a percentage. Range: 0 to 100%

Table 78. Pattern Scoring node parameters (Sheet 2 of 2)

Parameter	Description
Preferred Ions	Specifies the preferred adduct ions for matching the isotope patterns for compounds. When this selection is empty, the node evaluates all the adduct ions present across the input files. An empty selection for this parameter generates a validation prompt when you submit the analysis to the run queue.

Search Neutral Losses node

Table 79 describes the parameters for the Search Neutral Losses node. This node generates the Neutral Losses column in the Compounds table and the Neutral Losses table.

Table 79. Search Neutral Losses node parameters

Parameter	Description
1. General Settings	
Neutral Losses	Specifies the neutral losses for the search. The dropdown list includes all the neutral losses in the Lists & Libraries > Neutral Losses view. See "Neutral Losses view."
High Accuracy Mass Tolerance	Specifies the mass tolerance to be used for searching fragments within high-accuracy MS2 scans such as those from the Thermo Scientific Orbitrap MS.
Low Accuracy Mass Tolerance	Specifies the mass tolerance to be used for searching fragments within low-accuracy MS2 scans such as those from an ion trap mass analyzer.
S/N Threshold	Specifies the signal-to-noise threshold for the search. The application ignores spectral peaks (centroids) with an intensity value below this threshold.
Use DIA Scans for Search	Specifies whether to search data-independent scans such AIF scans for fragments in addition to searching the data dependent (DDF) scans.

Post-Processing nodes

These nodes provide additional information about the detected or found compounds.

- Descriptive Statistics node
- Differential Analysis node

- Export Xcalibur Inclusion or Exclusion List node
- Result Exporter node
- Scripting Node

Descriptive Statistics node

Use the Descriptive Statistics node to store descriptive statistics for each expected or unknown compound in the result file and add the following hidden columns to the Compounds and Expected Compounds tables: Mean Area, Median Area, Minimum Area, Q1 Area, and Q3 Area.

To store the descriptive statistics in the result file, the processing workflow must include the Group Expected Compounds node for targeted workflows and the Group Compounds node for untargeted workflows.

The Descriptive Statistics node has no parameters.

Note The Descriptive Statistics node generates the descriptive statistics for individual compounds; it has no effect on the Descriptive Statistics view that is available for a result file.

Differential Analysis node

Use the Differential Analysis node to calculate the statistics for a differential analysis (fold change, ratio, p-values, and so on), store this data in the result file, and create a volcano plot in the Differential Analysis view by using the data stored in the compounds table (Compounds table or Expected Compounds table). A volcano plot is a type of scatter plot for replicate data where the *x* axis represents the $\log_2$ of the fold change between two sample groups (generated ratio), and the *y* axis represents the negative $\log_{10}$ of the p-value (test of significance) of the fold change.

This node requires input from a compounds node for a sample set with replicate data points and generated ratios. If the Grouping & Ratios page of an analysis does not contain generated ratios, the following confirmation message appears:

No quan ratios defined in ‘Grouping & Ratios’ tab

Table 80 describes the parameter for the Differential Analysis node.

Table 80. Differential Analysis node parameters

Parameter	Description
1. General Settings	
Log10 Transform Values	Specifies whether to calculate $\log_{10}$ values of the chromatographic peak areas before storing the data in the result file. Default: True
2. Peak Rating Contributions	
These parameter settings determine how the node calculates the peak rating values for chromatographic peaks. See "Chromatographic peak rating filter." The maximum value for each contributing parameter is unlimited. The contribution of each individual parameter is as follows: (Contribution value for the individual parameter/Divided by the sum of all the contribution values)×10.	
Area Contribution	Specifies the chromatographic peak area contribution to the peak rating. Default: 3
CV contribution	Specifies the contribution of the coefficient of variation for the peak areas across replicate samples to the peak rating. If an analysis includes no replicates, the node sets the CV contribution to 0 during processing. Default: 10
FWHM to Base Contribution	Specifies the FWHM to base contribution to the peak rating. Default: 5
Jaggedness Contribution	Specifies the jaggedness contribution to the peak rating. Default: 5
Modality Contribution	Specifies the modality contribution to the peak rating.
Zig-Zag Index Contribution	Specifies the zig-zag index contribution to the peak rating. Default: 5

Export Xcalibur Inclusion or Exclusion List node

Use the Export Xcalibur Inclusion/Exclusion List node to create an Inclusion/Exclusion mass list for a Thermo Scientific mass spectrometer.

Table 81 describes the parameters for the Export Xcalibur Inclusion or Exclusion List node.

Table 81. Export to Xcalibur Inclusion/Exclusion List node parameters

Parameter	Description
1. General Settings	
File Name	Specifies the file name for the inclusion/exclusion list.
Selected Instrument	Bases the format of the inclusion/exclusion list on the selected MS. Selections: LTQ Orbitrap, Orbitrap Fusion, Q Exactive
2. Use Filter Set	
Add Filter Set	Specifies the filters sets (FILTERSET file type) that you want to apply to the generated inclusion list or exclusion list.
3. Advanced Settings	
Left RT [min]	Specifies the window to the left of the specified retention time for a mass. Default: 1 min; range: 0.001 to 1000 min
Right RT [min]	Specifies the window to the right of the specified retention time for a mass. Default: 1 min; range: 0.001 to 1000 min
Include Isotopic Peaks	Specifies whether to include isotopic peaks in the list. Default: False
4. LTQ Orbitrap Settings	
Maximum Concurrent Entries	Specifies the maximum number of entries with overlapping time windows. Default: 500; range: 1 to 2000
Mass Precision Decimals	Specifies the required number of decimal places for the mass values. Default: 5

Result Exporter node

Use the Result Exporter node to export the data in each result table to a spreadsheet or text file. The application exports separate files for each result table.

Table 82 describes the parameters for the Result Exporter node.

Table 82. Result Exporter node parameters

Parameter	Description
1. Output Data	
File Name	Specifies the base file name for the exported TXT or XLS files. When the file name is not specified, the application uses the name of the result file for the exported TXT or XLS files. Default: Empty—The application uses the name of the result file.
Export Format	Specifies the file format for the exported data. Default: No selection; selections: Excel or Text
Exports All Columns	Specifies whether all the columns in the result file tables are exported to the selected file type. Default: False—The application exports only the visible columns in the result file to the user-selected file format.
2. Text Export Options	
R-Friendly Columns	Specifies whether the column names are R-Friendly. Applies only to TXT files. Default: False

Scripting Node

Use the Scripting Node to perform custom post-processing actions on the data in the result tables.

Tip For information about using the Scripting node, go to the Resources page of the following web site: https://mycompounddiscoverer.com/.

Table 83 describes the parameters for the Scripting node.

Table 83. Scripting node parameters

Parameter	Description
Executable and Parameters	
Path to Executable	Specifies the path to the executable file, for example, c:\Python37\python.exe.
Command Line Arguments	Specifies command line arguments provided to the executable, for example, "d:\My Scripts\script.py \" %NODEARGS%.
Requested Tables and Columns	Specifies the requested result table columns for the executable. If you specify a table without specifying specific columns in the table, the node exports the entire table. Use a colon to separate the table name from the table columns, a comma to separate the table columns, and a semicolon to separate tables. Format: TableName1: Column1, Column2; TableName2: Column3, Column4 To enter this list, do the following: 1. Click the browse icon. The Edit Parameter Text for Requested Tables and Columns dialog box opens. 2. Do one of the following: • Enter the tables and columns requested. Use a new line for each table. • Click **Load File**, select a text file that contains the table and column information, and click **Open**. 3. Click **OK**.
Use R-Friendly Columns	Specifies whether the column names are R-Friendly. Default: True
Archive Datafiles	Specifies whether the node creates an archive containing the JSON files and the text (.txt) files. Default: False

8

Review the analysis results

The Compound Discoverer application stores the results of an analysis in a result file (CDRESULT).

The following topics describe how to open result files, filter the result tables, edit the compound annotations, propose custom structures, modify the layout of a result page, and export mass lists and spectral data.

- Open, close, and update result files
- Factory default layout for a result page
- Modify the result page layout for ease of use
- Custom color-coded tags for result table entries
- Save, restore, and manage layouts
- Edit compound annotations
- Add or delete proposed structures for a compound
- Replace an annotation with a structure proposal
- Apply FISh scoring
- Filter the data for data reduction
- View the result summaries
- Shortcut menu commands for the result tables
- Export the tabular data in a result file to an external file
- Export spectral data to a new or existing mzVault library
- Export compounds to a new or existing mass list
- Copy or save graphical views for publication
- Copy structures to the Clipboard for use in other applications

For details about each of the graphical views and result tables, see these chapters:

- Chapter 9, "Graphical views for a result file."
- Chapter 10, "Descriptive information for the result tables."

Open, close, and update result files

During an analysis, the Compound Discoverer application processes a set of input files (Xcalibur RAW files) by using a processing workflow and stores the processing results in a result file (CDRESULT).

Note Result files are also known as analysis results, as you can open them from the Analysis Results page of a Compound Discoverer study.

When you open a result file for the first time, you see a tabbed document with the default layout in the application window. You can modify the layout and save these changes with the result file. The next time you open the result file, it will open with your custom layout.

To open a result file from a previous version of the application, you must update the file to the current version.

For instructions on how to open, close, and update result files, see these topics:

- Open result files created in the current version of the application
- Open result files created in previous versions of the application
- Update modes for legacy result files
- Close a result file

Open result files created in the current version of the application

You can open a result file from the application window, the Start Page, the Job Queue page, or the Analysis Results page. A result file opens as a tabbed document. The tab displays the file name of the result file (*File Name* X).

❖ To open a result file created in the current version of the application

- From the application window, do one of the following:
  - From the menu bar, choose **File > Open Result**. In the Open dialog box, browse to the appropriate folder, select the result file of interest, and click **Open**.
  - From the menu bar, choose **File > Recent Results > *recent result file***.
- From the Start Page, do one of the following:
  - Under Recent Results, click the blue link for the result file of interest.

  - Under What Would You Like to Do?, click **Open Result**.

- From the Job Queue page, do one of the following:
  - Double-click the table row for a completed job.
  - Select the table row of a completed job and click **Open Results**.
- From the Analysis Results page, do one of the following:
  - Double-click the table row for a completed analysis.
  - Select the file of interest and click **Open Results**.

Tip You can also drag and drop result files (CDRESULT) from Windows Explorer into the application window.

You can open as many result files as you want. To view a particular result file, click its tab.

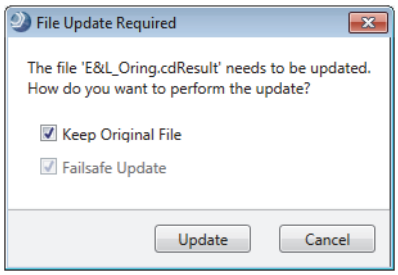
Open result files created in previous versions of the application

❖ **To open a result file from a previous version of the application**

1. From the menu bar, choose **File > Open Result**. In the Open dialog box, browse to the appropriate folder, select the result file of interest, and click **Open**.

   The File Update Required dialog box opens.

   Figure 85. File Update Required dialog box

2. Select one of the following update processes:
   - To retain the original result file, select the **Keep Original File** check box.

     The application then automatically selects the Failsafe Update check box.
   - To automatically delete the original file after the update process ends, select only the **Failsafe Update** check box.

     When the Failsafe Update check box is selected, the application automatically backs out of the update process if an error occurs.

   –or–

   - To minimize the processing time, clear both check boxes.

The application immediately processes the file without first creating a temporary file. Errors that occur during the update process can corrupt the file.

IMPORTANT To prevent loss of data when not using the fail-safe mode to update legacy result files, Thermo Fisher Scientific recommends that you manually store copies of these files in another directory.

3. To start the update process, click **Update**.

Update modes for legacy result files

When you attempt to open a legacy result file, the application prompts you to select an update process:

- Selecting the Keep Original File check box runs the update process in the fail-safe mode and renames the original result file with an appended version number. This option takes the most processing time, but it prevents data corruption of the original file.
- Selecting the Failsafe Update check box runs the update process in the fail-safe mode, but it does not save the original result file. If the update process fails, the application retains the original result file. You can make another attempt to update the file or you can open the file in a previous version of the application.

  Note You can install multiple versions of the Compound Discoverer application on the same data system computer.

- Clearing both check boxes turns off the fail-safe mode. This option takes the least amount of processing time, but it risks the possibility of corrupting the original file and making it unrecoverable.

In the fail-safe mode, the application does the following:

1. Creates a temporary file.
2. Runs the updates on the temporary file.
3. After completing the update process successfully, it does the following:
   a. Appends the application version to the file name of the original file. Because the application does not reprocess the original file, the file retains its original time stamp.
   b. Changes the file name extension of the temporary file to CDRESULT. The time stamp for the updated file corresponds to the completion of the update process.

   If the update process fails, the application does not rename the original file.

Close a result file

You can close a result file (CDRESULT) in one of two ways.

❖ **To close a result file**

- Right-click the tab and choose **Close**.

–or–

- Click the close icon on the document's tab ( ).

If the tab is not visible, click the Current Tabs icon, , and select the result file from the list. For details, see "Show, hide, and rearrange the tabbed pages of the application."

Factory default layout for a result page

When you open a result file, it appears as a tabbed page in the application window. See "Open, close, and update result files."

The factory default layout for a result page includes the following items:

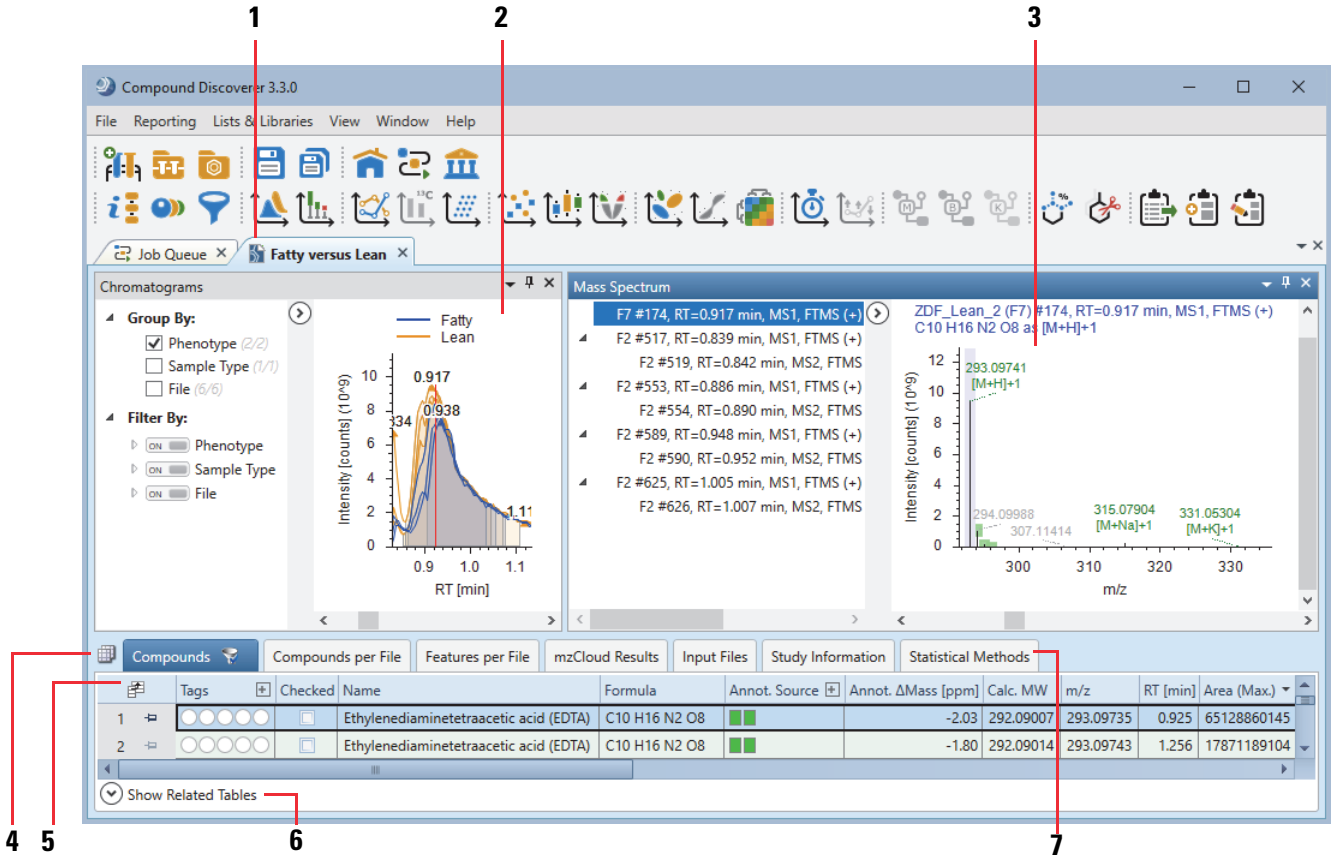
- A tab with the result file name
- For LC studies, the Chromatograms view on the top left is populated with XIC traces for the component with the largest chromatographic peak area across the input files—that is, the view is populated with the XIC traces for the compound listed in the first row of the Compounds table or the Expected Compounds table. The view is zoomed to the start and end points of the chromatographic peak.
- For LC studies, the Mass Spectrum view on the top right is populated with the MS1 scan with the highest resolution and highest intensity related to the preferred ions across the input files. The spectrum tree to the left includes the MS1 scans and the available fragmentation scans within the following time range for a compound:
  - Peak apex (RT) ± the peak's full width at half maximum (FWHM)

    –or–
  - Start and end points of the chromatographic peak, as determined by the peak detection algorithm

  –
- A set of tabbed main tables below the two graphical views
- A collapsed area for the related tables below the main tables

Figure 86 shows a result page for a result file generated with an untargeted processing workflow.

Figure 86. Default layout for a result page from an untargeted workflow (LC studies), numbered at the top left from 1 to 3 and from the bottom left from 4 to 7



No.	Description	No.	Description
1	Result file tab	5	Opens the Field Chooser dialog box for the current table
2	Chromatograms view with a collapsible pane at the left	6	Opens the related tables pane for the item that is currently selected in the active main table
3	Mass Spectrum view with a spectrum tree at the left	7	Main result tables
4	Opens the Select Visible Tables dialog box		

You can change the layout of a result file as follows:

- The views that you want to display and their location. See Chapter 9, "Graphical views for a result file."
- The main and related tables and table columns that you want to display and the order of the table columns from left to right. See Chapter 8, "Review the analysis results," "Show or hide result tables," and "Show or hide table columns."
- The data (table rows) displayed or hidden in the result tables. See "Filter the data for data reduction."

For more information, see "Modify the result page layout for ease of use."

Modify the result page layout for ease of use

The result file layout includes the relative positions of the graphical views, the visible result tables, the column arrangement and column fixing if it is enabled, and the applied result filters.

Tip For information about modifying the layout of the table columns and rows, see Chapter 15, "Common operations for manipulating data tables." This chapter describes how to hide or display specific table columns by using the Field Chooser dialog box, reorder or stack the table columns by using the mouse, and pin rows to the top of the tables.

These topics describe some of the ways that you can change the layout of a tabbed result page:

- Float a result page view
- Enlarge a result page view
- Use the collapsible pane options for filtering, grouping, coloring, and discriminating by
- Show or hide result tables

Float a result page view

❖ **To change a docked view on a result page to a floating view**

Do one of the following:

- Right-click the title bar of the view and choose **Floating**.
- Double-click the title bar of the view.

–or–

- Drag the view away from its docked position.

Enlarge a result page view

❖ **To enlarge a floating view for a result page to fill the screen**

Double-click the title bar of the view.

To restore the previous size of a floating window, double-click the title bar again.

Use the collapsible pane options for filtering, grouping, coloring, and discriminating by

These four views on a result page include a collapsible pane of filtering, grouping, coloring, or discriminating by options:

- Chromatograms view. See "Chromatograms view."
- Trend Chart view. See "Trend Chart view."
- Principal Component Analysis view. See "Principal Component Analysis view."
- Partial Least Squares Discriminant Analysis. See "Partial Least Squares Discriminant Analysis view."
- Descriptive Statistics view. See "Descriptive Statistics view."

Note If the analysis does not include samples with different study factor values or sample types, the application cannot group the samples, and only the Files check box appears in the Group By list.

Table 84 describes the effect of clearing and selecting the check boxes in the collapsible pane at the left of a view.

Table 84. Effect of clearing or selecting the check boxes in the collapsible pane

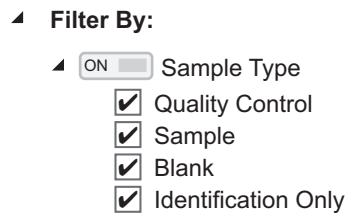
Objective	Selection
Remove or display data points	Use the check boxes under Filter By to remove or display data points by sample type, study factor value, or individual file. By default, the application selects all the check boxes under Filter By for the Chromatograms view. By default, the application does not select the Blank sample type or the Quality Control sample type check boxes for the statistics views, and the Identification Only sample type does not appear in the Sample Type list.
Visually distinguish data points by grouping them	For the Chromatograms view, use the check boxes under Group By to colorize the traces by group. The application duplicates the check boxes in the Study Variables area of the Grouping and Ratios page of the analysis. For the Trend Chart view, use the check boxes under Group By to change how the data points for the selected compound are grouped across the input files.
Distinguishing data point by color	For the Principal Component Analysis view, use the Color By check boxes to distinguish the principal components by color. For the Descriptive Statistics view, use the Color By check boxes to visually group the box plots by color.
Discriminate by specific study variables	For the Principal Least Squares–Discriminant Analysis view, use the Discriminate By check boxes to select the study variables for the supervised analysis.

Table 85 describes the Group By and Filter By options in the collapsible pane.

Table 85. Options in the collapsible left pane (Sheet 1 of 2)

Feature	Description
(*X*/*Y*)	The left integer is the number of samples that are selected under Filter By (and that also contain the selected compound). The right integer is the number of samples that contain the selected compound.
ON/OFF toggle for the Filter By items	ON—The check boxes are available. OFF—The check boxes are unavailable and the items are not filtered out.

Table 85. Options in the collapsible left pane (Sheet 2 of 2)

Feature	Description
Check boxes	
Group By *Study Variable*	Selecting one or more of these check boxes groups the samples with the same value or values for the selected study variable or variables and displays the groups in different colors. By default, the application duplicates the selection in the Study Variables pane on the Grouping and Ratios page of the analysis. Study variables include the study factor values and the sample types.
Group By Sample	Selecting this check box displays the data points for the selected samples in the Filter By area in different colors. Default: Clear
Filter By *Study Factor*	Select these check boxes to display data for one or more study factors. By default, the application selects all the study factors.
Filter By Sample Type	Select these check boxes to display data for one or more sample types. For the Chromatograms view, the application selects all sample types by default.  For the statistical views, the application excludes the Identification Only sample type and clears the Blank sample type check box. 
Filter By File	Select these check boxes to display data from one or more of the files. By default, the application selects all of the files.

For more information about using the options on the collapsible pane, see these topics:

- Filter the result data by the study variable values
- Filter the result data by input file
- Group the result data by the study variables or by individual files

Filter the result data by the study variable values

You can filter the data points displayed in a result page view by selecting or clearing the check boxes for the study variable values in the collapsible pane.

❖ To filter data points by the study variable values

1. If the collapsible pane is closed, click the icon,  , in the upper-left corner of the view.
2. Under Filter By, click the expand icon to the left of the study variable name to open the values list.
3. Clear the check boxes for the items that you want to hide or values that you want to remove from the statistical calculations.

Filter the result data by input file

You can filter the data points displayed in a result page view by selecting or clearing the check boxes for the input files in the collapsible pane.

❖ To filter the data by selected files

1. Under Filter By, click the expand icon to the left of File to open the File list.
2. Clear the check boxes for the files that you want to exclude from the display or the statistical calculations.

Note By default, for the statistical views, the check box for the Blank sample type under Filter By is clear.

Group the result data by the study variables or by individual files

You can group the data points displayed in a result page view by selecting or clearing the check boxes under Group By in the collapsible pane.

❖ To group the data points in a view

1. To group the data by the study variables or by the individual files, select a row in the active result table. Then, select one or more check boxes under Group By.
2. To view a color legend of the sample groups, right-click the Chromatograms view and choose **Display Options > Show Legend**.

Show or hide result tables

The set of result tables in a result file depends on the processing workflow. By default, some of the result tables are hidden.

❖ To show or hide result tables

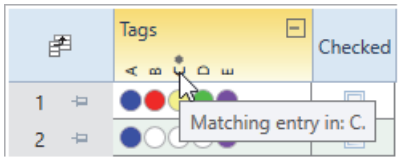
1. Open a result file. See "Open, close, and update result files."
2. Click the **Select Table Visibility** icon,  , to the left of the result table tabs.

   The Select Visible Tables dialog box opens.
3. Select the check box that corresponds to the table that you want to show, or clear the check box that corresponds to the table that you want to hide.
4. Click **OK** to accept the changes.

Custom color-coded tags for result table entries

In the result file tables that include the Tags column, you can label entries with color-coded name tags, and then use these tags to sort and filter the tables. You can customize the number of tags displayed (number of subcolumns in the Tags column), the tag names, and the tag colors.

Figure 87. Tags column showing selected tags with the standard colors and text labels



For details, see the following topics:

- Define custom tags by using the Custom Tags Editor
- Add or remove custom tags
- Filter a result table by the custom tags
- Import or export custom tags

Define custom tags by using the Custom Tags Editor

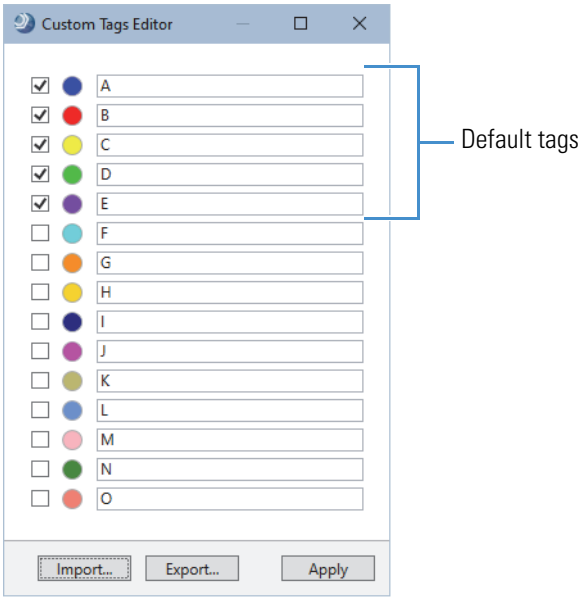
Use the Custom Tags Editor to customize the number of available tags and the colors and text labels for these color-coded tags in the Tags column of a result table.

By default, the Tags column contains five tags. From left to right, the subcolumn headings for the tags are labeled A, B, C, D, and E, and the tag colors are set to blue, red, yellow, green, and purple. You can change the number of tags to 0 or any integer value from 1 to 15 by selecting or clearing the check boxes in the Custom Tags Editor.

❖ To create a set of named and color-coded tags

1. Open a result file.
2. From the menu bar, choose **View > Custom Tags Editor**.

Figure 88. Custom Tags Editor with the default settings



3. (Optional) If you have created a stored custom tags file (.tags) and you want to edit it, do the following:

   a. Click **Import** and select the file that you want to edit.

   b. In the Custom Tags Editor, select the number of tags that you want to display in the Tags columns of the result tables in the current result file by selecting the check boxes.

4. To modify the colors and text labels for the tags, follow the instructions in Table 86.

   You use the Color dialog box to modify the colors.

Figure 89. Color dialog box

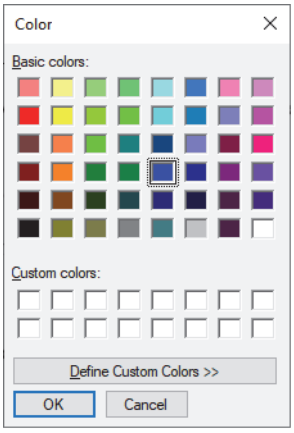
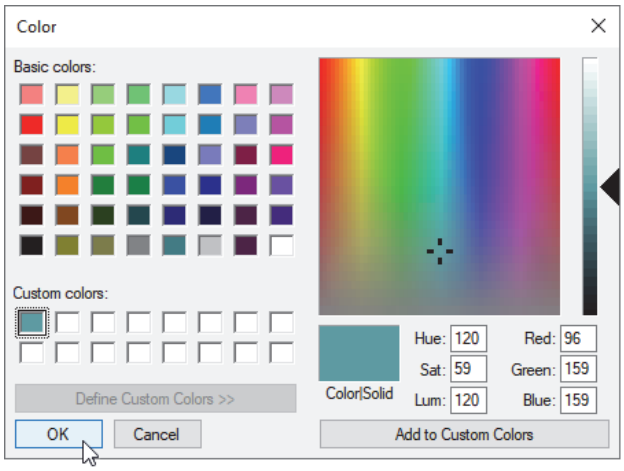


Table 86. Defining the tags for a result file

Task	Procedure
Change the color of a tag to a different standard color.	1. In the editor, click the color circle to the left of the name box. 2. In the Color dialog box, select a color from the set of basic colors and click **OK**.
Change the color of a tag to a custom color.	1. In the editor, click the color circle to the left of the name box. 2. In the Color dialog box, click **Define Custom Colors**. 3. Define a custom color by using the color gradient or entering the Red, Green, and Blue (RGB) values or the Hue, Saturation, and Luminosity (HSL) values, and then and click **Add to Custom Colors**. 4. Select the custom color and click **OK**.  The color of the selected tag in the Custom Tag Editor changes to the selected color.
Change the text label for a tag.	In the editor, select the current text in the text box, and then enter your custom text label.

5. To apply the custom settings in the Custom Tags Editor dialog box to the tags in the current result file, click **Apply**.

   The Custom Tags Editor dialog box remains open until you close it.

6. (Optional) To export the defined tags to an external file that you can use with any result file, do the following:
   a. Click **Export**.

      The Save Custom Tags Editor Settings dialog box opens.

   b. Name the file, select its storage location, and click **Save**.

Add or remove custom tags

The Tags column is available for most of the result tables in a result file. When the Tags column is available, the shortcut menu (also known as a context or right-click menu) includes the following commands: Add Tag, Remove Tag, Set Tags, Remove All Tags in All Tables.

Note For more information about the shortcut menus for result tables, see "Shortcut menu commands for the result tables."

Before you add tags to the result tables, define the names and colors of the tags. See "Define custom tags by using the Custom Tags Editor."

Table 87. Adding tags to and removing tags from items (Sheet 1 of 3)

Task	Procedure
Add a tag to an item in the current result table.	Click the circle for the tag in the Tags column for the item. Or, right-click the item in the result table, choose **Add Tag**, and then select the tag that you want to add.
Remove a specific tag from an item in the current result table.	Click the circle for the tag in the Tags column. Or, right-click the entry, choose **Remove Tag**, and then, select the tag that you want to remove.
Remove all the tags from all the entries in all the result tables.	Right-click any result table that has a Tags column and choose **Remove All Tags in All Tables**. Then, click **OK** at the prompt.

Note Use the Set Tags shortcut menu to remove selected tags from the following:
- Selected items in the current result table.
- Selected items in the current result table and all its subtables.
- All items in the current table.
- All items in the current result table and all its subtables.

Table 87. Adding tags to and removing tags from items (Sheet 2 of 3)

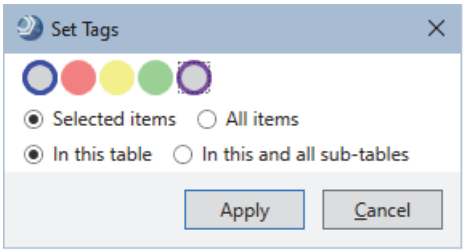
Task	Procedure
Remove specific tags from selected items in the current result table.	1. Select the items (rows) of interest by using the SHIFT key or the CTRL key. 2. Right-click a selected table row and choose **Set Tags**. The Set Tags dialog box opens. 3. Double-click the tags that you want to remove. The center of the selected tags turn gray. 4. Select the **Selected Items** option and the **In This Table** option. The following figure shows the settings for removing tags 1 and 5 from the selected items (rows) in the current result table.  5. Click **Apply**.
Remove specific tags from selected items in the current result table and all the subtables for the selected items.	1. Select the items (rows) of interest by using the SHIFT key or the CTRL key. 2. Right-click a selected table row and choose **Set Tags**. The Set Tags dialog box opens. 3. Select the tags that you want to remove. The color of the selected tags turns to gray. 4. Select the **Selected Items** option and the **In This and All Subtables** option. 5. Click **Apply**.

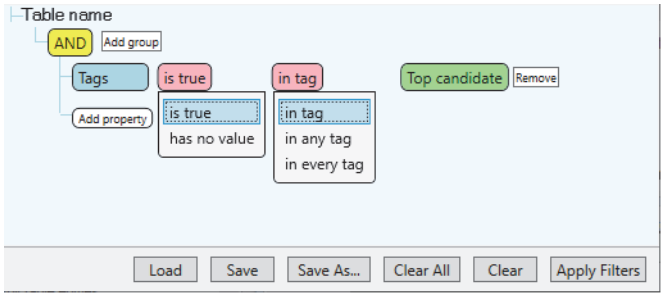
Table 87. Adding tags to and removing tags from items (Sheet 3 of 3)

Task	Procedure
Remove specific tags from all items in the current result table.	1. Right-click a selected table row and choose **Set Tags**. The Set Tags dialog box opens. 2. Select the tags that you want to remove. The color of the selected tags turns to gray. 3. Select the **All Items** option and the **In This Table** option. 4. Click **Apply**.
Remove specific tags from all items in the current result table and all items in the subtables for the current result table.	1. Right-click a selected table row and choose **Set Tags**. The Set Tags dialog box opens. 2. Select the tags that you want to remove. The color of the selected tags turns to gray. 3. Select the **All Items** option and the **In This and all Subtables** option. 4. Click **Apply**.

Filter a result table by the custom tags

Use the Result Filters view to filter the result tables by the custom tags. For general information about using the Result Filters view, see "Filter the data for data reduction."

Figure 90. Result Filters view (right side) showing the filters for the Tags column



❖ To filter the result tables in a result file by the custom tags

1. Open the result file of interest.
2. If you have not already defined and applied custom tags, follow the instructions in these topics:
   - Define custom tags by using the Custom Tags Editor
   - Add or remove custom tags
3. From the application menu bar, choose **View > Result Filters**.
4. On the left side of the Result Filters view, select the tables that you want to filter.
5. On the right side of the view, set up the filters for each table one-by-one.
6. To set up a single custom tags filter, select **Tags**, and then select the remaining filters as follows:
   - Is True or Has No Value > In Tag > *Tag Name*
   - Is True or Has No Value > In Any Tag
   - Is True or Has No Value > In Every Tag
7. To filter by multiple conditions, use the AND and OR conjunctions.
8. Click **Apply Filters**.

Import or export custom tags

When you create a set of custom tags, you can export the tag definitions to a TAGS file or import the tag definitions from a TAGS file to the current result file.

The Custom Tags Editor is not available until you open a result file.

Table 88. Importing or exporting custom tags

Task	Procedure
Export custom tags to a TAGS file	1. Open the result file that includes the definitions that you want to export. Or, open any result file. 2. From the application menu bar, choose **View > Custom Tags Editor**. The Custom Tags Editor opens. 3. Define the tags if you have not already done so. 4. Click **Export**. The Save Custom Tags Editor Settings dialog box opens. 5. Name the file, select where you want to store the file, and click **Save**.
Import custom tags from a TAGS file	1. Open the result file of interest. 2. From the application menu bar, choose **View > Custom Tags Editor**. The Custom Tags Editor opens. 3. Click **Import**. The Load Custom Tags Editor Settings dialog box opens. 4. Browse to and select the TAGS file of interest. Then, click **Open**.

Save, restore, and manage layouts

The layout of the result file includes the location of the graphical views, the result tables that you want to display, the columns and rows that you want to display in the result tables, the filter set, the custom annotations, and the Group By and Filter By settings.

In addition to the factory default layout, the application comes with the following custom layouts for LC studies:

- Stable Isotope Labeling—Opens the Isotopologues Distribution Chart, the Trend Chart, and the Metabolika Pathways view in the bottom right of the result page. In the Compounds table, hides the following columns: #Metabolika Pathways, Avg. Exchange, FISh Coverage, and Metabolika Pathways. Opens the Labeled Compounds per File table that is related to the currently selected compound in the main Compounds table.
- Statistics—Opens the Differential Analysis and Trend Chart views on the bottom left and the Principal Component Analysis, Partial Least Squares Discriminant Analysis, and Hierarchical Cluster Analysis views on the bottom right. Closes the Chromatograms and Mass Spectrum views. Closes the search and pathway result tables if they are visible.

For details about working with layouts, see the following topics:

- Save the current layout of a result file
- Reset the layout to the factory defaults
- Create a custom layout
- Apply a layout
- Manage the layouts

Save the current layout of a result file

After you modify the layout of a result file, you can save the current layout so that when you reopen the result file, it opens to the current layout.

❖ **To save the current layout of a result file**

With the result file selected as the active page, do one of the following:

- In the toolbar, click the **Save the Currently Active Item** icon, .
- From the menu bar, choose **File > Save**.

Reset the layout to the factory defaults

After you modify the layout of a result file, you can quickly restore the default layout.

❖ To reset the layout to the factory default settings

With the result file selected as the active page, choose **Window > Reset Layout** from the menu bar.

The application closes the result file, and then reopens the result file to the factory default layout.

Create a custom layout

If you frequently modify the layout of your result files, you might want to create a custom layout with the result tables, result table columns, and views that you prefer to display.

❖ To create a custom layout for a result file

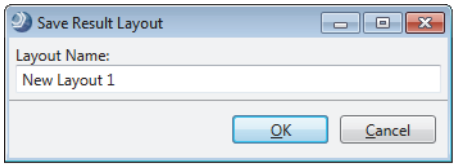
1. Open a result file and modify its layout.

   For details, see these topics:

   - Open, close, and update result files
   - Modify the result page layout for ease of use

2. From the menu bar, choose **Window > Save Layout**.

   The Save Result Layout dialog box opens.



3. Name the layout and click **OK**.

Apply a layout

A layout determines which of the available result tables and graphical views appear as well as where they appear in the application window when you open a result file.

❖ To apply a layout

1. With the result file selected as the active page, choose **Window > Apply Layout** from the menu bar.
2. Select a layout from the list or use the hot keys.

IMPORTANT The custom layouts—Statistics and Stable Isotope Labeling—are designed for LC studies that include statistical analysis results or stable isotope labeling results, respectively.

Manage the layouts

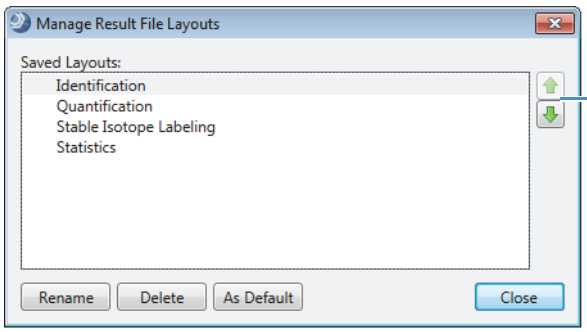
Use the Manage Result File Layouts dialog box to specify manage the list of layouts that appear in the Window > Apply Layouts list. From this dialog box, you can delete or rename each layout or specify the default layout.

❖ To manage the layouts

1. From the menu bar, choose **Window > Manage Layouts**.

   The Manage Result File Layouts dialog box opens. The list order corresponds to the hot keys in the Apply Layout list. For example, for this list, the hot key combination for the Statistics layout is CTRL+ALT+1.

   Figure 91. Manage Result File Layouts dialog box

   Use these buttons to change the order of the layouts.

   Changing the order changes the associated hot keys. The first 10 layouts in the list have associated hot keys.

2. Do the following as applicable:

   - To delete a layout, select it and click **Delete**.
   - To rename a layout, select it and click **Rename**. Then, in the Rename Result Layout dialog box, rename the layout and click **OK**.
   - To make the layout the default layout, select it and click **As Default**.
   - To change the list order, select a layout, and use the Up/Down buttons,  , to move the layout up or down in the list.

Edit compound annotations

Annotations include the compound name, formula, annotation source, FISh coverage score, and structure.

Use the Compound Annotation Editor dialog box to edit the annotations for compounds of interest in the compounds table (Compounds table or Expected Compounds table) and the Structure Proposals table.

Saving a custom annotation overwrites the original processing results.

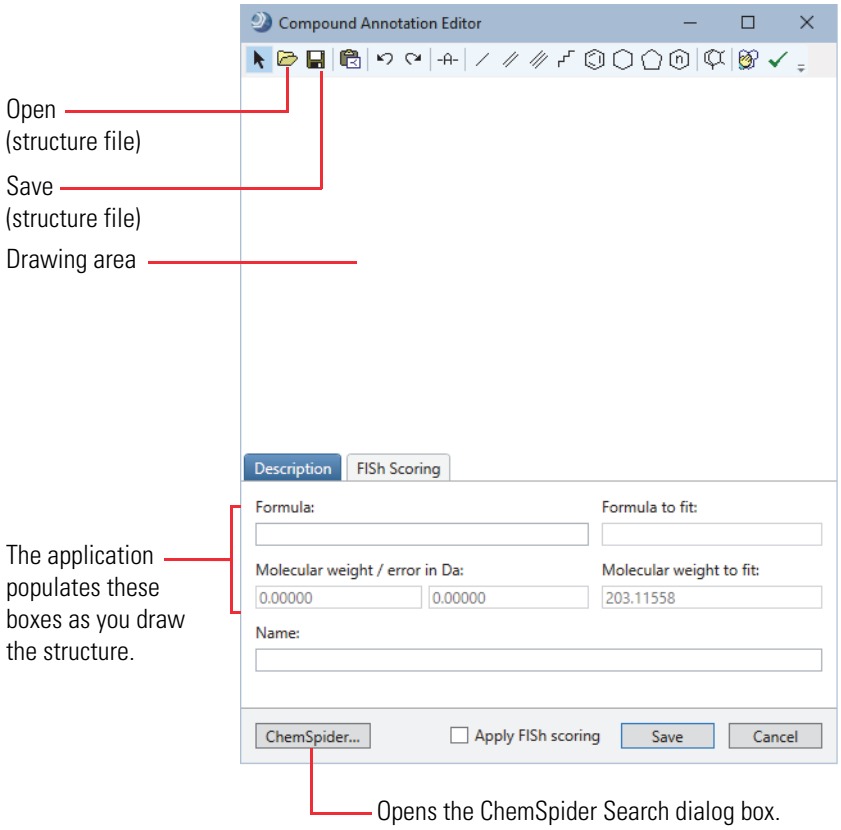
❖ To edit a compound annotation

1. Double-click the row of interest in the compounds table or related Structure Proposals table.

   The Compound Annotation Editor dialog box opens.

   The application automatically populates the Molecular Weight/Error in Da and Molecular Weight to Fit boxes. If the formula, structure, and name are available, the application also populates these fields.

   Figure 92. Compound Annotation Editor dialog box



2. To add a structure to the drawing area, do any of the following:
   - Use the structure drawing tools. See "Structure drawing tools and commands."
   - Open a structure file. See "Load a structure from a structure file."
   - Run a ChemSpider search and select one of the hits. See "Find a structure in the ChemSpider database."
3. Click **Save** to save your custom annotations in the result file.

Table 89 describes the parameters in the Compound Annotation Editor dialog box.

Table 89. Compound Annotation Editor parameters

Parameter	Description
Description page	
Formula	Displays the elemental formula of the structure in the drawing area or the assigned formula.
Formula to Fit	Displays the elemental formula of the component found by the Find Expected Compounds node in a targeted analysis for an LC study.
Molecular Weight/Error in Da	Displays the molecular weight (MW) of the structure in the drawing area and the difference between the structure's calculated MW and the MW for the selected compound—that is, the MW in the Molecular Weight to Fit box.
Molecular Weight to Fit	Displays the molecular weight (based on the formula) of the compound selected in the Compounds table or the Expected Compounds table.
Name	Displays the name of the compound from an online or local database search. To change the name, type alphanumeric text in this box.
Buttons and check box at the bottom of the dialog box	
ChemSpider	Opens the ChemSpider Search dialog box for searching the ChemSpider database.
Apply FISh Scoring	Select this check box and click **Save** to run the FISh Scoring algorithm.
Save	Saves the changes.
Cancel	Cancels the changes and closes the dialog box.
FISh Scoring page	
See "Apply FISh scoring."	

Add or delete proposed structures for a compound

In a result file, every compound in the compounds table (Compounds table or Expected Compounds table for an LC study) has a related Structure Proposals table.

For details about adding or deleting proposed structures for a compound, see the following topics:

- Add structure proposals
- Delete structure proposals

Add structure proposals

❖ **To add a structure proposal to a Structure Proposals table**

1. Select a compound in the main compounds table (Compounds table or Expected Compounds table).
2. Click **Show Related Tables** below the compounds table.
3. Do one of the following:
   a. Click the **Structure Proposals** tab.
   b. Right-click anywhere below the Structure Proposals tab and choose **Structure Proposals > Add Structure Proposal**.

   –or–

   a. Open any of the search results tables for the selected compound.
   b. Right-click the entry of interest in the search results table and choose **Add to Structure Proposals**.
4. Edit the structure proposal by following the instructions in "Edit compound annotations."

Delete structure proposals

In a result file, the Structure Proposals table is a related table for the compound selected in the main compounds table (Expected Compounds table or Compounds table).

❖ **To delete a structure proposal from a Structure Proposals table**

1. Select the compound of interest in the main compounds table.
2. Click **Show Related Tables** at the bottom left of the result page.
3. Click the **Structure Proposals** tab.
4. Right-click the entry and choose **Structure Proposals > Delete Structure Proposal**.

Replace an annotation with a structure proposal

In a result file, annotations include the name, formula, annotation source, FISh coverage score, and structure for a compound.

❖ **To replace the annotations for a compound in the main compounds table**

1. Select the compound of interest in the main compounds table (Expected Compounds table or Compounds table).
2. Click **Show Related Tables** at the bottom left of the result page.
3. Do one of the following:
   - Click the Structure Proposals tab. Then, right-click a row in the Structured Proposals table and choose **Structure Proposals > Use As Compound Annotation**.
   - Open any of the related results tables, right-click the entry of interest and choose **Use as Compound Annotation**.

Apply FISh scoring

You can apply FISh scoring to a selected entry in the compounds table (Expected Compounds table or Compounds table) or the entries in the following compound-related search result tables: Structure Proposals, mzCloud Results, mzVault Results, Mass List Search Results, BioCyc Results, Metabolika Results, and ChemSpider Results. You can also apply FISh scoring from the Compound Annotation Editor dialog box.

The FISh scoring algorithm uses the structure in the structure column of the result table or the drawing area of the Compound Annotation Editor dialog box. The selected entry in the compounds table must have MS2 data (check the indicator in the MS2 column).

For details about running the FISh scoring algorithm, see the following topics:

- Apply FISh scoring by using a shortcut menu command
- Apply FISh Scoring from the Compound Annotation Editor dialog box
- Specify the FISh scoring parameter settings

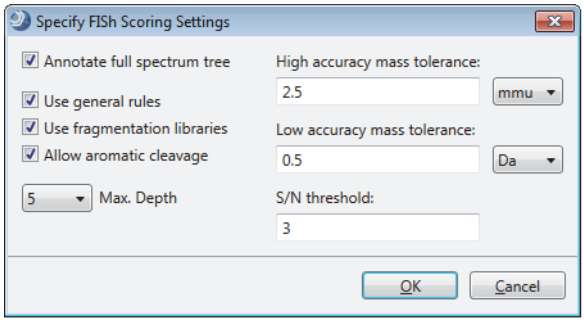
Apply FISh scoring by using a shortcut menu command

You can apply FISh scoring to a compound that has a structure and MS2 data from the compounds table, the related Structure Proposals table for the compound, or a related results table for the compound.

❖ To apply FISh Scoring from a result table

1. Make sure that the entries of interest include structures.
2. To open the Specify FISh Scoring Settings dialog box (Figure 93), do one of the following:
   - To submit a compound, right-click the selection and choose **Apply FISh Scoring**.
   - To submit a single selection in a Structure Proposals table, right-click the selection and choose **Structure Proposals > Apply FISh Scoring to Selection**.
   - To submit all of the entries in a Structure Proposals table, right-click the table and choose **Structure Proposals > Apply FISh Scoring to All**.
   - To submit an entry in a related search result table, right-click the table and choose **Add to Structure Proposals and Apply FISh Scoring**.

Figure 93. Specify FISh Scoring Settings dialog box



3. Set up the parameters. See "Specify the FISh scoring parameter settings."
4. Click **OK**.

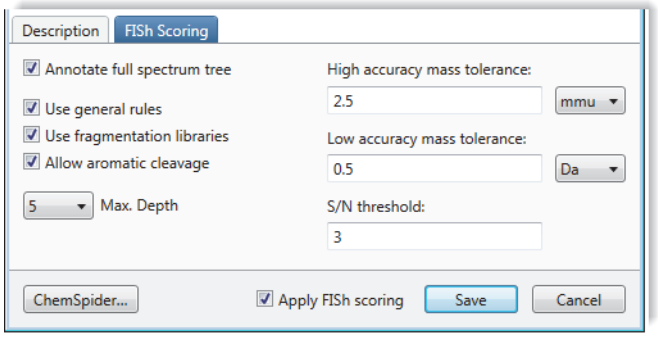
   In the FISh Scoring Queue view to the left of the table, one job appears for each selected entry. For each entry that includes a structure, the application runs the FISh scoring algorithm. The run time increases as the complexity of the structure increases. When an entry does not include a structure, the job ends in failure and is highlighted with a red border.

Apply FISh Scoring from the Compound Annotation Editor dialog box

❖ To apply FISh Scoring from the Compound Annotation Editor dialog box

1. To open the FISh Scoring page of the Compound Annotations dialog box, right-click an entry in the compounds table and choose **Edit Compound Annotation**.
2. Make sure that the drawing area on the Description page includes a structure.
3. Click the **FISh Scoring** tab.
4. Select the **Apply FISh Scoring** check box.

Figure 94. FISh Scoring page of the Compound Annotation Editor dialog box



5. Specify the parameter settings. See "Specify the FISh scoring parameter settings."
6. Click **Save**.

Specify the FISh scoring parameter settings

❖ To set up the FISh scoring parameters

1. In the Specify FISh Scoring Settings dialog box or on the FISh Scoring page of the Compound Annotation Editor dialog box, make the following selections:
   - To annotate the full spectrum tree, select the **Annotate Full Spectrum Tree** check box.
   - To use the general fragmentation rules, select the **Use General Rules** check box.
   - To use the fragmentation libraries, select the **Use Fragmentation Libraries** check box.

     Tip If time allows, select the **Use Fragmentation Libraries** check box. Using the fragmentation libraries provides significantly more structural information; however, it can also add a significant amount of processing time.

   - To allow aromatic cleavage as one of the fragmentation steps, select the **Allow Aromatic Cleavage** check box.
   - In the Max. Depth list, select the maximum number of steps allowed in the fragmentation pathway.
2. Use the default values or type new values in the following boxes:
   - For the FTMS scans, type a value in the High Accuracy Mass Tolerance box and select the appropriate units.
   - For the ITMS scans, type a value in the Low Accuracy Mass Tolerance box and select the appropriate units.
   - In the S/N Threshold box, type a value for the FTMS scans.

Table 90 describes the parameter settings for the FISh scoring algorithm.

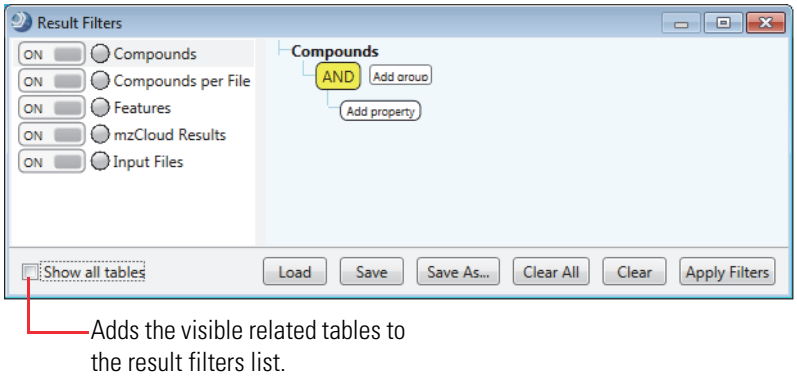
Table 90. FISh scoring parameters

Parameter	Description
Annotate Full Spectrum Tree	Annotates the full spectrum tree (MS/MS, MS^3, and so on) in the Mass Spectrum view.
Use General Rules	Uses the general fragmentation rules.
Use Fragmentation Libraries	Uses the fragmentation libraries.
Allow Aromatic Cleavage	Allows aromatic cleavage as one of the reaction steps.
Max. Depth	Specifies the maximum number of fragmentation reactions to consider in the fragmentation pathway. Default: 5; range: 1–20
High Accuracy mass tolerance and units	Specifies the mass tolerance for FTMS data. Default: 2.5 mmu
Low Accuracy Mass Tolerance and units	Specifies the mass tolerance for ITMS data. Default: 0.5 Da
S/N Threshold	Specifies the signal-to-noise threshold for FTMS data. The FT mass analyzer calculates the S/N level for each centroid.

Filter the data for data reduction

To show only the most pertinent data, use the Result Filters view to apply filters to the processed data. By default, the left pane of the Result Filters view lists the main tables in the current result file. The right pane displays the filters for the table that you select in the left pane.

Figure 95. Result Filters view with an empty filter for the Compounds table (LC study)



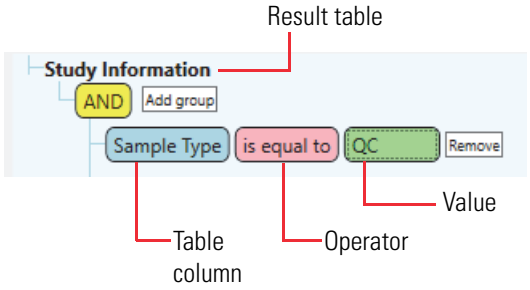
Note The filters for each table are independent of other table filters. For example, a retention time filter for the Merged Features table does not affect the entries in the other tables that include a retention time column. In addition, filtering only removes rows from the display; it does not update or change any of the calculated values.

To set up and apply the data reduction filters, see these topics:

- Set up, apply, and save filter sets
- Create a result filter with an AND logical conjunction
- Create a result filter with an OR logical conjunction
- Create a result filter with both of the logical conjunctions
- Load a saved filter set
- Result Filters view parameters

Components of a result table filter

You can filter each result table in a result file by one or more filters. Each filter consists of the property (table column in blue) and one or more operators or conditions (in pink). In addition, some filters take one or more values (in green) and a final data entry value or input file name.



Property

Specifies a column in the selected result table. The dropdown list contains all the columns in the selected result table.

The columns in a result table contain the following types of entries:

- Numeric (value)
- Alphanumeric (text)
- Status (for example, color indicators)
- Condition (for example, the check boxes in the Checked column and the tags in the Tags column) entries

One or more operators or conditions

After you select the result column to filter, you select the operator to filter by. Some filters are single operators and some filters require multiple operators. The available operators depend on the type of data that you are filtering: numeric values, alphanumeric text, indicators, or conditions.

When you set up filters with multiple operators, not all combinations of the operators make sense. For example, for the Gap Status column of a main compounds table, you can set up the following filter: Gap status > Has No Value > In Every File Holding a Value. This filter hides every compound in the table.

Value

Filters for numeric columns with numeric values— for example, the RT column—end with a text box for entering the numeric value or a selection list of the input files.

Filters for columns with alphanumeric strings—for example, the Name column—end with a text box for entering the string.

Set up, apply, and save filter sets

This topic describes how to set up, apply, and save a set of result filters (FILTERSET) for the result tables in a result file.

❖ To set up, apply, and save a filter set

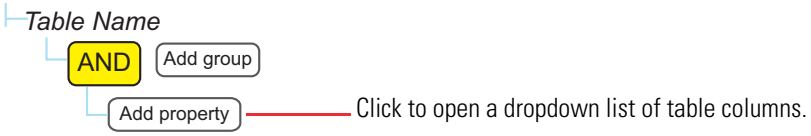
1. Open a result file.
2. From the application menu bar, choose **View > Result Filters**.

   The Result Filters view opens as a floating window or as a docked view and displays the filter tree for the current table.

   Each table has its own set of filter conditions.
3. (Optional) To display a filter tree that includes all the visible result tables in the result file, select the **Show All Tables** check box.

   Note To change which tables are visible, use the Select Visible Tables dialog box.
4. In the Result Filters view, select the table of interest in the left pane.

   The table name appears in the right pane. The following selection tree appears below the table name.



5. Click **Add Property**.

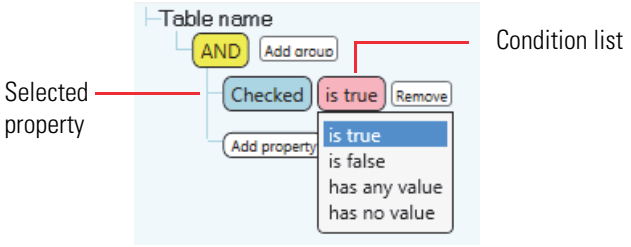
   A list that begins with the AND and OR logic selections followed by the columns in the selected table appears.

6. Select the table column (property) that you want to filter by.

7. Do any of the following:

   - For the Checked property, select a condition.

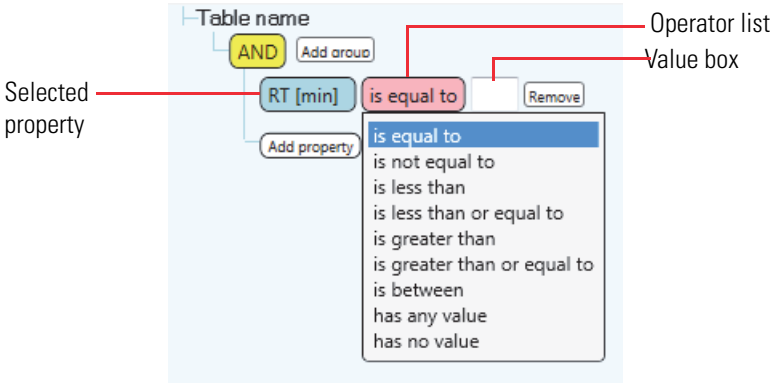
     This figure shows the condition list for the Checked property.



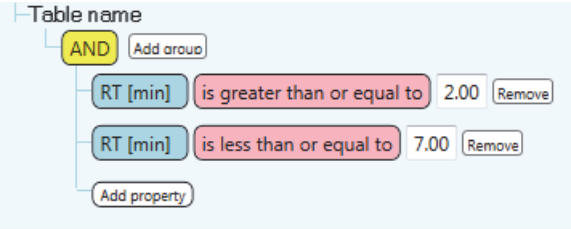
   - For a numeric-value property, such as retention time (RT), select an operator (mathematical relationship) and type a value in the adjacent box, if applicable.

     Tip When you select the Is Equal To operator, type a numeric value to a minimum precision of two decimal places or a minimum precision that is equal to the number of decimal places that are displayed in the column, whichever is greater. For example, for any of the Area columns, type a numeric value with two decimal places, even though the Area column displays a numeric value with no decimal places.

     This figure shows the operator list for numeric properties.

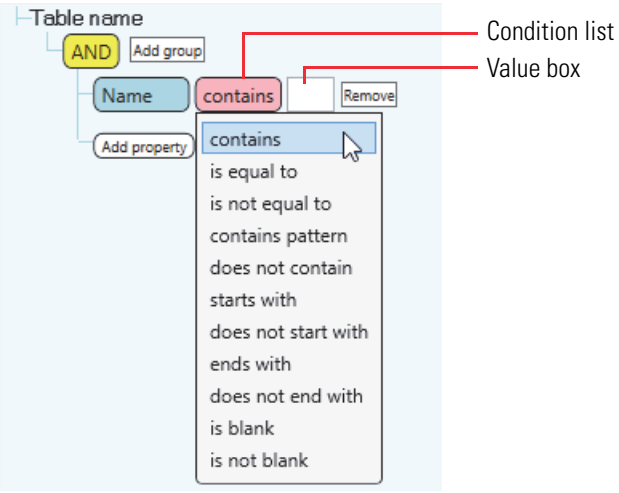


This figure shows a set of filter conditions that limits the displayed results to chromatographic peaks from 2 to 7 minutes.



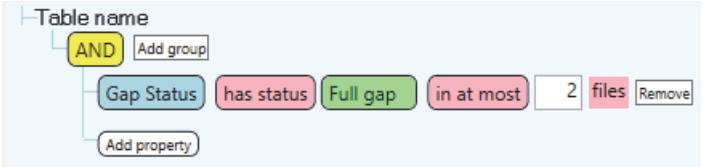
- For a non-numeric property (alphanumeric string), such as Name, select a condition and type a value in the value box if applicable.

  This figure shows the condition list for non-numeric properties.



- For a status property, such as Gap Status, select one or more conditions and values as applicable. For a multiple condition filter, not all combinations make sense. Clicking Remove at the end of a filter removes the individual filter.

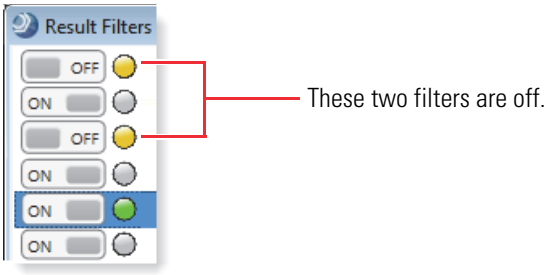
  This figure shows a filter for the Gap Status column.



8. Do any of the following:

   - To apply the filters in the current filter set, click **Apply Filters**.
   - To save a filter to a FILTERSET file, click **Save** or **Save As**. Then, browse to the location where you want to store the file, name the file, and click **Save**.
   - To turn off the filters for a specific table, click **ON** to the left of the table name in the left pane of the Result Filters view.

The indicator icon to the left of the table name turns from green to yellow, and the button displays OFF.



- To clear the filters for a specific table, select the table in the left pane of the Result Filters view. Then, click **Clear**.
- To clear all the filters in a filter set, click **Clear All**.

Create a result filter with an AND logical conjunction

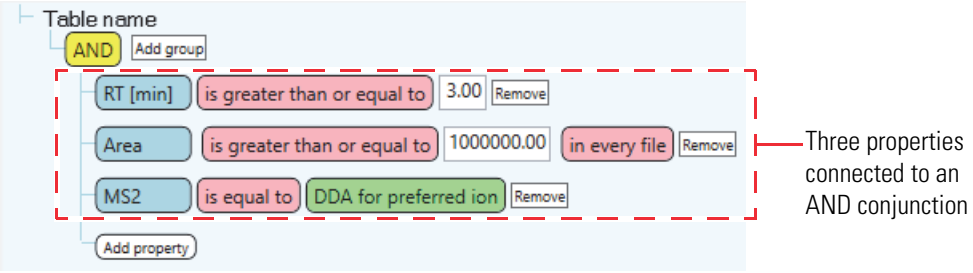
This topic describes how to use the AND logical conjunction in a result filter.

❖ To create a filter set using the AND logical conjunction

Note When you use the AND logical conjunction, all of the connected property conditions must be True.

1. In the Result Filter view, keep the **AND** logical conjunction as the first item in the filter tree.
2. For each property that you want to conjoin with the AND conjunction, click **Add Property**, select a property from the list, and set the property boundaries.

   This figure shows a filter set that uses three properties conjoined with an AND conjunction. When you apply this filter set to the data in a compounds table, only those rows that meet all three conditions remain; that is, you see only those detected chromatographic peaks with a retention time greater than 3.00 minutes, with an integrated peak area greater than 1 000 000, and where the compound has data-dependent scans for the preferred ion.



Create a result filter with an OR logical conjunction

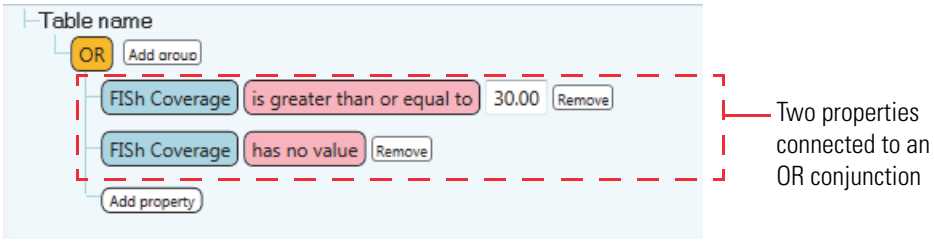
This topic describes how to use the OR logical conjunction in a result filter.

❖ **To create a filter set using the OR logical conjunction**

> **Note** When you use the OR logical conjunction, only one of the connected property conditions must be True.

1. Select the **OR** logical conjunction as the first item in the filter tree.
2. For each property that you want to conjoin with the OR conjunction, click **Add Property**, select a property from the list, and set up the property conditions.

   This figure shows a filter set that uses two properties conjoined with an OR conjunction. When you apply this filter set to the data in the result table, those rows that meet at least one of the conditions remain—that is, you see the rows where the FISh coverage value is greater than or equal to 30 or where the FISh coverage column has no reported value.

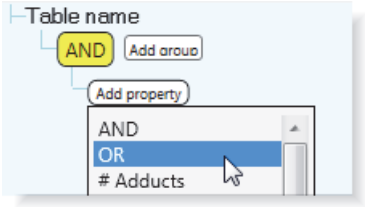


Create a result filter with both of the logical conjunctions

This topic describes how to use both of the logical conjunctions in a result filter.

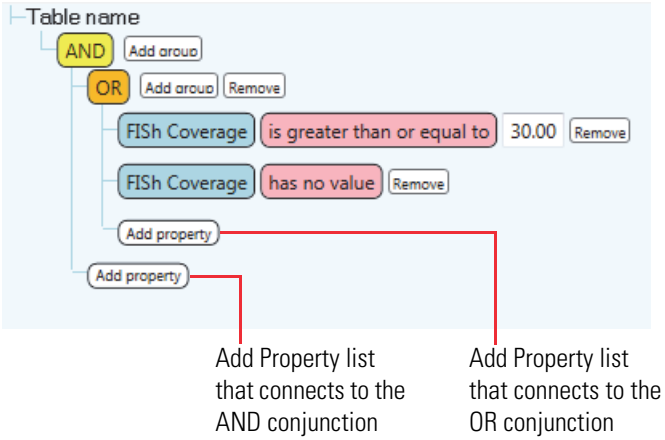
❖ **To create a filter set using both the AND and the OR logical conjunctions**

1. Keep the **AND** logical conjunction as the first item in the filter tree.
2. To conjoin two properties with the OR conjunction, do the following:
   a. Click **Add Property** and select **OR** from the dropdown list.



b. Set up the properties that you want to conjoin with the OR conjunction.

This example shows the condition where the FISh Coverage must be greater than or equal to 30 or have no value. (For LC studies, the FISh scoring algorithm does not calculate scores for DIA scans.)



3. For each property that you want to conjoin with the AND conjunction, click the **Add Property** list that connects to the AND conjunction, select a property from the list, and set up the property boundaries.

Figure 96 shows a result filter that keeps chromatographic peaks that meet the following conditions:

- A FISh Coverage score that meets one of these conditions:
  - A FISh Coverage score that is greater than or equal to 30

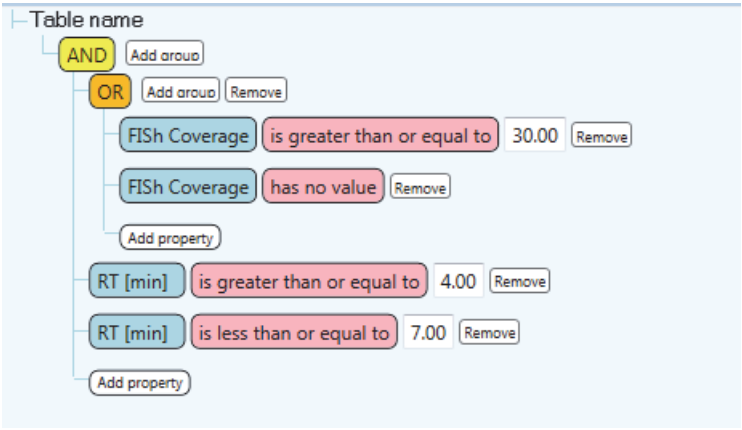
  –or–

  - No FISh Coverage score

–and–

- A Retention Time from 4 to 7 minutes

Figure 96. Filter that uses both AND and OR conjunctions



Load a saved filter set

This topic describes how to load the filters from a FILTERSET file.

❖ **To load a saved filter set**

1. In the Result Filters view, click **Load**.

   The Load Filter Set dialog box opens.

2. Browse to the appropriate folder and select the filter set of interest.

3. Click **Open**.

   If the filter set contains filter conditions for tables that are not in the current result file, the application automatically hides the unused filters. You can modify the filter conditions for the applicable tables only.

Result Filters view parameters

Use the Result Filters view to create data reduction filters for the tables in a result file. The Result Filters view is a floating window that can remain open while you work in other areas of the application.

Table 91 describes the panes, buttons, icons, and check box in the Result Filters view.

Table 91. Result Filters panes and buttons (Sheet 1 of 2)

Feature	Description
Left pane	Lists the main tables included in the current result file. An On/Off button and an indicator icon appear to the left of the table name.
ON/OFF button	Use to turn on or turn off the conditions for the associated main table.
Indicator icons	(○) Gray—Indicates that the table is unfiltered. (●) Green—Indicates that a filter has been applied to the table. (●) Yellow—Indicates that the table filter is off.
Right pane Displays the filter settings for the selected table. You can modify these settings as described in "Set up, apply, and save filter sets."	
AND or OR	Specifies the logical connection between properties or groups.
Add Group	Adds a group.
Add Property	Adds a property.

Table 91. Result Filters panes and buttons (Sheet 2 of 2)

Feature	Description
Check box	
Show All Tables	Selecting this check box adds the related tables to the table list.
Buttons	
Load	Opens the Load Filter Set dialog box where you can select a saved filter set and open it.
Save	If a saved filter set is open, clicking Save overwrites the original settings in the file with the current filters in the Result Filters window.
Save As	Opens the Save Filter dialog box where you can name the file and select a folder for a FILTERSET file.
Clear All	Clears all the filters for the current filter set.
Clear	Clears the current filter.
Apply Filters	Applies all the filters for the current filter set.

View the result summaries

In the Summaries view on a result page, you can view the following summaries:

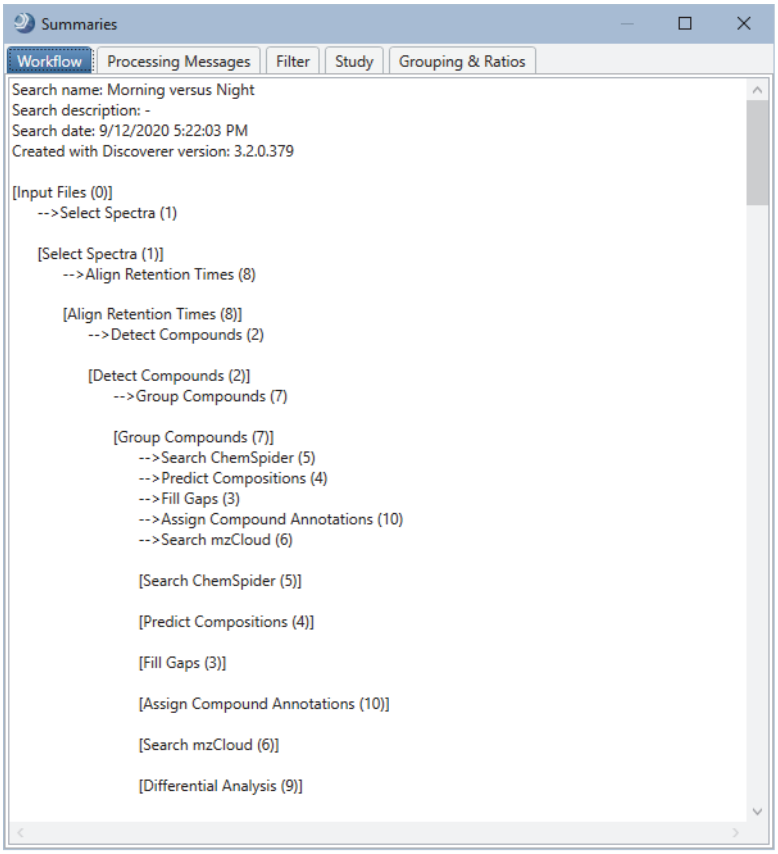
- Workflow summary
- Processing Messages summary
- Filter summary
- Study summary
- Grouping & Ratios summary

❖ To open the Summaries view

1. Open the result file of interest. See "Open, close, and update result files."
2. From the menu bar, choose **View > Result Summary**.

   The Summaries view includes these five pages: Workflow, Processing Messages, Filter, Study, and Grouping & Ratios.

Figure 97. Summaries view



Workflow summary

To view the processing workflow that the analysis used to create the active result file, open the Workflow page. This page lists the name of the processing workflow, the creation date for the result file (.cdResult), the raw data files (.raw) that were processed to create the result file, and the parameter settings for the workflow nodes.

For information about creating a processing workflow, see Chapter 6, "Create and edit processing workflows."

Processing Messages summary

To view a summary of the processing steps that the analysis used to create the active result file, open the Processing Messages page.

Filter summary

To view a summary of the filters used to reduce the data in the results window, open the Filter page. This page lists the name of the latest filter set (FILTERSET file type) that you applied to the result file and the filter conditions in the filter set. Use the Result Filters view to create filter sets. See "Filter the data for data reduction."

Study summary

To view a summary of the study settings for the input files that make up the result file, open the Study page. This page lists the following:

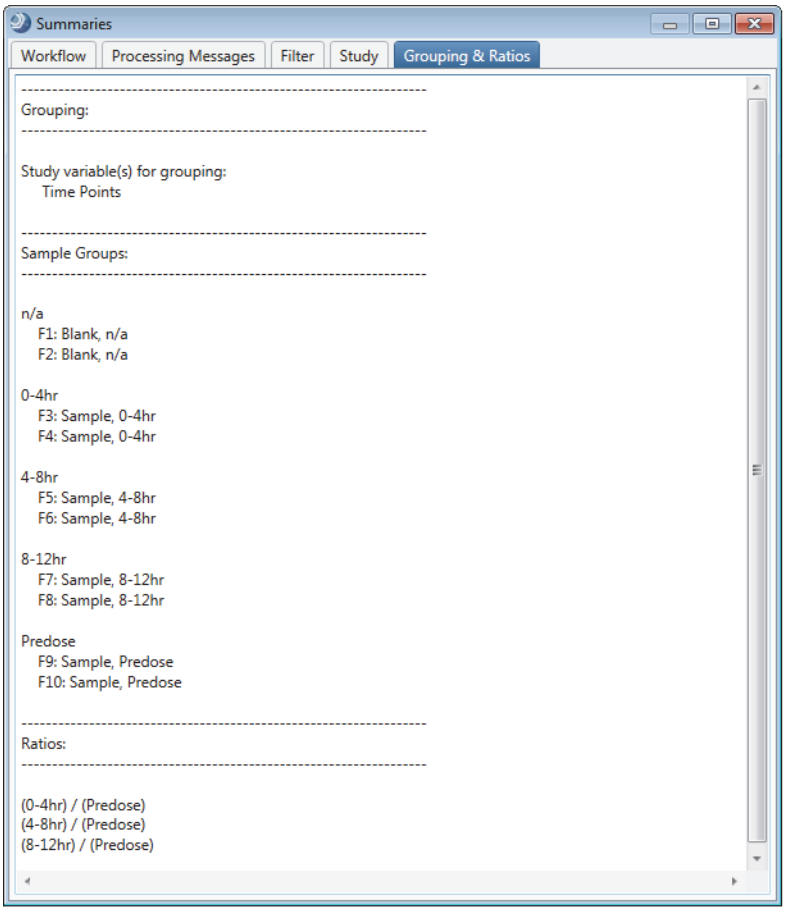
- Name and creation date of the study
- Directory location of the study
- Study factors and their values
- Sample names (Xcalibur RAW files) and their directory location

Grouping & Ratios summary

To view a summary of the sample groups and ratios for the analysis, open the Grouping & Ratios page.

Figure 98 shows an example summary of the sample groups and ratios for an analysis. The summary lists the selected study variables, sample groups, and ratios in order from top to bottom.

Figure 98. Grouping & Ratios Summary page



Shortcut menu commands for the result tables

To access the shortcut menu commands for a result table, right-click the result table.

Note Shortcut menus are also known as context menus or right-click menus.

For information about the shortcut menus for the result tables on a result page, see these tables:

- Table 92 describes the commands in the shortcut menus for the result tables in either type of study.
- Table 93 describes the shortcut menu commands that are specific to LC studies.

Table 92. Shortcut menu commands for the result tables (Sheet 1 of 4)

Command	Description
All main and related result tables	
Copy With Headers	Copies the current table row and its associated column headings to the Clipboard.
Copy	Copies the current table row to the Clipboard. Does not copy the column headings. See "Copy table entries to the clipboard."
Clear Selection	Undoes any row selections. Clears the Chromatograms view, the Mass Spectrum view, or both of these views if they are populated with data.
Cell Selection Mode	Turns on the cell selection mode. When the Cell Selection Mode is on, you cannot sort the table columns.
Enable Column Fixing or Disable Column Fixing	Turns on the column pins. Pinning (or freezing) a column moves it to the left of the Checked column. See "Freeze table columns."
Export > As Plain Text	Exports the data to a comma-separated values file. See "Export the result table contents to a text file."
Export > As Excel	Exports the data to an Excel™ spreadsheet file. See "Export the result table contents to a spreadsheet."
All result tables with a Structure column You can copy the structures in the following tables to the Clipboard: • For LC studies only: Compounds and Expected Compounds • For either study type: BioCyc Results, mzCloud Results, mzVault Results, ChemSpider Results, Mass List Search Results, Metabolika Results, and Structure Proposals	
Copy Structure > As MOL	Copies the selected structure in MOL format to the Clipboard.
Copy Structure > As InCHI	Copies the selected structure in InCHI format to the Clipboard.
Copy Structure > As InCHI Key	Copies the selected structure in InCHI Key format to the Clipboard.
All related tables with a Structure column	
Use as Compound Annotation	Uses the annotations in the selected entry for the related compound in the main compounds table (Expected Compounds table or Compounds table).

Table 92. Shortcut menu commands for the result tables (Sheet 2 of 4)

Command	Description
Add to Structure Proposals	Add the selected entry to the Structure Proposals table for the related compound in the main compounds table (Expected Compounds table or Compounds table).
Add to Structure Proposals and Apply FISh Scoring	Add the selected entry to the Structure Proposals table for the related compound in the main compounds table (Expected Compounds table or Compounds table) and runs the FISh scoring algorithm.
All result tables with a Tags column	
See "Add or remove custom tags."	
Add Tag	Adds the selected tag to the current row.
Remove Tag	Removes the selected tag for the current row.
Set Tags	Opens the Set Tags dialog box where you can add tags to multiple entries, all the entries in the current table, or all the entries in the current table and all its subtables.
Remove All Tags in All Tables	Clears all the tags in all the result tables in the current result file.
All result tables with a Checked column	
Check Selected	Places a check in the selected row's check box.
Check All	Selects the check boxes for all of the table rows.
Uncheck Selected	Clears the check box for the selected row.
Uncheck All	Clears the check boxes for all of the table rows.
Remove All Checkmarks in All Tables	Clears the check boxes in all the result tables.
All result tables with expanding table headings	
Expand All Column Headers	Expands the collapsed column headings.
Collapse All Column Headers	Collapses the expanded column headings.
Compounds table and Expected Compounds table	
Edit Compound Annotation	Opens the Compound Annotation Editor where you can name the compound, add a structure that matches the formula and molecular weight, run a ChemSpider search, and apply the FISh Scoring algorithm. If the table does not already include the Name and FISh Coverage columns, adds these columns.

Table 92. Shortcut menu commands for the result tables (Sheet 3 of 4)

Command	Description
Clear Compound Annotation	Removes the annotation, which includes the structure, name, formula, annotation source, and FISh coverage score if applied.
Apply FISh Scoring	Applies the FISh scoring algorithm to the selected entries and populates the FISh Coverage column with the calculated score.
Compounds table only	
Molecular Networks > Send to Viewer	Opens the molecular networking viewer in a web browser. See "Modify the simulation in the molecular networks viewer." The Generate Molecular Networks node adds this command to the shortcut menu for the result table.
Molecular Networks > Mark Selected > *tag selection*	If the Clipboard contains information from nodes (RT and MW for each node copied to the Clipboard) in the Molecular Network viewer, this command marks the matching compounds in the result table with the selected tag.
Structure Proposals table	
Structure Proposals > Add Structure Proposal	Adds a new row to the Structure Proposals table that includes the formula and molecular weight from the selected row in the main Compounds or Expected Compounds table. See "Add structure proposals." You can type a name in the Name column and a description in the Comments column. Double-click the new row to open the Compounds Annotation Editor where you can draw the compound's structure, open a structure file, or run a ChemSpider search.
Structure Proposals > Edit Structure Proposal	Opens the Compound Annotation Editor where you can name the compound, add a structure that matches the formula and molecular weight, run a ChemSpider search, and apply the FISh Scoring algorithm.
Structure Proposals > Delete Structure Proposal	Removes the selected row from the Structure Proposals table. See "Delete structure proposals."
Structure Proposals > Use as Compound Annotation	Replaces the annotations in the selected row of the main compounds table with the annotations in the current row of the Structure Proposals table.

Table 92. Shortcut menu commands for the result tables (Sheet 4 of 4)

Command	Description
Structure Proposals > Apply FISh Scoring to Selected	Opens a dialog box where you can specify the settings for the FISh scoring algorithm and submit the information in the selected row. See "Apply FISh scoring." To apply FISh scoring, the selected row in the Structure Proposals table must include a formula or a structure.
Structure Proposals > Apply FISh Scoring to All	Opens a dialog box where you can specify the settings for the FISh scoring algorithm and submit all the rows in the Structure Proposals table.
All related tables that have a corresponding main table	
Go to Same Item in Main Table	Opens the main table with the same name as the related table and selects the corresponding table row in the main table.

Table 93. Shortcut menu commands found only in LC studies (Sheet 1 of 2)

Command	Description
Compounds table and Expected Compounds table	
Export > As Xcalibur Inclusion/Exclusion List	Exports information about all of the compounds in the table or only the selected compounds in the table to a text file in the format required for the selected mass spectrometer. The information includes the *m/z* value of the monoisotopic ion and the start and stop times for the chromatographic peak. See "Export an Xcalibur inclusion or exclusion list from a compounds table."
Export > Add Compound to Existing mzVault Library	Exports a selected compound to an existing mzVault library. See "Add a compound to an existing mzVault library."
Export > As mzVault Library	Exports the selected compounds to a new mzVault library. See "Create a new mzVault library."
Compounds table	
Export > As TraceFinder List	Exports information about all of the compounds, only the named compounds, or only the checked compounds in the table to a CSV file in a format appropriate for the TraceFinder application. See "Export the contents of the Compounds table to TraceFinder."
Export > As Mass List	Exports the selected items to a new mass list. See "Export compounds from the Compounds table to a new mass list."
Add Selected Compounds to Existing Mass List	Adds the selected compounds to the specified mass list. See "Export compounds from the Compounds table to an existing mass list."

Table 93. Shortcut menu commands found only in LC studies (Sheet 2 of 2)

Command	Description
Expected Compounds table	
Reset Compound Annotation	Resets the annotations of the selected entries to the original data processing results.

Export the tabular data in a result file to an external file

These topics describe how to export the contents of a result table to an external file:

- Shortcut menu commands for the result tables
- Export the result table contents to a spreadsheet
- Export the result table contents to a text file
- Export an Xcalibur inclusion or exclusion list from a compounds table
- Export the contents of the Compounds table to TraceFinder
- Export spectral data to a new or existing mzVault library

Export the result table contents to a spreadsheet

Use the Export > As Excel command to export result table items to a spreadsheet application.

You can export the contents of any of the result tables to a spreadsheet file. When you open the Export to Excel dialog box from any of the main tables, the Level 1 selection in the dialog box defaults to the active result table. When you open the Export to Excel dialog box from any of the related tables, the Level 1 selection defaults to the main compounds table, which depends on the processing workflow.

For LC studies, the main compounds table is the Compounds table when the processing workflow includes the Detect Compounds node or the Detect Compounds node and the Expected Compounds node. When the processing workflow includes only the Expected Compounds node, the compounds table is the Expected Compounds table.

❖ To export the contents of a result table to a spreadsheet file

1. Right-click the result table that you want to export and choose **Export > As Excel**.

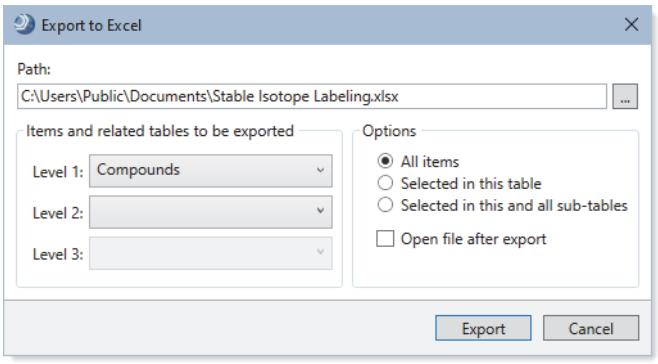
   The Export to Excel dialog box opens.

   The default storage path is C:\Users\Public\Documents*result file name*.

The default selection in the Level 1 box depends on where you opened the dialog box:

- If you opened the dialog box from a main table, the default selection in the Level 1 box is the name of the active result table.
- If you opened the dialog box from a related table, the selection in the Level 1 box is a main compounds table.

Figure 99. Export to Excel dialog box with the Compounds table selected



2. Make the appropriate selections in the Export to Excel dialog box as follows:

   If you open the Export to Excel dialog box from a main table, the Level 1 selection is the table where you opened the dialog box. If you open the Export to Excel dialog box from a related table, the Level 1 selection is a main compounds table.

   You can modify the export options in any order.

Table 94. Export options (Sheet 1 of 2)

Export option	Procedure
Change the directory folder, the file name, or both.	Click the browse icon, ..., next to the Path box. Then, select a directory folder and rename the file as appropriate, select the spreadsheet type (XLS or Microsoft Excel File), and click **Save**.
Select the result tables to export.	If necessary, select a different result table from the Level 1 list. Then, as appropriate, select an available table from the Level 2 list, followed by an available table from the Level 3 list.

Table 94. Export options (Sheet 2 of 2)

Export option	Procedure
In the Options area, select which items you want to export.	Select one of these options: **All Items**—Exports all the visible table rows in all the selected tables. **Selected in This Table and All Subtables**—Exports all the visible table rows in the main table where the check box in the Checked column is selected. Selected in This Table—Exports all the visible table rows in the main table and all the visible table rows in the selected related tables where the check box in the Check column is selected.
In the Options area, select whether you want the spreadsheet file to open after you click Export.	If you want the spreadsheet file to open in a spreadsheet application after you click Export, select the **Open File After Export** check box.

3. Click **Export** to export the data to a spreadsheet.

   When the export is complete, a confirmation prompt appears with the name and location of the file.

4. At the prompt, click **OK**.

Export the result table contents to a text file

You can export the contents of any of the result tables to a text file.

❖ To export the contents of a result table to a text file

1. Right-click the result table that you want to export and choose **Export > As Plain Text**.

   The Export to CSV File dialog box opens. The File Name box displays the name of the selected result table.

2. Select the folder where you want to store the file, name the file as necessary, and click **Save**.

   The text file (CSV) appears in the selected folder.

Export an Xcalibur inclusion or exclusion list from a compounds table

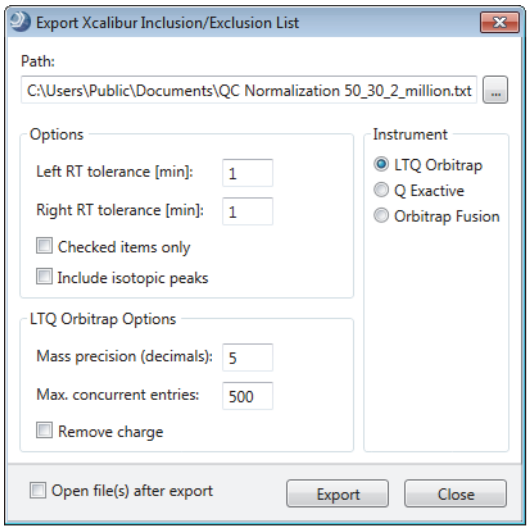
You can export the contents of the Compounds table or the Expected Compounds table to an Xcalibur Inclusion/Exclusion list and then import this list into an instrument method that controls your Thermo Scientific mass spectrometer.

❖ To export an Xcalibur inclusion or exclusion list

1. Right-click the Compounds table or the Expected Compounds table and choose **Export > As Xcalibur Inclusion/Exclusion List**.

   The Export Xcalibur Inclusion/Exclusion List dialog box opens.

   Figure 100. Export Xcalibur Inclusion/Exclusion List dialog box



2. Make the appropriate selections and entries (Table 95).
3. Click **Export**.

   The application attempts to save the text file to the specified location. If the file name conflicts with an existing file, a confirmation message appears. In the absence of a conflicting file, a completion message appears indicating that the exported file is in the selected folder.

4. If a confirmation message appears, do one of the following:

   - To overwrite the existing file, click **Yes**, and then click **OK** when the completion message appears.
   - To cancel the export, click **No**.

Table 95 describes the parameters in the Export to Xcalibur Exclusion List dialog box.

Table 95. Export to Xcalibur Inclusion/Exclusion List dialog box parameters (Sheet 1 of 3)

Parameter	Description
Path	Specifies the file name and directory path of the text file that contains the inclusion/exclusion list for your Xcalibur instrument method.

Table 95. Export to Xcalibur Inclusion/Exclusion List dialog box parameters (Sheet 2 of 3)

Parameter	Description
Options	
IMPORTANT An Orbitrap Fusion mass spectrometer accepts a retention time range of 0.01 to 999 minutes. Make sure that the retention time window for each compound falls within the retention time range of the instrument method. • Expected RT – Left RT Tolerance > Minimum retention time for the instrument method • Expected RT + Right RT Tolerance < Maximum retention time for the instrument method	
Left RT Tolerance [min]	Specifies the minimum start time for the chromatographic peak. If the Expected RT minus the Left RT Tolerance setting is less than zero, the application exports a value of zero. Default: 1 Range: 0.001 to 1000
Right RT Tolerance [min]	Specifies the maximum stop time the chromatographic peak. There is no error checking for the calculated maximum retention time. Default: 1 Range: 0.001 to 1000
Checked Items Only	Specifies that the application exports only the selected compounds to the named text file. Default: Clear
Include Isotopic Peaks	Adds an entry for each isotopic spectral peak.
LTQ Orbitrap Options	
Mass Precision (Decimals)	Specifies the mass precision. For the LTQ Orbitrap, the mass precision of the exported data must match the required mass precision for your Xcalibur instrument methods. You specify the required mass precision for Xcalibur instrument methods in the Instrument Configuration dialog box of the Foundation platform. Default: 5; range: 0 to 5

Table 95. Export to Xcalibur Inclusion/Exclusion List dialog box parameters (Sheet 3 of 3)

Parameter	Description
Max. Concurrent Entries	Specifies the maximum number of entries with overlapping time windows. Default: 500; range: 1 to 2000
Remove Charge	Specifies whether the application exports the *m/z* value of the best ion for each detected compound or the neutral mass of each detected compound. Default: Clear
Instrument	
LTQ Orbitrap	Exports the list in the appropriate format for the LTQ Orbitrap instrument control software.
Q Exactive	Exports the list in the appropriate format for the Q Exactive instrument control software. The mass list includes the formula of each compound in the Comment column when the formula is available.
Orbitrap Fusion	Exports the list in the appropriate format for the Orbitrap Fusion instrument control software. If the table contains both positive and negative scans, the application creates two mass lists. The maximum number of target compounds for an Orbitrap Fusion mass list is 50 000. If the table includes more than 50 000 compounds, filter the table or check the compounds of interest before you export the mass list.
Buttons and check box	
Open File(s) after Export	Specifies that the file opens after the application completes the export.
Export	Exports the specified information to a text file.
Close	Closes the dialog box.

Export the contents of the Compounds table to TraceFinder

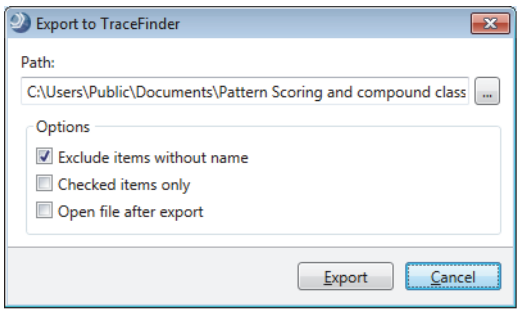
You can export the contents of the Compounds table to a CSV file that the TraceFinder application can use for data processing.

❖ **To export a compounds list for the TraceFinder application**

1. Right-click the Compounds table and choose **Export > As TraceFinder List**.

   The Export to TraceFinder dialog box opens. The default folder is either *drive*:\Users\Public\Documents or the last folder that you selected. The default file name is the name of the active result file.

   Figure 101. Export to TraceFinder dialog box

2. Select the folder where you want to store the file.
3. Do the following, as applicable:
   - To exclude unnamed compounds, select the **Exclude Items Without Name** check box.
   - To include only the checked compounds, select the **Checked Items Only** check box.
   - To automatically display the exported compounds list, select the **Open File After Export** check box.
4. Click **Export**.

   A status box appears when the export process finishes.
5. Click **OK**.

Export spectral data to a new or existing mzVault library

To export spectral data to a new or existing mzVault Library file, see the following topics:

- Add a compound to an existing mzVault library
- Create a new mzVault library

Add a compound to an existing mzVault library

From a Compounds table or an Expected Compounds table, use the Export > Add Compound to Existing mzVault Library shortcut menu command to export a selected compound to an existing mzVault library.

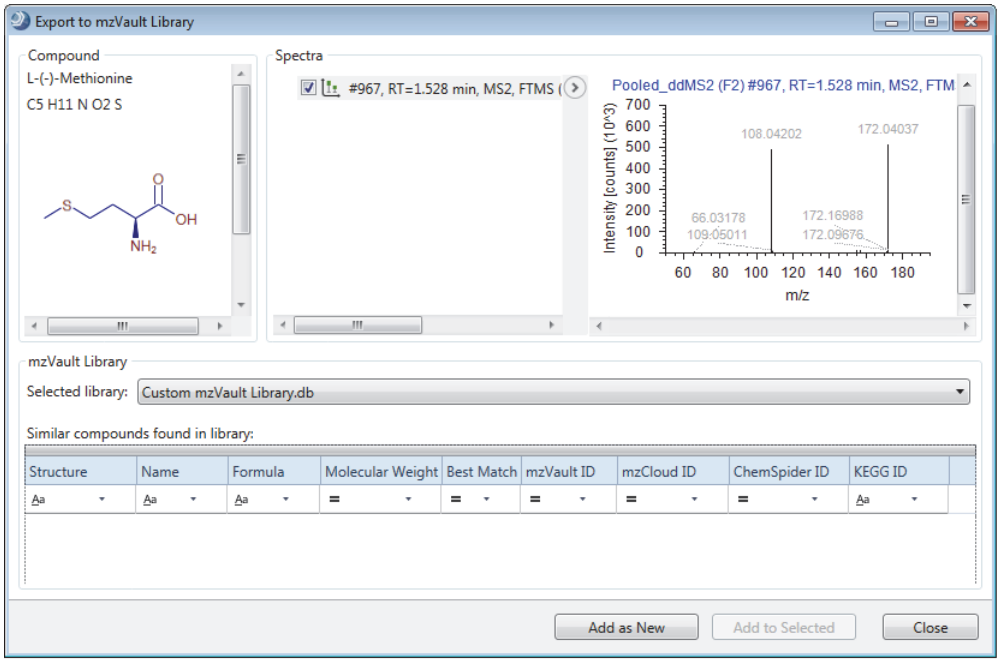
Tip The application comes with an empty library named Custom mzVault Library.db. For information about creating a new spectral library, see "Spectral Libraries view."

❖ To add a compound to an existing mzVault Library

1. Open a result file. See "Open, close, and update result files."
2. Open one of these tables by clicking its tab—Compounds table or Expected Compounds table.
3. Right-click a compound in the table and choose **Export > Add Compound to Existing mzVault Library**.

   The Export to mzVault Library dialog box opens. Its Spectra view displays the available fragmentation spectra for the selected compound.

   Figure 102. Export to mzVault Library dialog box populated with a Compounds table compound



4. Do the following:
   - In the spectrum tree, select the check boxes for the spectra that you want to add to the compound entry.
   - In the mzVault Library area, select the existing mzVault library from the Selected Library list.

5. Do one of the following:
   - To add the spectra to an existing compound entry in the library, select the entry in the Similar Compounds Found in Library list. Then, click **Add to Selected**.
   - To add the compound and the selected spectra as a new compound entry, click **Add as New**.
6. Close the dialog box.

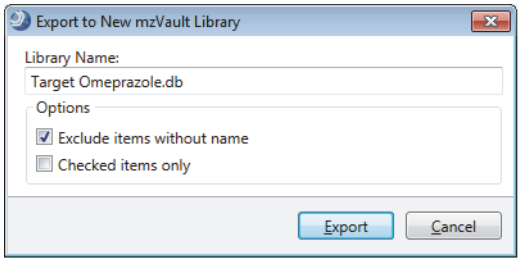
Create a new mzVault library

From a Compounds table or an Expected Compounds table, use the Export > Compounds to a New mzVault Library shortcut menu command to export all or selected compounds to new mzVault library.

❖ To export compounds to a new mzVault library

1. Open a result file. See "Open, close, and update result files."
2. Open one of these tables by clicking its tab—Compounds table or Expected Compounds table.
3. (Optional) Filter the table to display only the compounds of interest or select the check boxes for the compounds of interest.
4. Right-click the table and choose **Export > As mzVault Library**.

   The New mzVault Library dialog box opens. By default, the application populates the Library Name box with the name of the opened result file.



5. Do the following:
   - Type a new library name or keep the default name.
   - In the Options area, select whether to exclude compounds without a name, export only the compounds with selected check boxes, or both.
6. Click **Export**.

7. At the prompt, click **OK**.

   The new library appears in the Spectral Libraries list.

8. To modify a library with the mzVault 2.3 application, export it to another folder. Then, use the Replace command to replace the existing library with the modified library.

Export compounds to a new or existing mass list

You can create new mass lists or add compounds to existing mass lists by exporting compounds from the Compounds table of a result file. The application automatically adds exported mass lists to the table of available mass lists in the Lists & Libraries > Mass Lists view.

For details about exporting compounds to a mass list, see the appropriate topic:

- Export compounds from the Compounds table to a new mass list
- Export compounds from the Compounds table to an existing mass list

Export compounds from the Compounds table to a new mass list

❖ **To create a new mass list by exporting a set of compounds from the Compounds table**

1. Open the result file of interest.
2. Open the main Compounds table or a related Compounds table.
3. (Optional) To export only the checked compounds, select the check boxes for the compounds of interest in the Checked column.
4. Right-click the Compounds table and choose **Export > As Mass List**.
5. In the Export to New Mass List dialog box, do the following:
   a. In the Mass List Name box, type a name for the mass list.
   b. In the Options area, do any of the following:
      - To export only checked compounds, select the **Checked Items Only** check box.
      - To export only named compounds, select the **Exclude Items without Name** check box.
      - To include the retention time information in the mass list, select the **Export Retention Time** check box.
   c. Click **Export**.
6. At the prompt, click **OK**.

   The new mass list appears in your Mass Lists library.

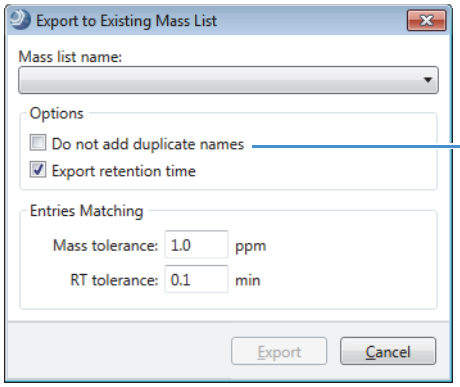
Export compounds from the Compounds table to an existing mass list

❖ To export compounds to an existing mass list

1. Open the result file of interest.
2. Open the main Compounds table or a related Compounds table.
3. Highlight the compounds of interest by using the SHIFT and CTRL keys.
4. Right-click your selection and choose **Export > Add Selected Compounds to Existing Mass List**.

   The Export to Existing Mass List dialog box opens.

   Figure 103. Export to Existing Mass List dialog box



If you select the Do Not Add Duplicate Names check box, the data entry boxes in the Entries Matching area become unavailable.

5. Do the following:
   - In the dropdown Mass List Name list, select the mass list where you want to add the selected compounds.
   - (Optional) To add the retention time information to the mass list, select the **Export Retention Time** check box.
6. To avoid exporting named compounds that are already in the mass list, do one of the following:
   - To exclude a named compound only if its mass and retention time match the duplicate compound in the mass list within specified tolerances, make sure that the **Do Not Add Duplicate Names** check box is not selected. Then, in the Entries Matching area, enter the tolerances that you want the application to use to exclude duplicate named compounds from being exported to the mass list.

     Note If you do not want to exclude a named compound unless both its mass and retention time are an exact match to the named compound in the mass list, set both tolerance values to 0.

- To exclude any named compound with a name that matches that of a named compound in the existing mass list, select the **Do Not Add Duplicate Names** check box.

Note This feature is case-sensitive.

Figure 104. Export to NIST Formatted File dialog box

Copy or save graphical views for publication

You can copy the contents of a graphical view to the Clipboard as editable text, as an image, or to an external file.

- To save a graphical view as a raster image, save it as one of these file types: PNG, GIF, JPG, TIF, or BMP.
- To save a graphical view as a vector image, save it as an EMF file.

For information about the graphical views that are available when a result page is active in the application window, see "Graphical views for a result file."

Table 96 lists the shortcut menu commands for copying data to the Clipboard or an external file.

Table 96. Commands for copying an image of a graphical view (Sheet 1 of 2)

Graphical view	Copy the image to the Clipboard	Copy the data points to the Clipboard	Copy the data to an image file	Copy the data to a TEXT or CSV file
Chromatograms view	Copy > Image	Copy > Points	Export > Image As	Export > Points As
Mass Spectrum view	Copy > Image	Copy > Points—Copies the scan label and the *m/z* and intensity values for annotated centroids to the Clipboard. Copy > Raw Points—Copies the *m/z* and intensity values for all centroids to the Clipboard. Does not copy the scan label.	Export > Image As	Export > Points As
Scatter Chart	Copy > Image	Copy > Data	Export > Image As	Export > Data As
Histogram Chart	Copy > Image	Copy > Data	Export > Image As	Export > Data As
Bar Chart	Copy > Image	Copy > Data	Export > Image As	Export > Data As
Pie Chart	Copy > Image	Copy > Data	Export > Image As	Export > Data As

Table 96. Commands for copying an image of a graphical view (Sheet 2 of 2)

Graphical view	Copy the image to the Clipboard	Copy the data points to the Clipboard	Copy the data to an image file	Copy the data to a TEXT or CSV file
Trend Chart	Copy > Image	Copy Information to Clipboard	Export > Image As	Export > Data As
Principal Component Analysis view	Copy > Image	Copy > Points	Export > Image As	Export > Points As (CSV file)
PLS-DA view	Copy > Image	Copy > Points Copy > Point Details	Export > Image As	Export > Points As (CSV file) Export > Point Details As
Descriptive Statistics view	Copy > Image	Copy Information to Clipboard	Export > Image As	Save Information As (CSV file)
Differential Analysis view	Copy > Image	Copy > Points Copy > Point Details (Use this command if the corresponding table includes structures.)	Export > Image As	Export > Points As Export > Point Details As
KEGG Pathways	Copy	N/A	Save Picture As (a PNG or BMP file)	N/A
Retention Time Correction	Copy > Image	Copy > Points	Export > Image As	Export > Points As
Compound Area Corrections	Copy > Image	Copy > Points	Export > Image As	Export > Points As

Copy structures to the Clipboard for use in other applications

You can copy structures from any result table that has a Structures column to the Clipboard for use in other applications.

❖ **To copy structures from a result table for use in other applications**

1. Open a result file from an analysis that included a structure search.

   For an LC study, any of the search node or mapping nodes can return a structure. For a GC study, a NIST library search or any of the search nodes or mapping nodes can return a structure.

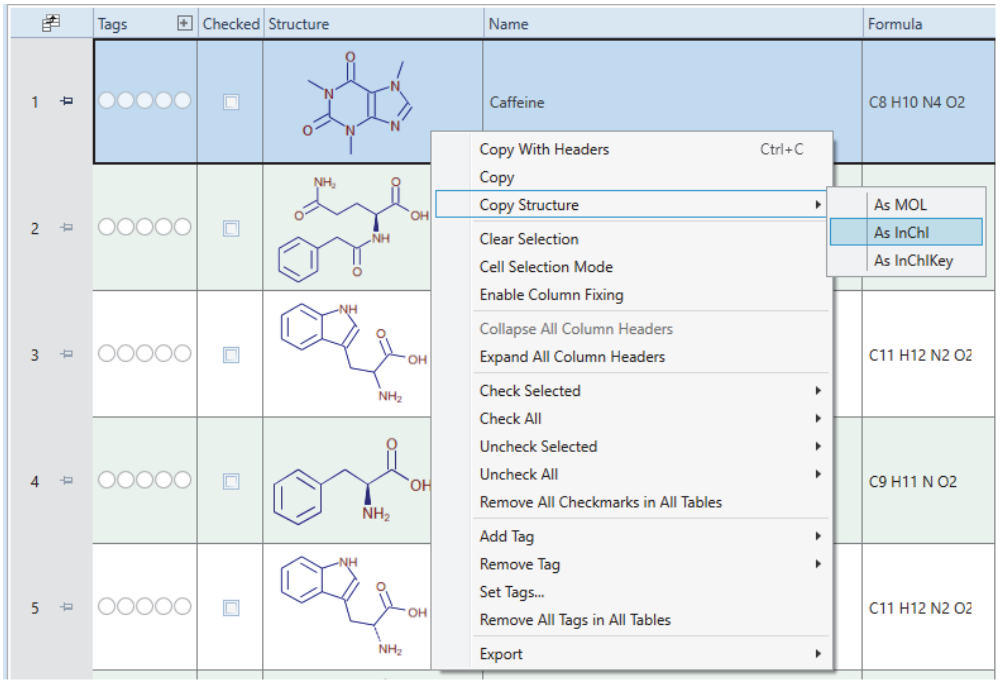
2. Open the result table of interest.

3. If the Structures column is hidden, do the following:
   a. Click the **Field Chooser** icon, , for the table.
   b. In the Field Chooser dialog box, select the check box for the Structure column.
   c. Close the Field Chooser dialog box.

> **Tip** You can copy structures without opening the Structure column. But opening the Structures column lets you confirm that the entry you want to copy has a structure annotation.

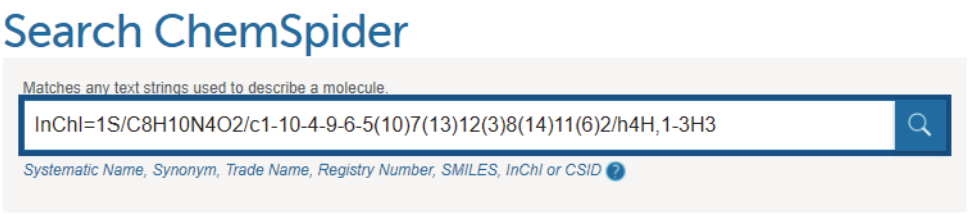
4. Right-click the entry of interest and choose **Copy Structure > As Mol**, **As InChi**, or **As InchIKey**.

Figure 105. Shortcut menu for a result table with a Structure column



5. Open the application where you want to paste the structure and press CTRL+V.

Figure 106. ChemSpider search box with pasted InChi string



9

Graphical views for a result file

The following topics describe how to use the graphical views that are available from the View menu:

- Chromatograms view
- Mass Spectrum view
- Result Charts view
- Trend Chart view
- Isotopologues Distribution Chart view
- Mass Defect Plot view
- Principal Component Analysis view
- Descriptive Statistics view
- Differential Analysis view
- Partial Least Squares Discriminant Analysis view
- KEGG Pathways view
- BioCyc Pathways view
- Metabolika Pathways view
- Retention Time Corrections view
- Compound Area Corrections view
- Hierarchical Clustering Analysis view
- mzLogic Analysis view
- FISh Scoring Queue view

Note Use the Result Charts view to create histograms, bar charts, pie charts, and scatter plots of the result data.

For details about the Result Filters view, see "Filter the data for data reduction." For details about viewing a summary of the analysis parameters for a result file, see "View the result summaries."

Chromatograms view

For LC studies, when you initially open a result file, the Chromatograms view displays the XIC traces for the compound in the first row of the Compounds table or the Expected Compounds table. By default, the display zooms in on the detected peaks for the selected rows.

The Chromatograms view consists of a collapsible pane on the left and the graphical view on the right. Right-clicking the graphical view opens a shortcut menu (see Table 98).

The following topics describe how to review the chromatographic data:

- View a chromatogram
- Add a chromatogram plot
- Overlay multiple chromatogram plots
- Change the grouping in the collapsible pane of an opened result file
- Hide the traces for a study variable value
- Update all the chromatogram plots simultaneously
- Manually integrate chromatographic peaks
- Chromatograms view shortcut menu commands

View a chromatogram

In an opened result file, you can display chromatogram traces (a plot of intensity versus time) by selecting a row in any of these result tables:

- Untargeted LC/MS workflow
  - Compounds
  - Compounds per File
  - Features
- Targeted LC/MS workflow
  - Expected Compounds
  - Expected Features per File
  - Expected Compounds per File

  - Merged Features
  - Expected Formulas
- General LC/MS traces
  - FISh Trace Fragments
  - Specialized Traces: TIC, BPC, XIC, isotope pattern, and FISh
  - Manual Peaks

❖ To view a chromatogram

1. Open a result file that contains chromatographic data.
2. If the Chromatograms view is closed, open it by choosing **View > Chromatogram** from the menu bar.

   Note When you select a row for a filtered study file, the Chromatograms view does not display a trace. For example, if the Blank check box is clear under Filter By Sample Type and you select a row for a Blank sample, the Chromatograms view remains empty. By default, the Blank Sample Type check box is clear until you select it.

3. Do one of the following:
   - Click the **Compounds** tab or the **Expected Compounds** tab and select a row.

     The Chromatograms view displays overlaid traces of the chromatographic peaks that were detected across the input files for the molecular weight and retention time (MW × RT dimensions) listed in the selected table row. Each trace is a composite of the adducts found. For the Expected Compounds table, the chromatographic peak for each row is also derived from the same parent compound and reaction steps.
   - Click the **Expected Formulas** tab and select a row.

     The Chromatograms view displays overlaid traces for all of the chromatographic peaks found for an expected elemental composition (same MW, parent compound, and elemental composition).
   - Click the **Merged Features** tab and select a row.

     The Chromatograms view displays overlaid traces of the chromatographic peaks detected by the Detect Compounds and Find Expected Compounds nodes for the selected feature (same *m/z* × RT dimensions).
   - Click the **Features** tab or the **Expected Features** tab and select a row.

     The Chromatograms view displays the integrated chromatographic peak for the selected table row (*m/z* × RT dimensions).

- Click the **Compounds per File** tab or the **Expected Compounds per File** tab and select a row.

  The Chromatograms view displays the integrated chromatographic peak for the selected table row (MW × RT dimensions). Each trace is a composite of its related adducts, and the peak area for a compound is the sum of the areas for its related adducts (parent area for the adducts listed in the Expected Features table or the Features table).

- Click the **FISh Trace Fragments** tab and select a row.

  The Chromatograms view displays a trace for the structure displayed in the selected table row. The FISh Trace Fragments table appears in the main table set when you select True for Individual Traces in the Create FISh Trace node of a processing workflow.

- Click the **Specialized Traces** tab and select a row.

Note The Specialized Traces table contains traces generated by these nodes: Create Mass Trace, Create Analog Trace, Create Pattern Trace, and Create FISh Trace.

Table 97. Workflow nodes that generate specialized traces

Workflow node	Generates any of these trace
Create Mass Trace	An extracted ion (mass range) chromatogram (XIC), a base peak chromatogram (BPC), or a total ion chromatogram (TIC)
Create Analog Trace	A UV-Vis trace from a UV-Vis or PDA detector, up to three traces from a PDA detector, or an analog trace from an LC detector that you connected to one of the analog input channels of a Thermo Scientific mass spectrometer
Create Pattern Trace	A TIC trace of the summed intensities of the mass spectral peaks (across the entire scan) that match the user-defined isotope pattern
Create FISh Trace	• A summed FISh trace of all the matching fragment ion scans (data-dependent acquisition [DDA] or data independent acquisition [DIA]) when you select True in the Summed Trace list. • An individual FISh trace for each fragment ion when you select True in the Individual Traces list. To view the individual trace for each fragment ion, see the FISh Trace Fragments table.

- Open the related tables, click the **Filled Gaps** tab, and select a row.

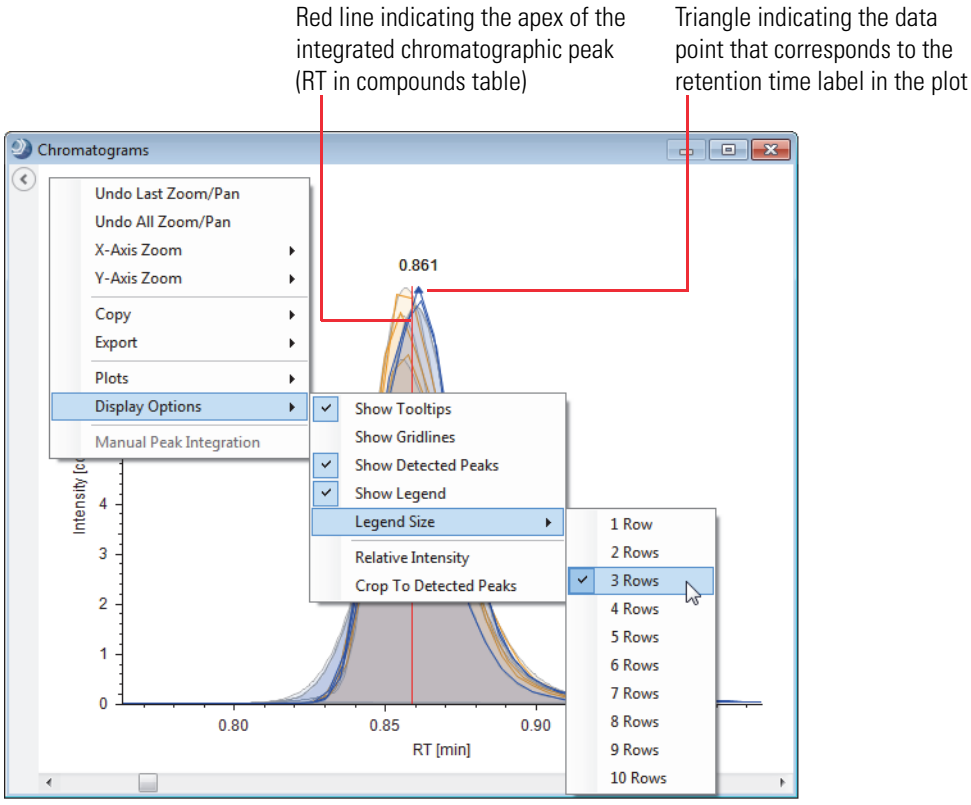
> **Tip** By default, the Filled Gaps table is hidden. To display this table, open the Select Visible Tables dialog box, select the **Filled Gaps** check box, and click **OK**. For more information, see "Filled Gaps table."

4. To determine the origin of a trace in a result file that includes multiple input files, right-click the Chromatograms view and choose **Display Options > Show Legend**.

5. To decrease or increase the number of legends displayed, right-click the Chromatograms view and choose **Display Options > Legend Size > #Rows**, where # is an integer value from 1 to 10.

   In Figure 107, the vertical red line indicates the peak apex of an integrated chromatographic peak. The triangle below the retention time label indicates the corresponding data point in the XIC trace.

Figure 107. Chromatograms view showing the shortcut menu (LC/MS data)



When the number of legend lines becomes too large for the available display space, the application displays an empty view with the following text:

Not enough space for drawing the chart properly.

Add a chromatogram plot

❖ To add a plot to the Chromatograms view

1. Open a result file that contains chromatographic data.
2. Right-click the Chromatograms view and choose **Plots > Add Plot**.

   The new plot appears below the original plot.

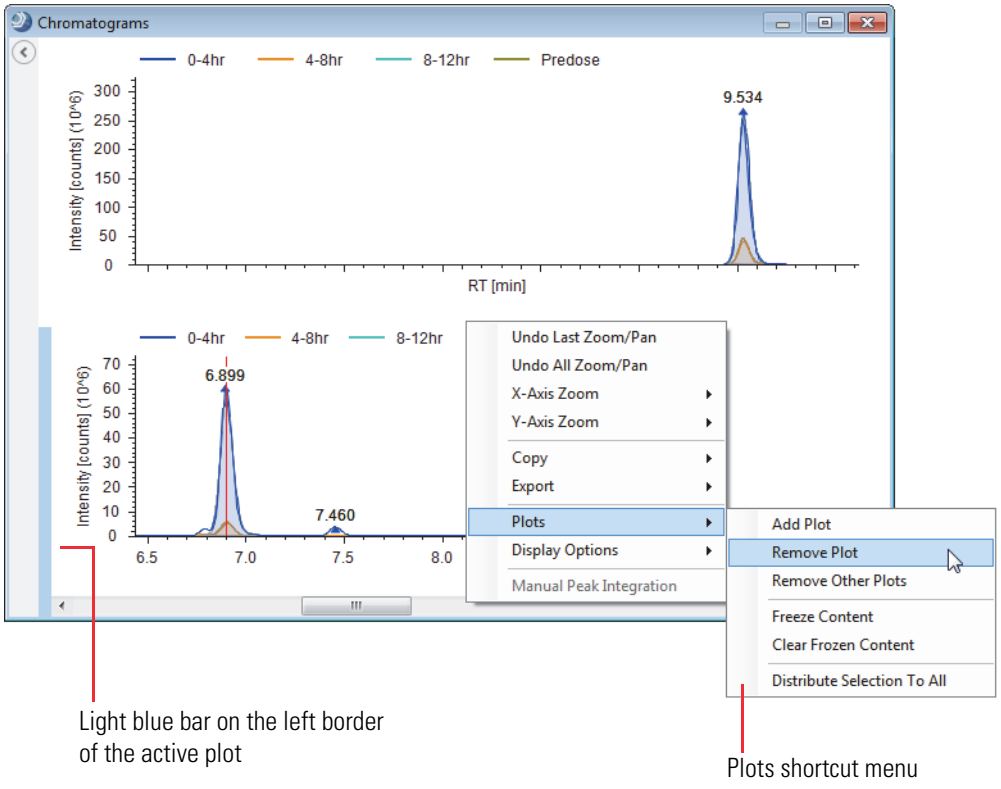
Note The size of the Chromatograms view limits the number of plots the view can display. When the application can no longer draw the plots properly, the following message appears:

> Not enough space for drawing plot properly

To display more plots, you can resize the view or drag the view to a second monitor and expand the view to fill the monitor.

In a Chromatograms view with more than one plot, a light blue bar on the left border highlights the active plot (see Figure 108). If you right-click the Chromatograms view and choose Plots > Remove Plot, the application removes the active plot.

Figure 108. Chromatograms view with two plots



Note Manual Peak Integration is available only for specialized traces in LC studies.

Overlay multiple chromatogram plots

❖ **To overlay multiple chromatograms in one chromatogram plot**

1. Open a result file that contains chromatographic data.
2. Do one of the following:
   - Hold down the Shift key and select a range of contiguous rows.
   - Hold down the CTRL key and select contiguous or noncontiguous rows one by one.
   - Hold down the Shift key and press the down arrow on the keyboard.

Tip Take care to avoid clicking an editable column in the result table, as doing so undoes the row selection and sets the focus to the table cell.

Change the grouping in the collapsible pane of an opened result file

❖ **To change the grouping of the chromatogram traces**

1. Open the collapsible left pane by clicking the icon,  .
2. Under Group By, select or clear one or more of the check boxes.
3. To display all of the study file traces in different colors, clear all of the check boxes under Group By, or under Group By, select only the **Samples** check box.

Hide the traces for a study variable value

❖ **To hide the chromatogram trace or traces for a study variable value**

Under Filter By, clear the check box for the study variable value.

Update all the chromatogram plots simultaneously

❖ **To simultaneously update all the plots in the Chromatograms view**

1. Open a result file that contains chromatographic data.
2. Add two or more plots to the Chromatograms view.
3. Right-click the view and choose **Plots > Distribute to All Selections**.

   As you select different table rows, all of the plots update. When Distribute to All Selections is not enabled, only the active plot updates.

Manually integrate chromatographic peaks

❖ To manually integrate chromatographic peaks

1. Open a result file that contains specialized traces.

   Note These workflow nodes generate specialized traces: Create Mass Trace, Create Analog Trace, Create Pattern Trace, and Create FISh Trace.

2. In the Specialized Traces table, select the trace of interest.
3. Right-click the Chromatograms view and choose **Manual Peak Integration**.

   Two red dashed lines appear and the integrated peak area appears in blue.

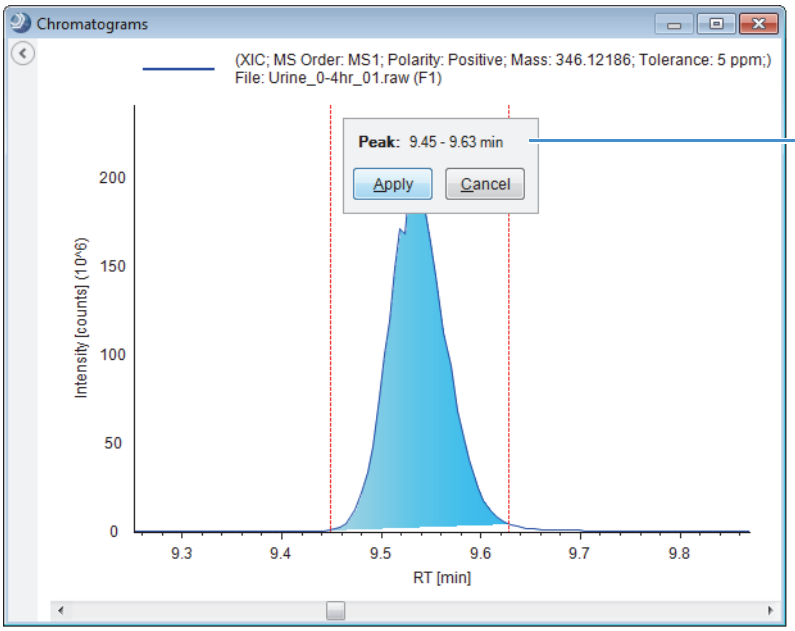
4. Drag one line to the beginning of the chromatographic peak and the other line to the end of the chromatographic peak.

   The integrated peak area changes as you move the start and end points of the chromatographic peak.

5. Place the cross-hair cursor on the peak.

   A pop-up box appears with the selected retention time range and the Apply and Cancel buttons.

Figure 109. Manually integrated chromatographic peak



6. To add the manual peak to the Manual Peaks table, do one of the following:
   - Click **Apply**.
   - On the keyboard, press **A**.

   If the result file did not already contain a Manual Peaks table, the new table appears in the main table tab set. The Manual Peaks table contains a row for the new manual peak.

Chromatograms view shortcut menu commands

Table 98 describes the shortcut menu commands for the Chromatograms view.

Table 98. Shortcut menu commands for the Chromatograms view (Sheet 1 of 5)

Command	Description
Note The default zoom settings are as follows: • X-axis Zoom > To Detected Peaks (Active Plot) • Y-axis Zoom > Auto Scale Y-axis	
Undo Last Zoom/Pan	Undoes the last zoom or pan movement.
Undo All Zoom/Pan	Zooms out to the full data acquisition time for the chromatogram on the *x* axis and the height of the largest chromatographic peak on the *y* axis.
X-axis Zoom > Keep Zoom	Maintains the same *x*-axis zoom range as you select different table rows. Overrides the Zoom to Detected Peaks command.
X-axis Zoom > Full Range	Displays the full data acquisition time for the chromatogram.
X-axis Zoom > To Detected Peaks (Active Plot)	Zooms the *x* axis to the detected peaks for the selected table rows.
X-axis Zoom > To Detected Peaks (All Plots)	Zooms the *x* axis to display the detected peaks in all of the plots.
Y-axis Zoom > Auto Scale Y-Axis	Default selection—Scales the *y* axis to the maximum intensity within the current *x*-axis (retention time) zoom range. Manual zooming of the *y* axis is unavailable in this mode.
Y-axis Zoom > Manual (Synchronize All Plots)	Scales the *y* axes of all the plots to the same scale. Manual zooming on both axes is available. To reset the *y*-axis scaling, choose **Y-axis Zoom > Auto Scale Y-Axis**, and then choose **Undo All Pan/Zoom**.
Y-axis Zoom > Manual (Each Plot Individual)	Only changes the *y*-axis scaling of the current plot. Manual zooming on both axes is available.

Table 98. Shortcut menu commands for the Chromatograms view (Sheet 2 of 5)

Command	Description
Copy > Image	Copies an image of the Chromatograms view (including the legend) to the Clipboard. You can paste the image into a Microsoft Office document as a raster image or into a vector-drawing program as a vector image.
Copy > Points	Copies the data as a two-column list of data points and copies the scan header. The first column lists the retention time and the second column lists either the relative intensity or the counts.
Export > Image As	Opens the Save As dialog box where you can specify a file name and save the contents of the Chromatograms view as one of these selectable image formats: EMF, PNG, GIF, JPG, TIFF, or BMP. The EMF format is a vector image.
Exports > Points As	Opens the Save As dialog box where you can specify a file name and save the contents of the Chromatograms view as a text file. The default file name is Chart.txt. When the chromatogram is a plot of relative intensity versus retention time, the application saves the data points as a two-column list. The first column lists the retention time and the second column lists the relative intensity (%). When the chromatogram is a plot of area (in counts) versus retention time, the second column lists the area for the peaks.
Plots > Add Plot	Adds an empty, active plot to the Chromatograms view. Only the screen size limits the maximum number of displayed plots. When you reach the screen's limit, the Chromatograms view appears to be empty and the following message appears: Not enough space for drawing chart properly.
Plots > Remove Plot	Removes the active plot, which has a gray border. Adding more than one plot makes this command available.
Plots > Remove Other Plots	Removes all of the plots in the Chromatograms view. Adding more than one plot to the Chromatograms view makes this command available.

Table 98. Shortcut menu commands for the Chromatograms view (Sheet 3 of 5)

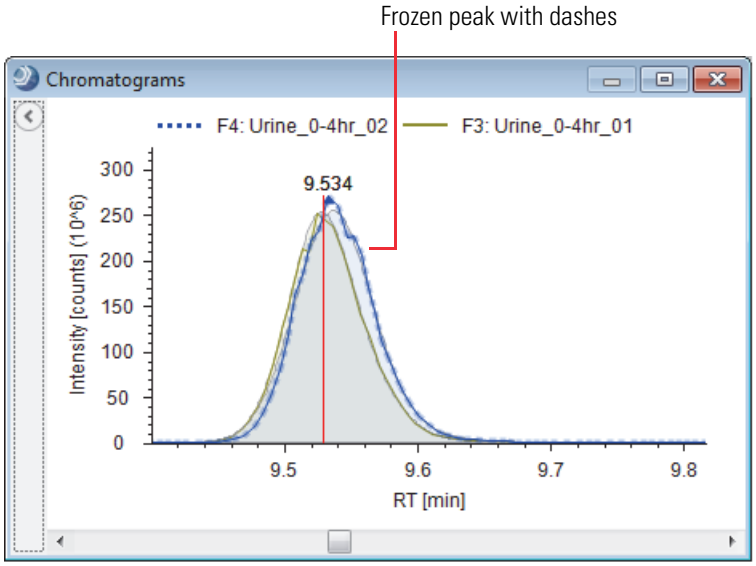
Command	Description
Plots > Freeze Content	Keeps the chromatogram of the currently selected row in the view when you select another row (in the current table or another result table). The application uses dashes to distinguish the frozen chromatogram trace. 
Plots > Clear Frozen Content	Clears the frozen chromatogram from the view.
Plots > Distribute Selection to All	Updates all of the plots simultaneously as you select different table rows. When Plots > Distribute Selection to All is not enabled, only the active plot updates.
Display Options > Show Tooltips	Displays a pop-up box with the following information, from top to bottom, when you place the cursor, +, over a chromatographic peak: • Parent compound and any applicable transformations for an expected compound • Chemical formula for an expected compound • Adduct ion (feature) • m/z value (feature) • Molecular weight (compound or expected compound) • Selected retention time, in minutes • Intensity (height), in counts, of the selected point on the chromatogram trace • File name of the input file

Table 98. Shortcut menu commands for the Chromatograms view (Sheet 4 of 5)

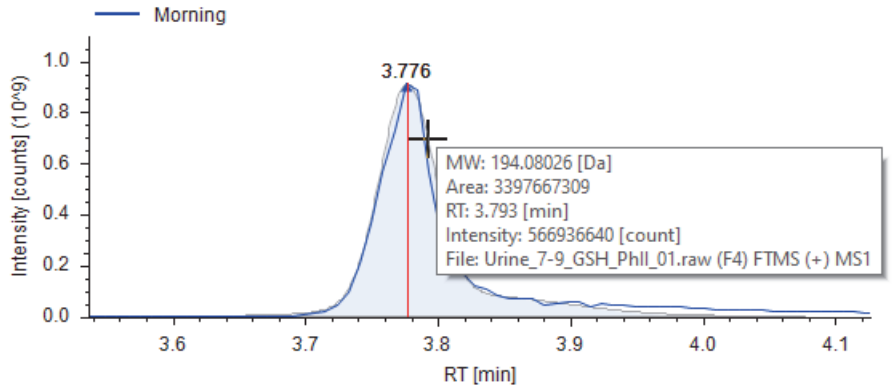
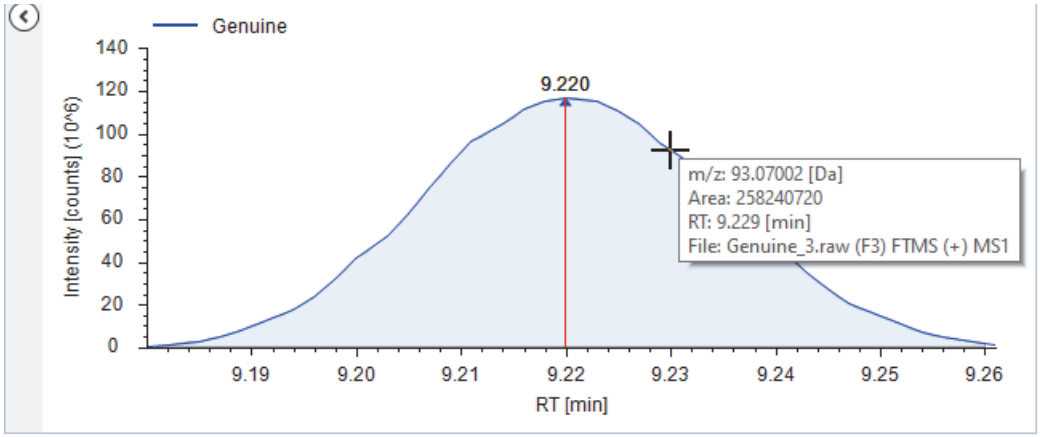
Command	Description
Chromatogram with a tooltip for an entry in the Compounds per File table. 	
Chromatogram with a tooltip for an entry in the GC EI Compounds per File table 	
Display Options > Show Gridlines	Adds grid lines to the Chromatograms view.
Display Options > Show Detected Peaks	Uses a fill color for the integrated area under the detected chromatographic peaks. Turning off this command removes the fill color. **Tip** To see the peaks underneath the larger peaks in a set of overlaid traces, turn off the Show Detected Peaks command.
Display Options > Show Legend	Displays a legend for the sample groups at the top of the view.
Display Options > Legend Size	Specifies the number of legend lines that you want the application to display. Selections: 0 to 10

Table 98. Shortcut menu commands for the Chromatograms view (Sheet 5 of 5)

Command	Description
Display Options > Relative Intensity	Displays the *y*-axis scale as relative intensity (0 to 100%). The legend changes to Intensity [%]. The default *y*-axis scale is an absolute scale; the *y*-axis legend is intensity [counts].
Display Options > Crop to Detected Peaks	Redraws only the chromatographic peaks of the displayed traces. Does not redraw the baseline portions of the traces as you select different table rows.
Manual Peak Integration	Use to add a manual peak to a specialized trace. Adding a manual peak adds the Manual Peaks table to a result file. See "Manually integrate chromatographic peaks." Selecting a trace in the Specialized Traces table makes this command available.

Table 99 describes the traces that you can display in the Chromatograms view.

Table 99. Chromatograms view traces (Sheet 1 of 2)

Trace type	Description
UV	Displays a chromatogram created from the UV signal from a UV-Vis detector or the analog channel of a PDA detector.
Analog	Displays a trace of response versus time. Raw data files can contain analog data from a device that is hard-wired to the analog channels of a Thermo Scientific mass spectrometer.
PDA total scan	Displays a chromatogram of the total absorbance for the entire scan wavelength range for each time point.
PDA spectrum maximum	Displays a chromatogram of the highest absorbance reading in the wavelength range for each time point.
PDA wavelength range	Displays a chromatogram of the total absorbance for the specified wavelength range for each time point.
Base peak chromatogram (BPC)	Displays a chromatogram of the most intense mass spectral peak in the specified mass range for each time point.
Total ion chromatogram (TIC)	Displays a chromatogram of the total intensity from all the mass spectral peaks in the specified mass range for each time point.

Table 99. Chromatograms view traces (Sheet 2 of 2)

Trace type	Description
Extracted ion chromatogram (XIC)	Displays an XIC trace, which is a mass range trace, when you select a row in any of these tables: Merged Features, Expected Compounds, Expected Compounds per File, Expected Compound Features, Compounds, Compounds per File, Unknown Compound Features, FISh Trace Fragments, or Specialized Traces. The XIC trace is made up of the mass spectral peaks that match the specified mass value within the specified mass tolerance.
Pattern trace	Displays a TIC trace of the summed intensities of the mass spectral peaks that match a specified pattern for each time point.
FISh trace	Displays a TIC trace of the summed intensities of the mass spectral peaks in a fragmentation scan (MS/MS or MS^3) that match the predicted fragments of the selected library compound and its transformation products for each time point.

Mass Spectrum view

The Mass Spectrum view displays the spectral tree of a selected component in the result table and the mass spectrum of the selected scan in the spectral tree.

For details, see these topics:

- Display a mass spectrum
- Change the zoom level of the Mass Spectrum view
- View annotated fragment structures for targeted compounds
- View annotated fragment structures for untargeted compounds
- Create a mirror plot
- Search the mzCloud database for a matching fragmentation spectrum
- Spectral tree pane of the Mass Spectrum view
- Isotope pattern matching for compounds with formulas
- Mass Spectrum view shortcut menu commands

Display a mass spectrum

❖ **To display a specific mass spectrum**

1. Open a result file.
2. If the Mass Spectrum view is closed, choose **View > Mass Spectrum** from the menu bar.
3. Do the following:
   a. Select an entry in any of these result tables.

LC studies	
• Compounds table	• Features table
• Compounds per File table	• Expected Features table
• Expected Compounds table	• mzCloud Results table
• Expected Compounds per File table	• Structure Proposals table

   The Mass Spectrum view displays the matching spectral tree and a zoomed-in view of the full MS scan.

   b. Select the scan of interest from the spectral tree.

Change the zoom level of the Mass Spectrum view

In the Mass Spectrum view for a result file, you can independently zoom in or out on the *x* or *y* axis by dragging the cursor horizontally or vertically, respectively, or you can zoom in or out of a rectangular section of the plot.

Table 100. Working with the zoom level in the Mass Spectrum view

Task	Procedure
Zoom in on the *x* axis.	Drag the cursor to the right over the *m/z* range of interest.
Zoom out on the *x* axis.	Drag the cursor horizontally to the left over the *m/z* range of interest.
Zoom in on the *y* axis.	Drag the cursor vertically down the *y* axis.
Zoom out on the *y* axis.	Drag the cursor vertically up the *y* axis.
Zoom in on a section of the plot.	Drag the cursor diagonally across the section.
Undo the last zoom-in action.	Right-click the plot and choose **Zoom Out**.
Change the zoom level to the full *m/z* range on the *x* axis and the full response range on the *y* axis.	Right-click the plot and choose **Undo All Zoom/Pan**.

View annotated fragment structures for targeted compounds

For studies where you are targeting specific compounds, you can add the FISh Scoring node to the processing workflow or apply the FISh scoring algorithm to expected compounds in the result file.

❖ To review the matching fragment structures predicted by the FISh scoring algorithm

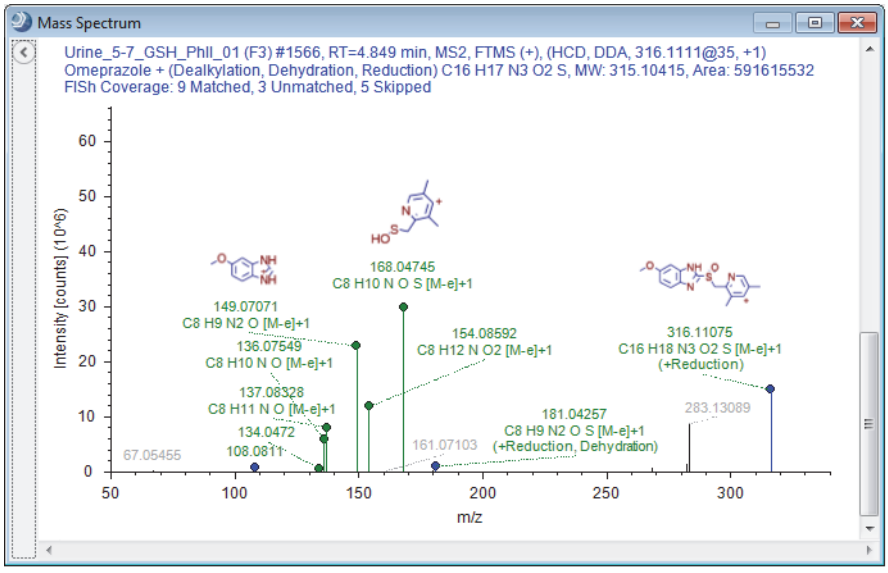
1. Open a result file generated by a processing workflow that included the Expected Compounds node and the FISh Scoring node. Then, select a compound in the Expected Compounds table.
2. (Optional) Enlarge the Mass Spectrum view.
3. In the spectral tree, select an MS2 or higher scan.
4. Review the color-coded mass spectral peaks, the theoretical fragment structures, and the transformations for the shifted mass spectral peaks.

   The FISh Scoring node annotates centroids that match the *m/z* value of a theoretical fragment ion with its theoretical structure and color-codes the centroids in a fragmentation scan as follows.

Color	Meaning
(●) Green	Direct match—Matches the *m/z* value of a theoretical fragment ion.
(●) Blue	Shifted match—Matches the *m/z* value of a theoretical fragment ion with at least one transformation applied.

Figure 110 shows an annotated fragmentation spectrum.

Figure 110. Fragmentation spectrum with FISh annotations (targeted analysis)



View annotated fragment structures for untargeted compounds

For LC studies, you can apply the FISh scoring algorithm to compounds in the Compounds table and the related Structure Proposals table that have MS2 spectra and assigned structures.

❖ **To run the FISh scoring algorithm on an untargeted compound and view the structure annotations in the Mass Spectrum view**

1. Open a result file from an untargeted analysis that returns structures.

   For LC studies, the processing workflow must include the Detect Compounds node, Group Compounds node, Predict Compositions node, Assign Compound Annotations node, and any of the identification or pathway mapping nodes that return structures. In addition, the input files must include fragmentation scans.

2. Display the FISh Coverage and Structure columns as follows:

   a. Open the Field Chooser dialog box by clicking the icon,  , in the upper-left corner of the Compounds table.

   b. Select the FISh Coverage and Structure check boxes, and then close the Field Chooser dialog box.

3. Right-click a compound of interest that has a structure and fragmentation spectra and choose **Apply FISh Scoring**.

   The Specify FISh Scoring Settings dialog box opens.

4. Specify the fragmentation settings and click **OK**.

   The FISh Scoring Queue opens, and the application starts processing the MS2 scans against the structure. When processing is completed, the calculated FISh coverage score appears in the FISh Coverage column.

5. If the Mass Spectrum view is closed, open it by choosing **View > Mass Spectrum** from the menu bar.

6. In the spectral tree at the left of the Mass Spectrum view, select an MS2 scan.

   The annotated spectrum appears in the Mass Spectrum view. The spectrum header displays the number of centroids that the FISh scoring algorithm matched to theoretical fragments, the number of theoretical fragments that had no matching centroid, and the number of fragments that it did not attempt to match (skipped) because their expected intensity was below the signal-to-noise setting.

The FISh scoring algorithm annotates each centroid that matches the *m/z* value of a theoretical fragment ion with its theoretical structure, *m/z* value, and formula. In addition, the application displays matching centroids in green with a green circle at the top.

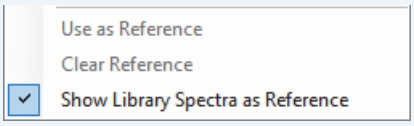
Create a mirror plot

In a result file that includes MS2 scans, you can create a mirror plot to compare an experimental spectrum to a reference spectrum.

❖ To create a mirror plot of two fragmentation scans

1. Open a result file with fragmentation scans.
2. If the Mass Spectrum view is closed, choose **View > Mass Spectrum** from the menu bar.
3. In the spectral tree pane, select a reference scan.
4. Right-click the Mass Spectrum view and turn off the **Show Library Spectra as Reference** command if it is available.

Note The Use As Reference command is unavailable when the Show Library Spectra As Reference command is available.



5. Right-click the Mass Spectrum view and choose **Use As Reference**.
6. Select the fragmentation scan that you want to compare.

   The reference scan appears on the bottom and the comparison scan appears on the top.
7. To remove the reference scan from the plot, right-click the Mass Spectrum view and choose **Clear Reference**.

Search the mzCloud database for a matching fragmentation spectrum

From the Mass Spectrum view, you can submit a query fragmentation spectrum to the online mzCloud mass spectral database.

❖ To manually search the mzCloud database for a matching fragmentation spectrum

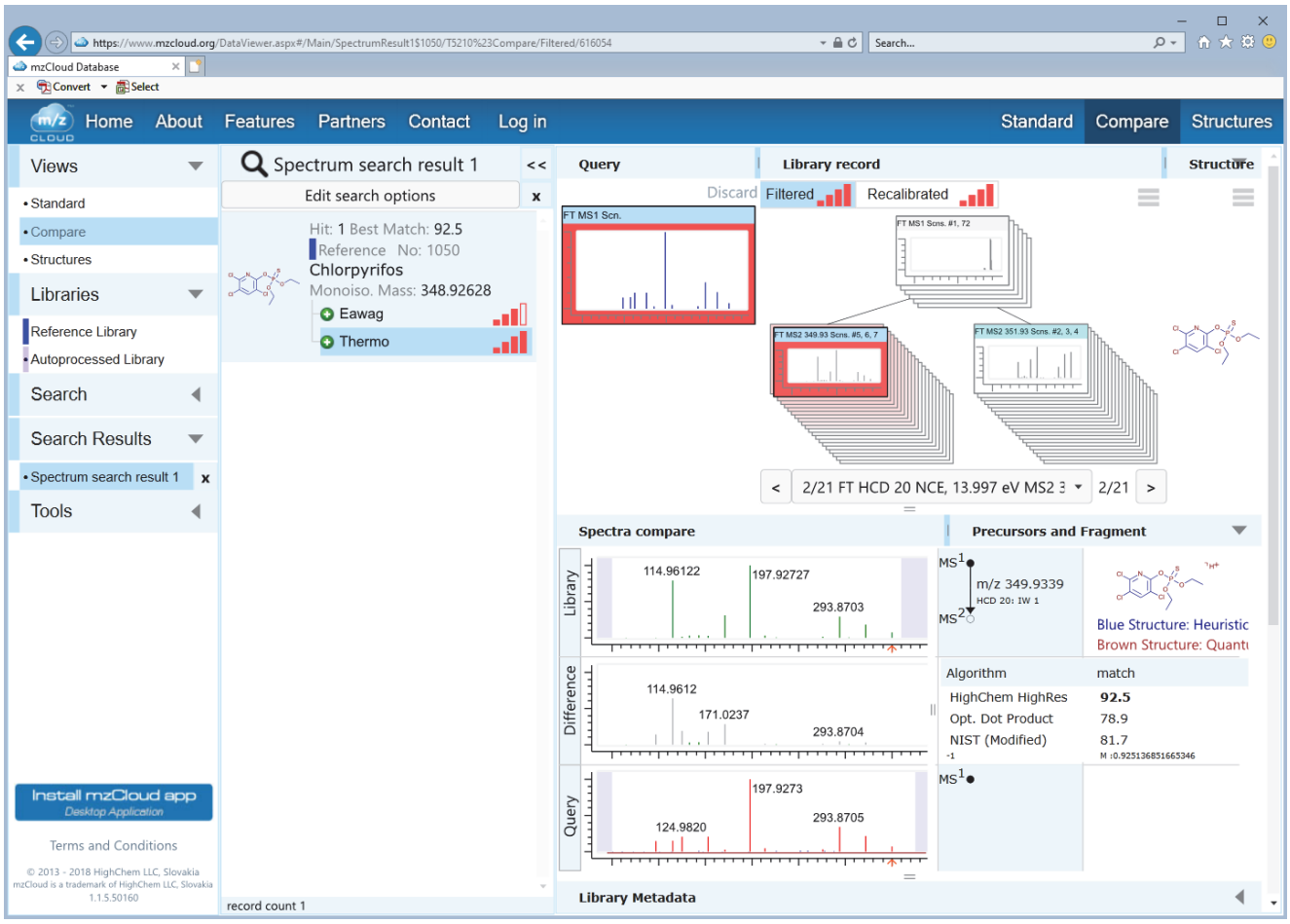
Note The mzCloud database is compatible only with the Internet Explorer™ web browser. To access the mzCloud spectral database from the Compound Discoverer application, set Internet Explorer as your default Internet browser.

1. Open a result file with data-dependent fragmentation data.

2. In the spectral tree pane of the Mass Spectrum view, select a fragmentation scan.
3. Right-click the spectrum plot and choose **Submit To mzCloud**.

   The online mzCloud application opens to the Select Spectrum dialog box and displays the selected query spectrum.
4. Optimize the settings and click **OK**.

Figure 111. mzCloud search for a query spectrum of Chlorpyrifos



Spectral tree pane of the Mass Spectrum view

For an LC study, the collapsible pane on the left of the Mass Spectrum view contains a spectral tree with the high-resolution scans for preferred ions that elute within the following retention time window:

- Peak apex (RT) ± the peak's full width at half maximum (FWHM)

–or–

- From the start time to the end time for the chromatographic peak as defined by the peak detection algorithm

For MS1 scans, the tree lists the scan number, the retention time at the apex of the chromatographic peak, the mass analyzer, and the scan polarity.

For MSn scans, the tree lists the scan number, the retention time at the apex of the chromatographic peak, the mass analyzer, the scan polarity, and the fragmentation information, including the scan power, collision cell type, and the fragmentation type (data-dependent acquisition [DDA] or data-independent acquisition [DIA]).

Isotope pattern matching for compounds with formulas

For LC studies, selecting an entry in the following result tables populates the Mass Spectrum view with a spectral tree for the entry in the left pane and the first MS1 scan for the selected compound or feature in the right pane.

- Expected Compounds
- Expected Compounds per File
- Expected Features
- Compounds

If the analysis predicts a formula for the compound or feature, the MS1 scan shows the isotope pattern fit for the detected compound. Colored rectangles highlight the mass spectral peaks (centroids) that match the theoretical isotope pattern. These rectangles have a minimum display width to ensure that they are still visible when you zoom out or use the Undo All Zoom/Pan shortcut menu command.

Note The isotope pattern fit algorithm is “resolution aware”; that is, in addition to the list of elemental compositions provided by the Generate Expected Compounds node or the Predict Compositions node, it uses the resolution information provided with the scan data to perform an isotope pattern fit and calculate a spectral distance score.

If the resolution information is unavailable, it uses the setting for the Unrecognized MS Resolution parameter in the Select Spectra node.

Figure 112. MS1 scan with color-coded mass peaks and the shortcut menu (LC study)

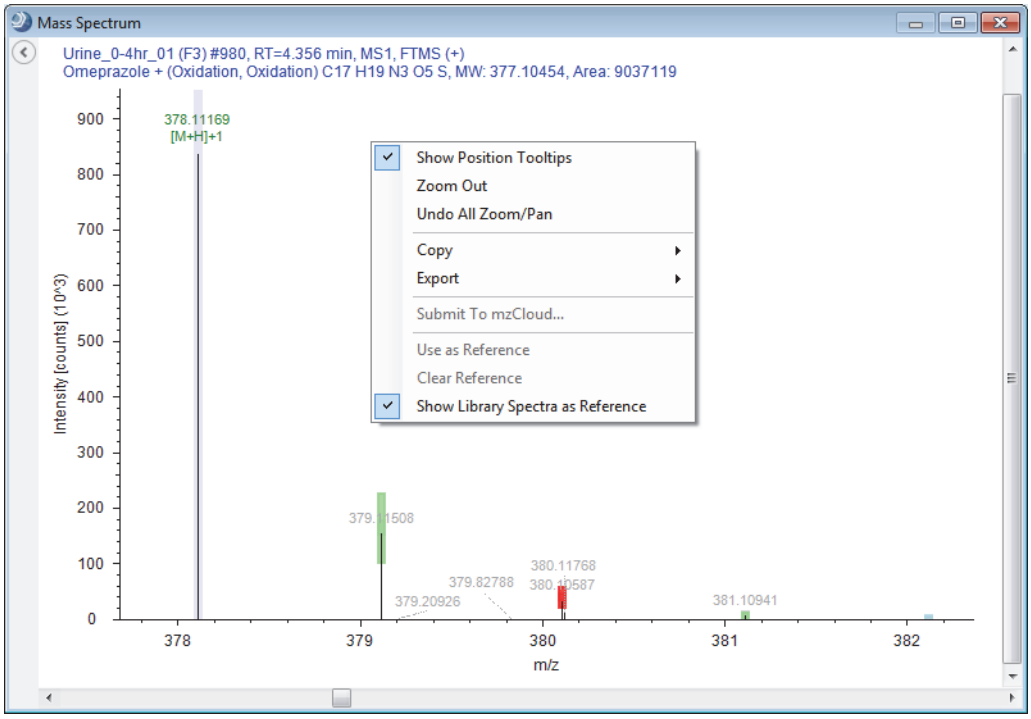


Table 101 describes the color coding for the centroids in an MS1 spectrum.

Table 101. Color coding for the centroids in an MS1 spectrum for a compound with a formula annotation

Color	Meaning
( ) Lavender	Indicates the most intense centroid in the spectrum.
	Note The A0 isotope (monoisotopic ion) is always the isotope with the lowest *m/z* value, but it is not necessarily the isotope with the highest intensity. For example, for compounds with more than one bromine atom, a bromine atom and a chlorine atom, or more than four chlorine atoms, the M + 2 (A2) isotope is the most intense isotope.
( ) Green	The labeled centroid matches the delta mass and the relative intensity of the theoretical isotope pattern for the formula annotation within the specified tolerances.
( ) Red	The expected centroid for this *m/z* value is missing or its intensity does not fall within the tolerance range for the theoretical isotope pattern for the formula annotation.
( ) Light blue	The expected centroid for this *m/z* value (for the formula annotation) might be missing because its theoretical intensity is at the level of the baseline noise.

Mass Spectrum view shortcut menu commands

Table 102 describes the shortcut (right-click) menu commands for the Mass Spectrum view.

Table 102. Mass Spectrum view shortcut menu commands (Sheet 1 of 2)

Command	Description
Show Position Tooltips	Displays the *m/z* value and intensity of the mass spectrum peaks as you point to them.
Zoom Out	Undoes the last zoom-in action.
Undo All Zoom/Pan	Changes the zoom level to the full *m/z* range on the *x* axis and the full response range on the *y* axis.
Copy > Image	Copies the mass spectrum as a bitmap (raster) image to the Clipboard.
Copy > Points	Copies the data points and the scan header for the selected scan to the Clipboard. Also copies all text annotations, such as the FISh fragment annotations and the adduct information. Use this command to copy the FISh annotations to the Clipboard.
Copy > Raw Points	Copies the data points for the selected scan to the Clipboard. Use this command to copy points to a library search application.
Export > Image As	Opens the Save As dialog box, where you can type a name and select a file type for the current scan. The available file types are BMP, EMT, GIF, JPG, PNG, and TIF.
Export > Points As	Opens the Save As dialog box, where you can type a name and select a file type for the current scan. The available file type is TXT.

Table 102. Mass Spectrum view shortcut menu commands (Sheet 2 of 2)

Command	Description
Submit to mzCloud	Opens the Spectrum Search dialog box for the mzCloud database where you can submit a search for the selected fragmentation scan. Available for an MS/MS data-dependent scan. **IMPORTANT** The mzCloud web application is compatible only with the Internet Explorer™ web browser. **Tip** To test your computer's ability to connect to the mzCloud database, choose **Help > Communication Tests** from the application toolbar. Click the **mzCloud** tab, and then click **Run Tests**. To set up the mass tolerances for manual searches, choose **Help > Configuration** from the application toolbar. In the left pane, select **Submit Single Spectrum to mzCloud Options**. Edit the settings as applicable.
Use As Reference	Creates a mirror plot that initially consists of the currently selected scan. When you select another scan, the reference scan remains in the $-y$-axis portion of the graph and the new scan appears in the $+y$-axis portion of the graph. Unavailable when the Show Library Spectra Reference command is enabled.
Clear Reference	Removes the reference plot from the Mass Spectrum view.
Show Library Spectra as Reference	Displays the recalibrated library spectrum from the mzCloud database in the bottom portion of the mirror plot. Available when you select a row in the mzCloud Results table.

Result Charts view

Use the Result Charts view to plot the data in a result table as a scatter plot, histogram, bar chart, or pie chart.

For details about the Result Charts view, see the following topics:

- Open the Result Charts view
- Use the copy, export, and zoom commands for the Result Charts view
- Display and pin the Options Pane for the Result Charts view
- Histogram charts
- Bar charts
- Pie charts
- Scatter plots

Open the Result Charts view

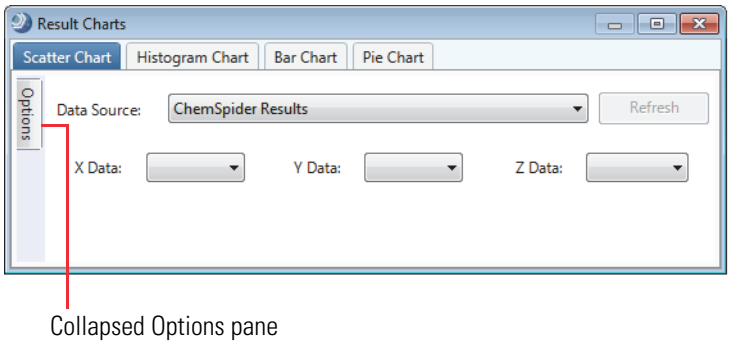
❖ **To open the Result Charts view**

1. Open a result file. See "Open, close, and update result files."
2. In the menu bar, choose **View > Result Charts**.

   By default, the Result Charts view opens as a floating window. You can resize the window, drag the window to another screen, or dock the window. See "Rearrange the tabbed pages and graphical views."

   The Options pane for modifying the appearance of a chart view is a collapsible pane to the left of each chart.

Figure 113. Floating Result Charts view with the collapsed (unpinned) Options pane at the left



Use the copy, export, and zoom commands for the Result Charts view

❖ **To access and use the shortcut menu commands for a Result Charts page**

1. On the selected page of the Result Charts view, select the variables that you want to plot.
2. Click **Refresh** to plot the data.
3. Right-click the chart and choose one of the commands listed in Table 103.

Table 103. Common shortcut menu commands for the Result Chart views[a]

Command	Availability	Function
Undo All Pan/Zoom	Scatter Chart, Histogram Chart, and Bar Chart	Undoes all panning and zooming. Returns the view to the default magnification.
Zoom Out	Scatter Chart, Histogram Chart, and Bar Chart	Undoes the last zoom-in action.
Copy > Image	All	Copies a raster image of the plot to the Clipboard.
Copy > Data	All	Copies a list of the data points to the Clipboard.
Export > Image As	All	Saves the plot in the selected file format. File types: EMF, PNG, GIF, JPG, TIF, and BMP
Export > Data As	All	Exports a list of data points to a text file.

[a] The shortcut menu for the Scatter Chart view has additional commands.

Display and pin the Options Pane for the Result Charts view

The Options pane of the Result Charts view contains the formatting options for the grid lines, fonts, and so on.

❖ **To display and pin the Options pane**

1. Point to the vertical Options tab on the left.
2. To keep the pane open, click the pin icon, ⊣, in the upper-right corner of the Options pane.

Histogram charts

Use the Histogram Chart page of the Result Charts view to plot the frequency distribution of a variable (result table column). You can display the data as a column chart, a bar chart, a line, or a stepped line chart.

❖ To display the data as a histogram

1. Open a result file.
2. Choose **View > Result Charts**.
3. Click the **Histograms Chart** tab.
4. From the Data Source list, select the variable (result table column) that you want to plot.
5. Click **Refresh**.
6. (Optional) To change the appearance of the histogram, do the following:
   a. Open the Options pane.
   b. Modify the settings for the colors, labels, and legends of the display, as necessary.

      –or–

      Click **Load** to load the settings that you most recently saved.
   c. To save the settings, click **Save** in the Options pane.

      The new settings overwrite any previously saved settings. The application loads these new settings when you click Load.
   d. To return the settings to the original default settings, click **Factory Defaults** in the Options pane.

Table 104 describes the parameters for the Histogram Chart page.

Table 104. Histogram Chart parameters (Sheet 1 of 6)

Parameters	Description
Data Source	Specifies the source of the data that you want to plot. The available data sources are the result table columns in the result file.
Refresh	Refreshes the display with data points from the selected data source.
Options pane commands	
Load	Loads the Option pane settings that you saved with the Save command.
Save	Saves the settings that you selected in the Options pane.
Factory Defaults	Resets the settings of the options in the Options pane to the defaults in effect when you installed the application.

Table 104. Histogram Chart parameters (Sheet 2 of 6)

Parameters	Description
1. Chart Options	
Chart Type	Determines how the application plots the data. • (Default) Column: Displays the data as columns extending from bottom to top. • Bar: Displays the data as bars extending from left to right. • Line: Displays the data as a line. Reported and excluded items are not stacked as they are in column and bar types. • StepLine: Displays the data as a line drawn in a series of 90-degree angles.
Show Cumulative	Determines whether the application displays a cumulative histogram, which can be useful if you want to compare distribution curves. For these charts, the application calculates the column height as the height of the current column plus the sum of all previous columns. The rightmost column height is therefore the total count or 100%, depending on the *y*-axis settings. • (Default) True: displays a cumulative histogram. • False: Displays a non-cumulative histogram.
Horizontal Grid Lines	Determines whether the histogram displays horizontal grid lines and specifies the style of these lines. • (Default) None: Displays no horizontal grid lines on the histogram. • Solid: Displays solid horizontal grid lines on the histogram. • Dotted: Displays dotted horizontal grid lines on the histogram.
Vertical Grid Lines	Determines whether the histogram displays vertical grid lines and specifies the style of these lines. • (Default) None: Displays no vertical grid lines on the histogram. • Solid: Displays solid vertical grid lines on the histogram. • Dotted: Displays dotted vertical grid lines on the histogram.

Table 104. Histogram Chart parameters (Sheet 3 of 6)

Parameters	Description
2. Column Options	
Show Column Amount	Determines whether the chart displays the amount or count of items. • True: Displays the amount or count of items in the chart. • (Default) False: Does not the display the amount or count of items in the chart.
Show Percentages	Determines whether percentage values appear above the columns or to the right of the bars. • True: Displays percentage values above the columns or to the right of the bars. • (Default) False: Does not display percentage values above the columns or to the right of the bars.
Column Display	Specifies the appearance of the columns or bars. • (Default) Flat: Displays the columns or bars as flat rectangles. • Cylinder: Displays the columns or bars as cylinders. • Emboss*: Displays the columns or bars as three-dimensional rectangles. • LightToDark: Displays the columns or bars as shaded rectangles. *Emboss is misspelled as Embross in the dropdown list.
Column Width	Specifies the relative width of the columns as a decimal between 0 and 1. Default: 0.8
Column Label Font	Specifies the font of the column labels that appear on top of the bars in the histogram. These labels are visible if you set Show Column Amount to True. Default: 8-point Arial
3. Axis Options	
X-Axis Number Format	Specifies the notation of the numbers used for the *x* axis. • (Default) Decimal: Uses decimal notation. • Scientific: Uses scientific notation.

Table 104. Histogram Chart parameters (Sheet 4 of 6)

Parameters	Description
X-Axis Title	Specifies the label for the *x* axis. The default *x*-axis title is the category selected from the Data Source list.
Y-Axis Type	Specifies the axis type (scale) of the *y* axis. • (Default) Linear: Plots the data on a linear scale. • Log: Plots the data on a logarithmic scale. • Percent: Plots the data as a percentage of the number of items.
Y-Axis Title	Specifies the label for the *y* axis. The default *y*-axis title is Count.
Reduce Number of Axis Labels	Determines whether the application increases readability by reducing the maximum number of axis labels to 30. If the chart includes more than 30 values, it displays only every second or every third label. • (Default) True: Reduces the maximum number of axis labels to 30. • False: Does not reduce the maximum number of axis labels to 30.
Axis Title Font	Specifies the font used to denote the labels of the *x* and *y* axes. Default: 12-point Arial
Axis Scale Font	Specifies the font used to denote the scale of the *x* and *y* axes. Default: 10-point Arial
4. Binning Options	
Binning Method	Specifies the number of data groups to display or the width of a single data group. • (Default) Auto: Groups the data by estimating the number of columns to display the number of data items. • FixedWidth: Groups the data according to the Width value. • FixedNumber: Groups the data according to the Number of Categories value.
Number of Bins	Specifies the number of categories used to group the data. Default: 20 **Note** For discrete numbers, the actual group number might be different.

Table 104. Histogram Chart parameters (Sheet 5 of 6)

Parameters	Description
Bin Width	Specifies the width of a single category used to group the data. Default: 1 **Note** For discrete numbers, the actual group number might be different.
Use Full Series Value Range	Determines the range of data values that the application uses to compile the histogram. • (Default) True: Uses all data for the histogram. • False: Uses only the data between the values specified by the Minimum Value option and the Maximum Value option.
Minimum Value	Specifies the minimum value of the displayed data range. When you use this parameter and the Maximum Value parameter, set Use Full Data Range to False. Use these two parameters when you want to show only a subrange of the data in a histogram.
Maximum Value	Specifies the maximum value of the displayed data range. When you use this option and the Minimum Value option, set the Use Full Data Range parameter to False.
5. Legend Options	
Show Legend	Determines whether a legend appears and where it appears. • (Default) None: Does not display a legend. • Top: Displays a legend at the top of the histogram. • Left: Displays a legend to the left of the histogram. • Bottom: Displays a legend at the bottom of the histogram. • Right: Displays a legend to the right of the histogram.
Legend Font	Specifies the font for the legend. Default: 8-point Arial

Table 104. Histogram Chart parameters (Sheet 6 of 6)

Parameters	Description
6. Series Options	
Show Only Checked Items	Determines whether the chart is compiled from data in all result rows or only data in result rows marked by check marks. • True: Compiles the chart only from data in result rows marked by check marks. • (Default) False: Compiles the chart from data in all result rows.
Target Series Color	Specifies the color of the target series. Default: Firebrick

Bar charts

Bar charts plot categorical and ordinal data types in columns with the count of the data types as the column height.

The Data Source list contains the numerical data categories that are available for the bar chart. The Options pane contains the different options that you can use to customize the bar chart. Moving the cursor over the columns in the chart activates a tooltip with information about the data category.

❖ To display the data as a bar chart

1. In an open result file, choose **View > Result Charts**.
2. Click the **Bar Charts** tab in the Result Charts view.
3. From the Data Source list, select the type of data to display as a bar chart.
4. Click **Refresh** to draw the chart.
5. (Optional) To change the chart's appearance, do the following:
   a. Open the Options pane and adjust the colors, labels, and legends of the display. Or, click **Load** to load the option settings that you most recently saved.
   b. To save all the settings, click **Save** in the Options pane.

      The new settings overwrite any previously saved settings. The application loads these new settings when you click Load.
   c. To return the Options pane settings to the original default settings, click **Factory Defaults i**n the Options pane.

Table 105 describes the parameters on the Bar Chart page of the Result Charts view.

Table 105. Bar Chart parameters (Sheet 1 of 3)

Command or option	Description
Options pane	
Load	Loads the Option pane settings that you saved with the Save command.
Save	Saves the settings that you selected in the Options pane.
Factory Defaults	Resets the options in the Options pane to the default settings in effect when you installed the application.
Chart Options	
Chart Type	Determines how the application plots the data. • (Default) Column: Displays the data as columns extending from bottom to top. • Bar: Displays the data as bars extending from left to right.
Horizontal Grid Lines	Determines whether the bar chart displays horizontal grid lines and specifies the style of these lines. • (Default) None: Displays no horizontal grid lines in the bar chart. • Solid: Displays solid horizontal grid lines in the bar chart. • Dotted: Displays dotted horizontal grid lines in the bar chart.
Axis Options	
X-Axis Title	Specifies the label for the *x* axis. The default *x*-axis title is the category selected from the Data Source list.
Y-Axis Title	Specifies the label for the *y* axis. The default *y*-axis title is Count.
Y-Axis Type	Specifies the axis type (scale) of the *y* axis. • (Default) Linear: Plots the data on a linear scale. • Log: Plots the data on a logarithmic scale. • Percent: Plots the data as a percentage of the number of items.
Axis Title Font	Specifies the font used to denote the labels of the *x* and *y* axes. Default: 12-point Arial
Axis Scale Font	Specifies the font used to denote the scale of the *x* and *y* axes. Default: 10-point Arial

Table 105. Bar Chart parameters (Sheet 2 of 3)

Command or option	Description
Bar Options	
Show Rotated Scale	Determines whether the scale labels along the *x* axis are slightly rotated to the right. • (Default) True: Rotates the scale labels. • False: Does not rotate the scale labels.
X-Axis Scale Angle	Specifies the angle between the label and the *x* axis for the labels when the Show Rotated Labels parameter is set to True. Range: –90 to 90 degrees Default: 30
Bar Display	Specifies the appearance of the columns or bars. • (Default) Flat: Displays the columns or bars as flat rectangles. • Cylinder: Displays the columns or bars as cylinders. • Emboss*: Displays the columns or bars as three-dimensional rectangles. • LightToDark: Displays the columns or bars as shaded rectangles. *Emboss is misspelled as Embross in the dropdown list.
Bar Width	Specifies the relative width of the columns. Range: 0.1–1.0 Default: 0.8
Show Amount	Determines whether the amount, or count of items, is displayed in the chart. • True: Displays the amount or count of items in the chart. • (Default) False: Does not the display the amount or count of items in the chart.
Show Percentage	Determines whether percentage values are displayed above the columns or to the right of the bars. • True: Displays percentage values above the columns or to the right of the bars. • (Default) False: Does not display percentage values above the columns or to the right of the bars.

Table 105. Bar Chart parameters (Sheet 3 of 3)

Command or option	Description
Column Label	Specifies the font of the column labels that appear on top of the bars in the bar chart. Default: 8-point Arial
Legend Options	
Show Legend	Determines whether a legend appears and where it appears. • (Default) None: Does not display a legend. • Top: Displays a legend at the top of the bar chart. • Left: Displays a legend to the left of the bar chart. • Bottom: Displays a legend at the bottom of the bar chart. • Right: Displays a legend to the right of the bar chart.
Legend Font	Specifies the legend font. Default: 8-point Arial
Series Options	
Show Only Checked Items	Determines whether the chart is compiled from data in all result rows or only data in result rows marked by check marks. • True: Compiles the chart only from data in result rows marked by check marks. • (Default) False: Compiles the chart from data in all result rows.
Series Color	Specifies the color of the bars. Default: CornflowerBlue
Data Source	Displays the result category used to plot the data.

Pie charts

The Pie Chart page shows several categories of data as a solid circle composed of slices (a pie) or as a ring (a doughnut). You can use a pie chart or a doughnut chart to indicate the relative size of quantities of data.

❖ To display the data as a pie chart

1. With an active result file, choose **View > Result Charts** from the menu bar.
2. Click the **Pie Chart** tab in the Result Charts view.

3. From the Data Source list, select the type of data to display.
4. Click **Refresh** to draw the chart.
5. (Optional) To change the chart's appearance, do the following:
   a. Open the Options pane and adjust the colors, labels, and legends of the display and specify how the chart displays small slices. Or, click **Load** to load the option settings that you most recently saved.

      Tip By default, the application consolidates small slices of 5% or less. To change this setting, do one of the following:

      - Select **False** for Collect Small Segments.

      –or–

      - Change the Small Slice Threshold (%) setting.

   b. To save all the settings, click **Save** in the Options pane.

      The new settings overwrite any previously saved settings. The application loads these new settings when you click Load.

      When you close the Result Charts view, the application stores the chart settings that you selected. When you reopen the chart, it displays these stored settings if they are available.

   c. To return the Options pane settings to the original default settings, click **Factory Defaults** in the Options pane.

Table 106 describes the parameters on the Pie Chart page of the Result Charts view.

Table 106. Pie Chart page parameters (Sheet 1 of 3)

Command or Option	Description
Options pane	
Load	Loads the Option pane settings that you saved with the Save command.
Save	Saves the settings that you selected in the Options pane.
Factory Defaults	Resets the options in the Options pane to the default settings in effect when you installed the application.
Chart Options	
Chart Type	Specifies the type of chart to display: • (Default) Pie: Displays the chart as a solid circle composed of slices. • Doughnut: Displays the chart as a ring.

Table 106. Pie Chart page parameters (Sheet 2 of 3)

Command or Option	Description
Vertical Rotation	Specifies the angle of rotation around the vertical axis. Default: 0
Angle of First Slice	Specifies the location of the first chart slice. Default: 0
Pie Slice Options	
Show Type Name with Value	Determines whether the application displays the name of the data group next to the value. • True: Displays the name of the data group next to the value. • (Default) False: Does not display the name of the data group next to the value.
Show Slice Amount	Determines whether the application displays the amount of each slice. • (Default) True: Displays the amount of each slice. • False: Does not display the amount of each slice.
Show Slice Percentage	Determines whether the application displays the percentage of each slice. • (Default) True: Displays the percentage of each slice. • False: Does not display the percentage of each slice.
Label Style	Specifies the label style of the chart segments. • Disabled: Does not display a label. • (Default) Inside: Displays the label on top of the chart segment. • Outside: Displays the label outside the chart segment.
Labels Font	Specifies the font of the data set labels. Default: 9-point Microsoft Trebuchet bold
Small Slices Options	
Collect Small Segments	Determines whether the application consolidates small segments together into a single slice. • (Default) True: Consolidates small segments into a single slice. • False: Leaves small segments as is.

Table 106. Pie Chart page parameters (Sheet 3 of 3)

Command or Option	Description
Small Slice Threshold (%)	Specifies a percentage threshold for the slices to be consolidated into a single slice. Default: 5%
Small Slice Collection Label	Specifies the label for the pie segment composed of consolidated segments. Default: Other
Small Slice Collection Color	Specifies the color of the pie segment composed of consolidated segments. Default: Gray
Show as Supplemental Pie	Determines whether to display small segments as a supplemental pie chart. • True: Displays small segments as a supplemental pie chart. • (Default) False: Leaves small segments as is.
Supplemental Pie Size	Specifies the size of the supplemental pie chart relative to the original pie chart. • Largest: Displays the supplemental pie chart as much larger than the original pie chart. • Larger: Displays the supplemental pie chart as larger than the original pie chart. • Comparable: Displays the supplemental pie chart as about the same size as the original pie chart. • (Default) Smaller: Displays the supplemental pie chart as smaller than the original pie chart. • Smallest: Displays the supplemental pie chart as much smaller than the original pie chart.
Data Source	Displays the result category used to plot the data.

Scatter plots

Use the Scatter Chart page to set up a scatter plot for visualizing whether there is a linear or logarithmic relationship between two or three variables (columns) in a result table.

For details about working with scatter plots, see these topics:

- Set up a scatter plot
- Use a filter set to filter the scatter plot
- Customize the appearance of a scatter plot
- Customization options for a scatter chart plot
- Scatter Chart page parameters
- Scatter Chart page shortcut menu commands

Set up a scatter plot

❖ **To set up a scatter plot**

1. Open a result file.
2. In the menu bar, choose **View > Result Charts**.

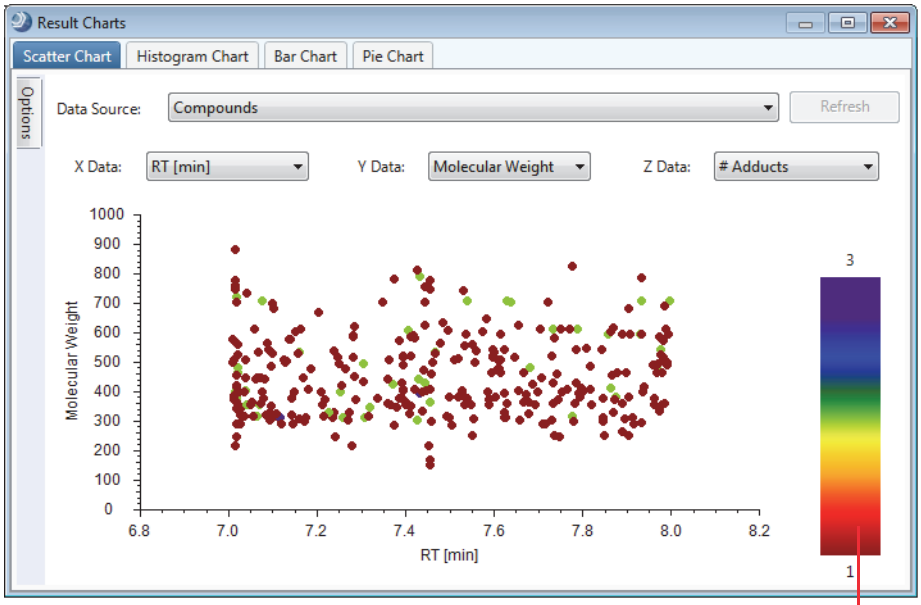
   By default, the Result Charts view opens as a floating window.
3. Click the **Scatter Chart** tab.
4. In the Data Source list, select one of the available result tables.

   The available selections depend on the workflow nodes in the processing workflow.
5. Select the variables as follows:
   a. In the X Data list, select the variable that you want to plot against the *x* axis.
   b. In the Y Data list, select the variable that you want to plot against the *y* axis.
   c. To create a three-dimensional scatter plot, select the variable in the Z Data list that you want to plot against the *z* axis.

      Selecting a data value for the *z* axis adds a color gradient to the plotted data points ranging from the lowest to the highest Z data value.
6. Click **Refresh**.

Depending on your selections, a two- or three-dimensional linear plot of the data points appears. With the default appearance settings, the data points appear as blue circles in a 2D plot and as circles of varying colors in a 3D plot. For a 3D plot, a color legend for the lowest to the highest Z data value appears to the right of the scatter chart.

Figure 114. Three-dimensional scatter chart



Use a filter set to filter the scatter plot

❖ **To interactively filter the scatter plot by using the Result Filters view**

1. Set up and apply a set of result filters in the Result Filters view.

   On the Scatter Chart page of the Result Charts view, the Refresh button turns orange.

2. Click **Refresh** to refresh the scatter chart plot.

Customize the appearance of a scatter plot

❖ **To customize the appearance of a scatter plot**

1. Open the Options pane on the Scatter Plot page of the Result Charts view and pin it. See "Display and pin the Options Pane for the Result Charts view."

2. In the Options pane, do any of the following:

   - To change the scaling, colors, labels, and legends in the display, under Axis Options, make the appropriate changes.

   - The application applies the changes as you make them.

- To change the font size or font type of the axis labels, click the expand icon to the left of Axis Scale Font or Axis Title Font. Then, make the appropriate selections or click the browse icon to open the Font dialog box where you can make your selections.
- A browse icon and a set of font parameters appear.
- To return the option settings to the original default settings, click **Factory Defaults**.

Customization options for a scatter chart plot

Table 107 describes the formatting options for the Scatter Chart page.

Table 107. Options pane for a Scatter Chart (Sheet 1 of 2)

Parameter	Description
Buttons	
Load	Loads the saved Options pane settings. Only click Load to apply a set of saved settings; otherwise, the view reverts to the last saved set.
Save	Saves the new settings.
Tip The Scatter Chart view automatically updates as you change the settings in the Options pane. However, the application does not save the settings until you click Save. If you click Load before saving the new settings, the view reverts to the previously saved settings.	
Factory Defaults	Resets the options in the Options pane to the default settings in effect when you installed the Compound Discoverer application.
Axis Options	
X Axis Type	Specifies the axis type (scale) of the *x* axis: Linear or Logarithmic.
Y Axis Type	Specifies the axis type (scale) of the *y* axis: Linear or Logarithmic.
Z Axis Type	Specifies the axis type (scale) of the *z* axis: Linear or Logarithmic.
Axis Scale Font	Specifies the font used to denote the scale of the *x* and *y* axes.
Axis Label Font	Specifies the font used for the titles of the *x* and *y* axes.
X-Axis Title	Specifies the title of the *x* axis.
Y-Axis Title	Specifies the title of the *y* axis.
Series Options	
Points	Specifies the appearance of the points in the scatter chart. Also specifies whether to show the points in the scatter chart.
Selected Points	Specifies both the appearance of the selected points in the scatter chart and whether to show the points in the scatter chart.

Table 107. Options pane for a Scatter Chart (Sheet 2 of 2)

Parameter	Description
Filtered-out Points	Specifies the appearance of the filtered-out points in the scatter chart and whether to show the points in the scatter chart.
Excluded Points	The Compound Discoverer workflow nodes do not generate excluded data points.

Scatter Chart page parameters

Table 108 describes parameters that are visible on the Scatter Chart page. Use these parameters to set up the scatter plot.

Table 108. Scatter Chart parameters

Parameter	Description
Data Source	Specifies the data source for the plot. The data source is one of the available result tables produced by the processing workflow.
Note The X, Y, and Z Data boxes list the available variables for the selected data source. The variables are the available columns in the selected data source (result table).	
X Data	Specifies the variable to plot against the *x* axis.
Y Data	Specifies the variable to plot against the *y* axis.
Z Data	Specifies the variable to plot against the *z* axis.
Plot grid	Two-dimensional grid where the application plots the data points. By default, the plot area has no grid lines. To add horizontal and vertical lines to the plot, make the appropriate selection under Options in the Options pane.
Axis labels	The default axis labels are the selected variable names.
Color legend	When you create a 3D plot, the scatter chart includes a color legend for the *z*-axis color gradient. The numeric value of the highest *z*-axis data point appears above the color legend.
Options pane	Use the parameters in this pane to customize the Scatter Chart page. For more information, see Table 107.
Buttons	
Refresh	Refreshes the content of the chart area.

Scatter Chart page shortcut menu commands

Table 109. Scatter Chart shortcut menu commands (Sheet 1 of 2)

Command	Description
Show Position Tooltips	Displays a tooltip when you place the cursor over a data point.
Zoom Out	Decreases the zoom of both axes.
Undo All Zoom/Pan	Displays the full *x*-axis range of the plot.
Copy > Image	Copies the scatter chart plot as a bitmap (raster) image to the Clipboard.
Copy > Data	Copies the data points for the selected variables to the Clipboard.
Export > Image As	Saves the plot to any of these file types: EMF, PNG, GIF JPG, TIF, and BMP
Export > Data As	Opens the Save As dialog box where you can save the data as a plain text file. By default, the application saves the file to the last open folder and uses the following convention to name the file: *ResultTable*_x_*XDataSelection_Range_YDataSelection_Range*_z_*ZDataSelection_Range_DataPointType*.txt Use the Browse icon to select a different folder. Exporting data from a scatter plot creates three text files: *File name* Filtered-out Points.txt, *File name* Points.txt, and *File name* Selected Points.txt.
Select Item for Point	Highlights the appropriate row in the result table (selected Data Source).
Check Point	By default, changes the selected point to a red diamond and selects the check box in the Checked column for the selected point (row in the selected Data Source result table). You can change the appearance of selected points by making the appropriate selections in the Series Options > Checked Points area of the Options pane. When you save the data to a text file, the Selected Points.txt file lists the selected points. To select a point, right-click the point of interest on the plot and choose **Check Point**.
Uncheck Point	Undoes the selection of a selected point. You can change the appearance of points by making the appropriate selections in the Selected Options > Points area of the Options pane.

Table 109. Scatter Chart shortcut menu commands (Sheet 2 of 2)

Command	Description
Check All Visible Points	Selects all of the visible points in the scatter plot.
Uncheck All Visible Points	Undoes the selection of the visible points in the scatter plot.

Trend Chart view

Use the Trend Chart view to compare the chromatographic peak areas for compounds by sample group.

You define the sample groups by selecting one or more check boxes under Group By in the collapsible pane to the left of the chart. In addition, you can change the sort order of each sample group and the hierarchy of the sample groups.

You can use the Trend Chart view to plot the data for a compound (or feature) in these result tables: Compounds, Expected Compounds, and Merged Features. For a single compound, the chart can plot the data as a trendline plot or a box-and-whisker plot. For two or more compounds, the chart displays the data only as a trendline plot, with one trendline for each compound.

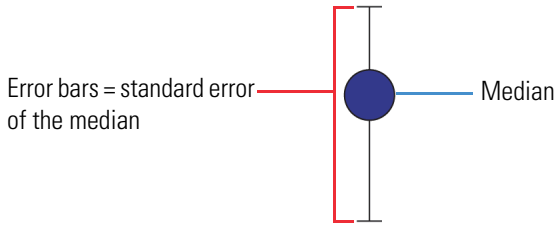
Note The trendline plot can plot sample groups that include only one data point; however, to plot the error bars for a group, it requires a minimum of two data points. With two data points, the circle represents the calculated median and the error bars represent the minimum and maximum areas.

The box-and-whisker plot requires a minimum of two data points to plot the box for a sample group. It does not plot sample groups that include only one data point. If none of the sample groups includes the minimum number of data points, the following text appears in the chart area: No results available to plot.

By default, the trendline plot type plots the median peak area for the selected component on the *y* axis against equally spaced sample groups on the *x* axis and connects the data points with straight lines. Each data point appears as a solid circle with two error bars. The circle represents the median. If the group includes a least three data points, the application uses the following equation to calculate the standard error of the median and draw the error bars:

$$\text{standard error of the median} = \sqrt{\pi/2} \times \text{std. dev (x)} / (\sqrt{\text{N}})$$

Figure 115. Trendline display of the data distribution



The box-and-whisker chart plots the peak area for a selected component on the *y* axis as a rectangle against equally spaced sample groups on the *x* axis. The height of the rectangle represents the peak areas in the interquartile range (see Figure 116). The application uses the following equations to calculate the upper and lower whiskers:

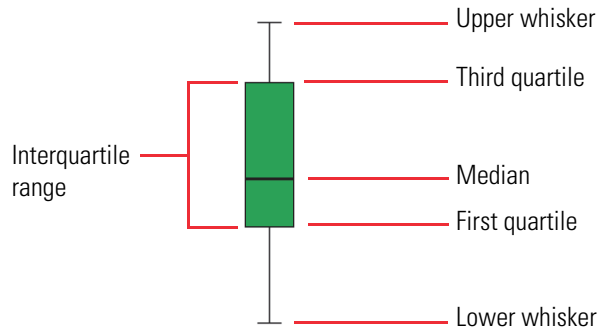
Interquartile range (IQR) = Quartile 3 (Q3) – Quartile 1 (Q1)

Upper whisker = Q3 + IQR × 1.5

Lower whisker = Q1 – IQR × 1.5

When the data set contains a small number of data points, the whiskers typically end at the highest and lowest data points. If the data set does not include a data point between the top of the interquartile range and the calculated value for the upper whisker, the application does not draw an upper whisker. If the data set does not include a data point between the bottom of the interquartile range and the calculated value for the lower whisker, the application does not draw a lower whisker.

Figure 116. Box-and-whisker display of the data distribution



Note To calculate the quartiles, the application uses a method that is similar to the type 6 method in the R statistical computing software.

For details about working with the Trend Chart view, see the following topics:

Open the Trend Chart view

❖ To open the Trend Chart view

1. Open the result file of interest.
2. From the menu bar, choose **View > Trend Chart**.

   The Trend Chart view opens as a docked window to the right of the result tables.

   - If the active result table does not contain a consolidated compounds list, the following text appears in the graph area: No Results Available to Plot. The Compounds, Expected Compounds, and Merged Features tables contain a consolidated compounds list.
   - If the active result table contains a consolidated compounds list and you select a row, a box-and-whisker plot appears in the graph area with data from the first table row.

Define the sample groups to compare

❖ To define the sample groups for a trend chart plot

1. Open the result file of interest, and then open the Trend Chart view.
2. In the left pane, under Group By, select the appropriate check boxes to define the sample groups.

Compare the peak areas for a single compound by sample group

❖ To compare the peak areas for a single compound by sample group

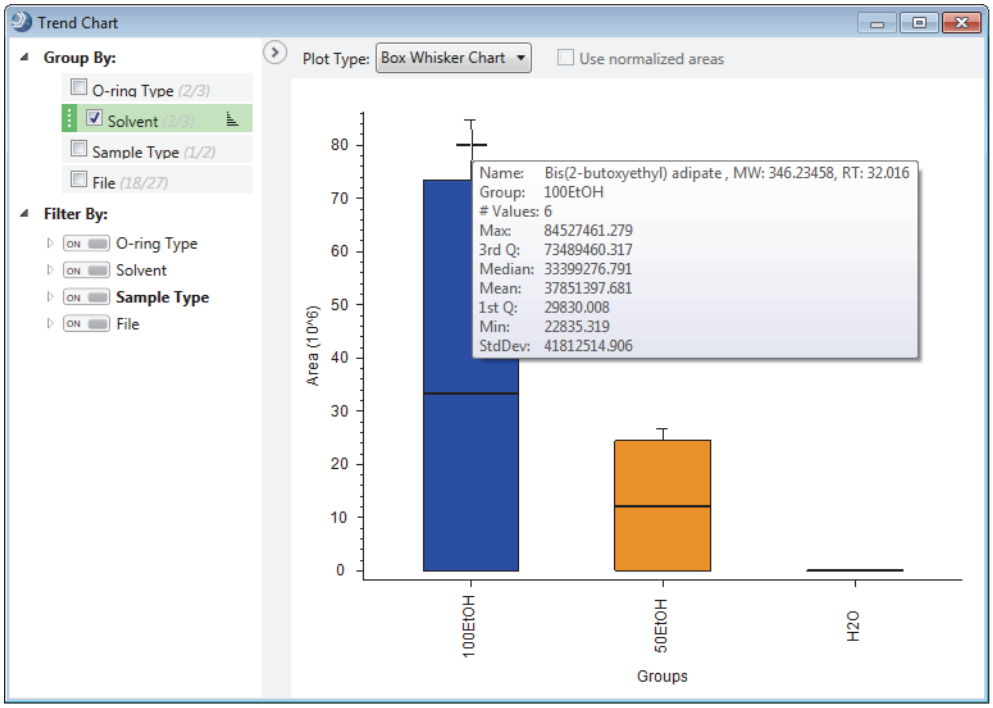
1. Open a result file, open the Trend Chart view, and define the sample groups that you want to compare.
2. In the Compounds, Expected Compounds, or Merged Features table, select the compound (or feature) of interest.
3. Right-click the graph area and choose **Show Legend**.

   The legend displays the sample group colors.
4. In the Plot Type list, select **Trendline Chart** or **Box Whisker Chart**.

   Depending on the selection, either a trendline plot or a box-and-whisker plot appears in the graph area. A tooltip opens when you place the cross-hair cursor anywhere on a box or whisker in the box-and-whisker plot or on data point in a trendline plot.

   Figure 117 shows a box-and-whisker plot. Placing the cross-hair cursor on a box or whisker opens a tooltip with descriptive statistics.

Figure 117. Box-and-whisker plot for one compound



Change the sort order of the defined groups

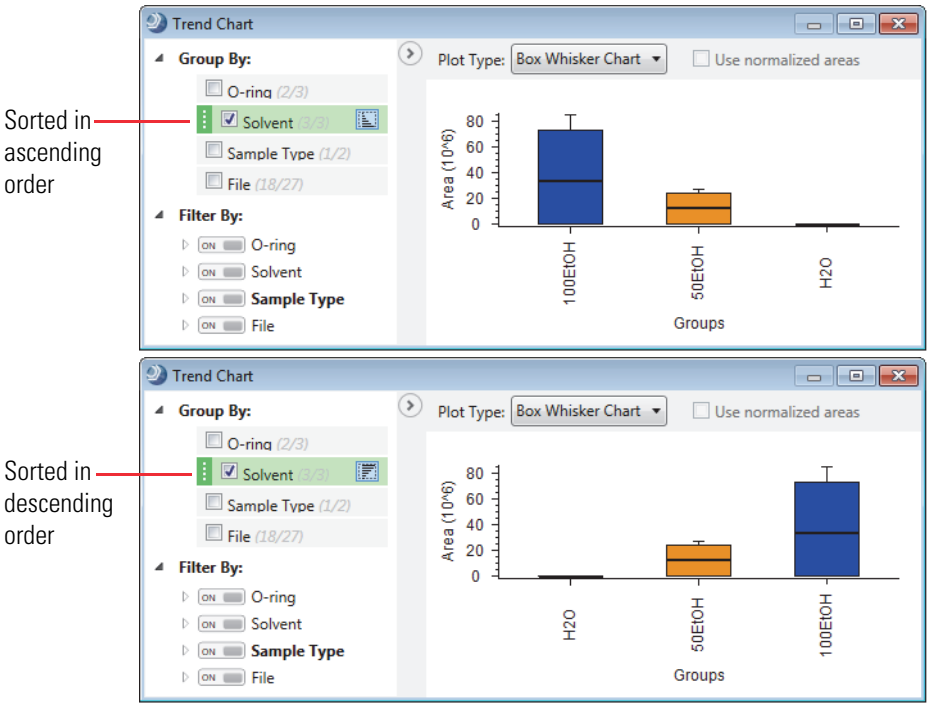
In the Trend Chart view, you can display the defined groups from left to right in ascending or descending order by chromatographic peak area.

❖ **To change the sort order of the defined groups in the Trend Chart view**

In the left pane, under Group By, click the sorting icon, , next to the study variable to sort and choose **Sort Ascending** or **Sort Descending**.

Changing the sort order changes the order of the groups on the *x* axis (Figure 118).

Figure 118. Trend chart with compounds grouped by solvent and sorted in ascending or descending order by chromatographic peak area



Compare the peak areas for multiple compounds by group

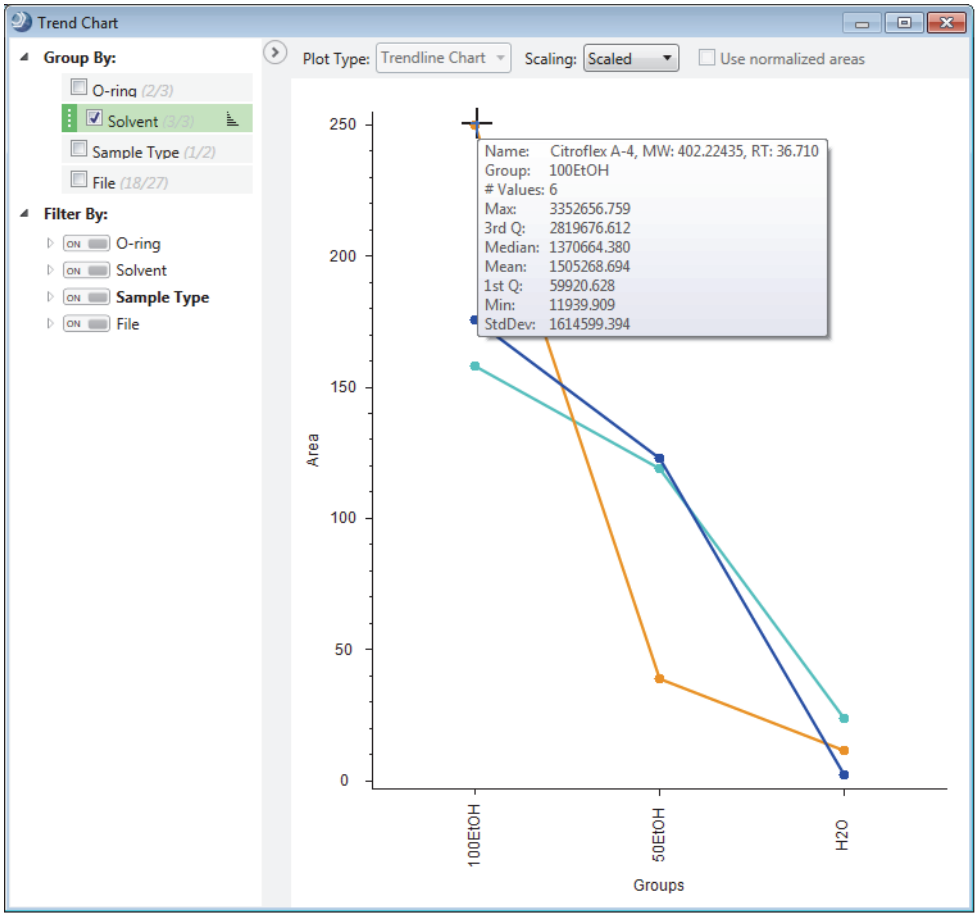
❖ **To compare the peak areas for multiple compounds by group**

1. Open the result file of interest, open the Trend Chart view, and define the sample groups.
2. To select the compounds to plot, press the CTRL key and select rows in the result table (Compounds, Expected Compounds, or Merged Features), taking care to avoid clicking an editable table cell.

   The plot changes to a scaled trendline. The data points represent the group median. The legend displays the name (if available), molecular weight, and retention time of each selected compound.

   Figure 119 shows a scaled trendline chart. To view descriptive statistics for the data points, click anywhere in the plot to activate the cross-hair cursor, and then place the cross-hair cursor on each data point of interest.

Figure 119. Trendline chart with three compounds



Change the hierarchy of the variables used for grouping

Changing the hierarchy of the variables used for grouping in the Trend Chart view modifies the sample grouping.

❖ **To change the hierarchy of the variables used for grouping**

Use the handle (⋮) next to the variable to drag the variable up or down in the list.

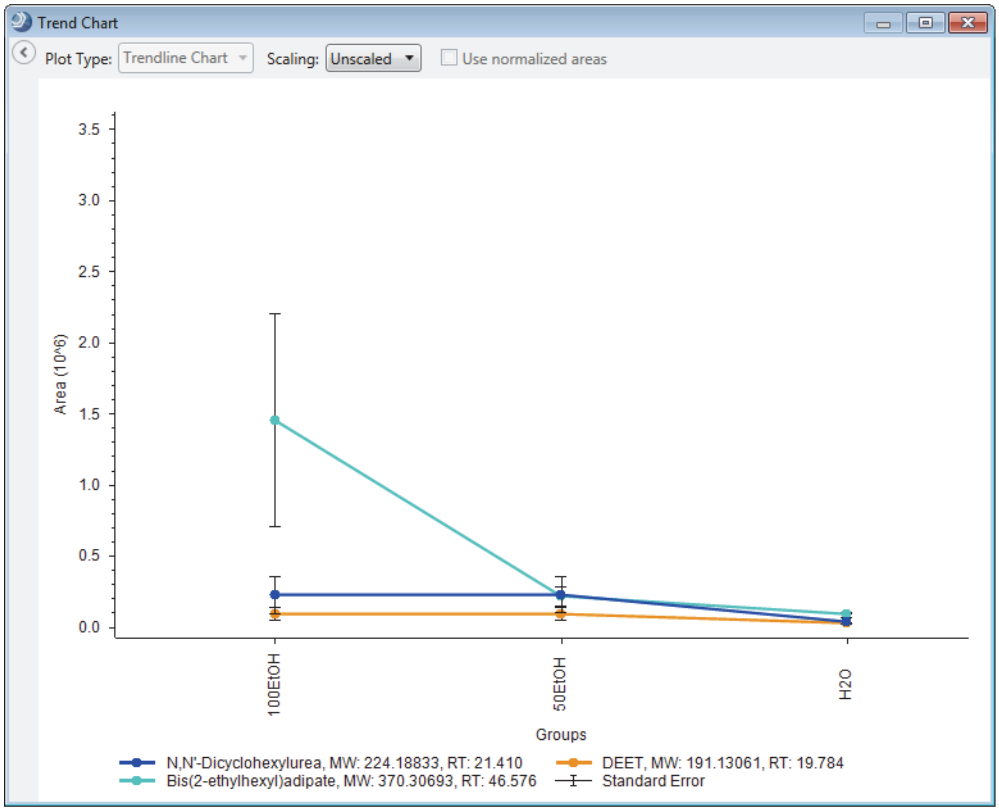
Show the error bars in a trendline chart

❖ **To view error bars for each data point in a trendline chart**

1. In the Scaling list above a trendline plot in the Trend Chart view, select **Unscaled**.
2. Right-click the plot and choose **Show Standard Errors**.

   The application plots the group median with error bars for the standard error of the median (Figure 120).

Figure 120. Trendline chart with error bars



Trend Chart view parameters

Table 110 describes the parameters in the Trend Chart view.

Table 110. Trend Chart view parameters

Parameter	Description
Plot Type	Controls the plot type in the graph area. Selections: Trendline Chart or Box Whisker Chart The Box Whisker Chart selection is only available for displaying a single compound.
Scaling (for the trendline chart)	Select the chart scaling: • Unscaled—Enables the Show Standard Errors command in the shortcut menu. • Scaled • Scaled to *Study Factor Value*
Use Normalized Areas	Displays the normalized areas for the data. Available when the processing workflow included the Normalize Areas node.

Isotopologues Distribution Chart view

For LC studies, if the analysis included the Analyze Labeled Compounds node, labeled samples, and at least one unlabeled reference sample, you can view a distribution chart of the detected isotopologues.

❖ To open the Isotopologues Distribution Chart and review the isotopologues

1. Open a result file for a stable isotope labeling analysis.
2. From the application menu bar, do one of the following:

   • Choose **Window > Apply Layout > Stable Isotope Labeling**.

   The Isotopologues Distribution Chart, Trend Chart, and Metabolika Pathways view open as a tabbed group to the right of the result tables. Under Group By, the File check box is selected.

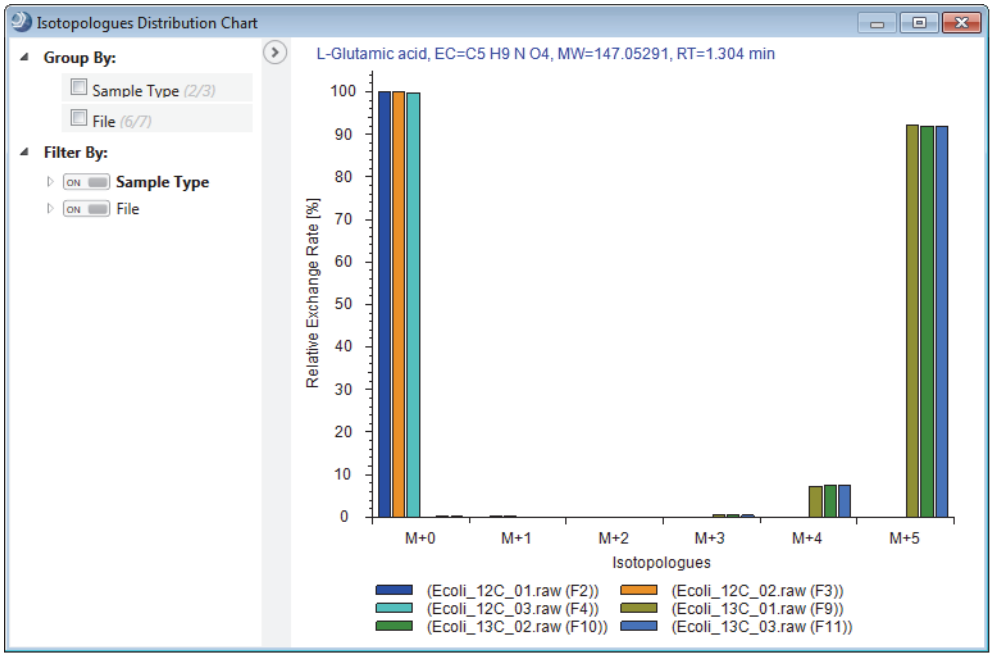
   –or–

   • Choose **View > Isotopologues Distribution Chart**.

   The Isotopologues Distribution Chart opens to the right of the result tables. Under Group By, all the check boxes are clear.

The compound's name, elemental composition, MW, and RT appear above the graph (Figure 121). The bars are colorized by input file.

Figure 121. Isotopologues Distribution Chart with no grouping selected

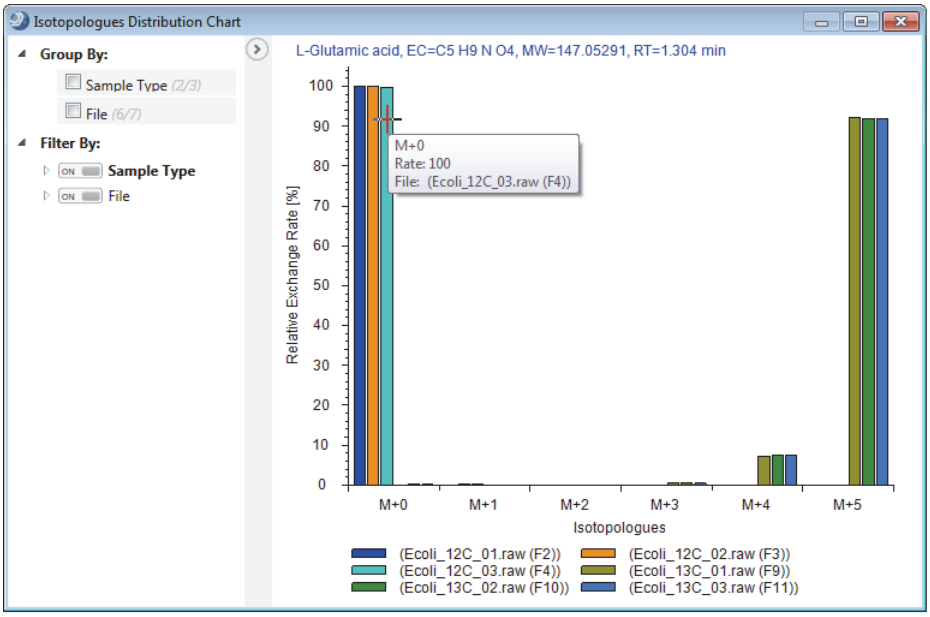


3. Do any of the following:

   - To display a tooltip for a bar, point to the bar.

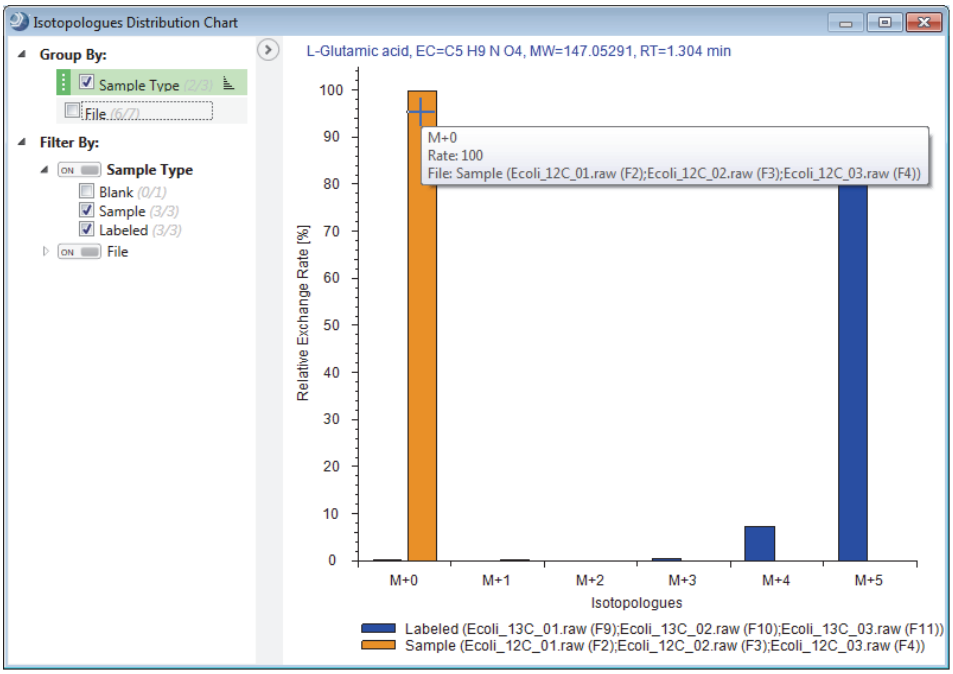
     Tip By default, the Show Position Tooltips feature is turned on. If a tooltip does not appear, click the chart. If a tooltip still does not appear, right-click the chart and choose **Show Position Tooltips**.

Figure 122. Isotopologues Distribution Chart with a tooltip



- To group the isotopologues by input file, under Group By, select the **File** check box.
- To group the isotopologues by sample type, under Group By, select the **Sample Type** check box.

Figure 123. Isotopologues grouped by sample type



Mass Defect Plot view

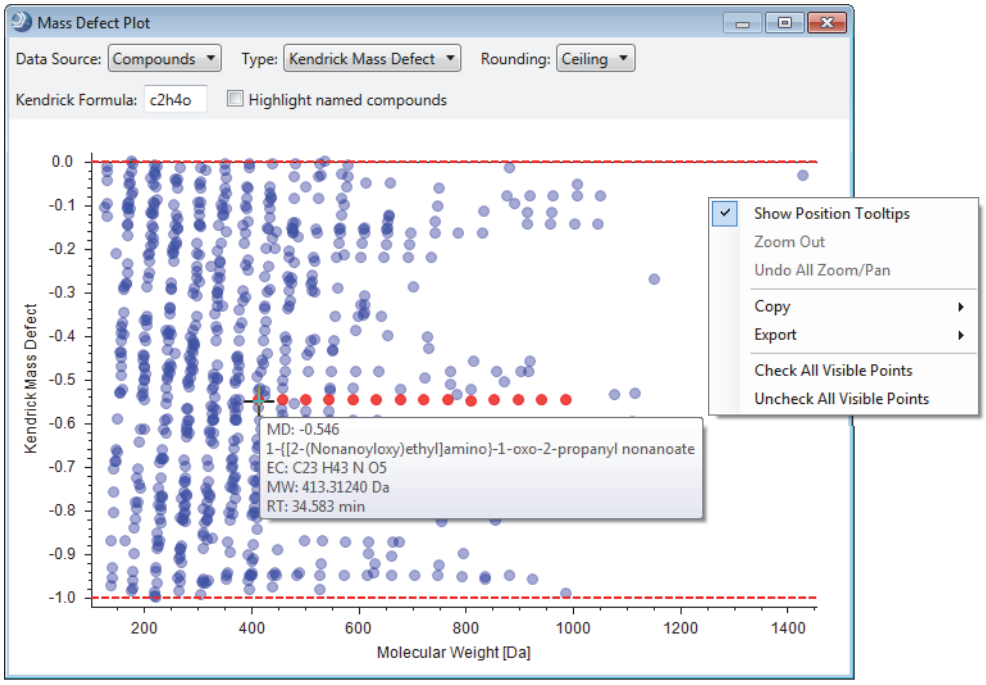
Use the Mass Defect Plot view to find similar compounds by visualizing the calculated mass defects for a set of compounds against their molecular weights. Your choices for calculating the mass defect in this view are the same as those for the Calculate Mass Defect and Filter By Mass Defect nodes.

❖ To set up the mass defect plot and examine it for similar compounds

1. Open a result file from a processing workflow that included the Detect Compounds node.
2. From the application menu bar, choose **View > Mass Defect Plot**.

   The compounds listed in the Compounds table appear as blue circles in the Mass Defect plot. The *y*-axis label displays the mass defect type, and the red dashed lines indicate the valid range of the mass defect values.
3. To specify how to calculate the mass defect, do the following:
   - From the Type list, select the mass defect calculation. Then, if you selected Kendrick Mass Defect, enter the Kendrick formula.
   - From the Rounding list, select **Ceiling**, **Floor**, or **Round**.
4. To highlight the compounds that have an assigned name in orange, select the **Highlight Named Compounds** check box.
5. To work interactively with the plot, do the following:
   - Use the shortcut menu commands for the view to do any of the following:
     - Zoom in or out of the plot.
     - Copy the image or the data points to the Clipboard.
     - Export the image or the data points to an external file.
     - Check or clear the visible data points. Checking a data point highlights the data point in red and places a check mark in the Checked column for the compound in the Compounds table.
   - Double-click a data point to navigate to the compound in the Compounds table.
   - Point to a compound to display a tooltip with information about the compound's mass defect, name, elemental composition, molecular weight, and retention time.

Figure 124. Mass Defect Plot view with its shortcut menu displayed



For more information, see "Mass defect types and visualization techniques."

Principal Component Analysis view

Use the Principal Component Analysis view to visualize the correlation between multivariate data in a set of observations. A principal component analysis transforms a set of observations for possibly correlated variables into an artificial set of independent linear combinations of the original variables known as principal components (PC1, PC2, PC3 and so on). PC1 has the most variation and the highest principal component has the least variation.

The Principal Component Analysis view contains three pages: Scores Plot, Loadings Plot, and Variances Plot. The scores plot shows the correlation among the observations. The loadings plot shows the relationship among the variables for a given pair of principal components. The variance plot shows the percentage and cumulated percentage of the variance that a principal component accounts for. In general, as the proportion of variance increases for the first two or three principal components, the dissimilarity between the sample groups increases.

For details about working with the Principal Component Analysis view, see the following topics:

- Set up a principal component analysis
- Interpret the scores plot
- Interpret the loadings plot
- Work interactively with the loadings plot

- Interpret the variance plot
- Principal Component Analysis view parameters

Set up a principal component analysis

❖ **To set up a principal component analysis**

1. Open a result file that contains any of these result tables:
   - Compounds
   - Expected Compounds
   - Merged Features
2. From the menu bar, choose **View > Principal Component Analysis**.

   If the result file contains a Compounds table, the Principal Component Analysis view opens with the Compounds table selected as the data source.
3. Do the following:
   - In the Data Source list, select the appropriate result table as appropriate for the data set.
   - In the X Data list, select **PC1**, **PC2**, **PC3**, **PC4**, or **PC5**.

     In most cases, select PC1 or PC2, as these principal components have the most variation.
   - If the data points differ by several orders of magnitude, select the **Center and Scale** check box.
   - If the processing workflow included the Normalize Areas node, select the **Use Normalized Areas** check box as appropriate.
   - To remove points from the plot, clear the check boxes under Filter By as appropriate.

   Using the new population, the application recalculates the principal components, including their contribution to the variance, and shifts the coordinates of the remaining data points.
4. To view additional information, do any of the following:
   - To display a legend at the bottom of the plot, right-click the plot and choose **Show Legend**.
   - To show a tooltip when you place the cross-hair cursor on a data point in the plots, right-click the plot and choose **Show Position Tooltips**.

Interpret the scores plot

Use the scores plot of the Principal Component Analysis view to interpret the relationship among the sample groups. Sample groups that are near each other are similar.

The Principal Component Analysis view is available for result files that include any of these tables: Compounds, Expected Compounds, or Merged Features.

❖ To review and interpret the scores plot

- Check the percentage values for the principal components. The labels on the *x* and *y* axes include the proportion of variance that the principal components add to the total variance as a percentage.
- Place the cross-hair cursor on a data point to view its coordinates.

  Figure 125 shows the scores plot for the compounds that leach out of four o-ring types soaked in ethanol. The black, brown, and white O-rings show a similar variance for PC1, while the red O-rings show a significant variance in the other direction for PC1. The brown and white O-rings show a similar variance for PC2.

  Figure 125. Scores plot for four O-ring types (white, brown, red, and black)

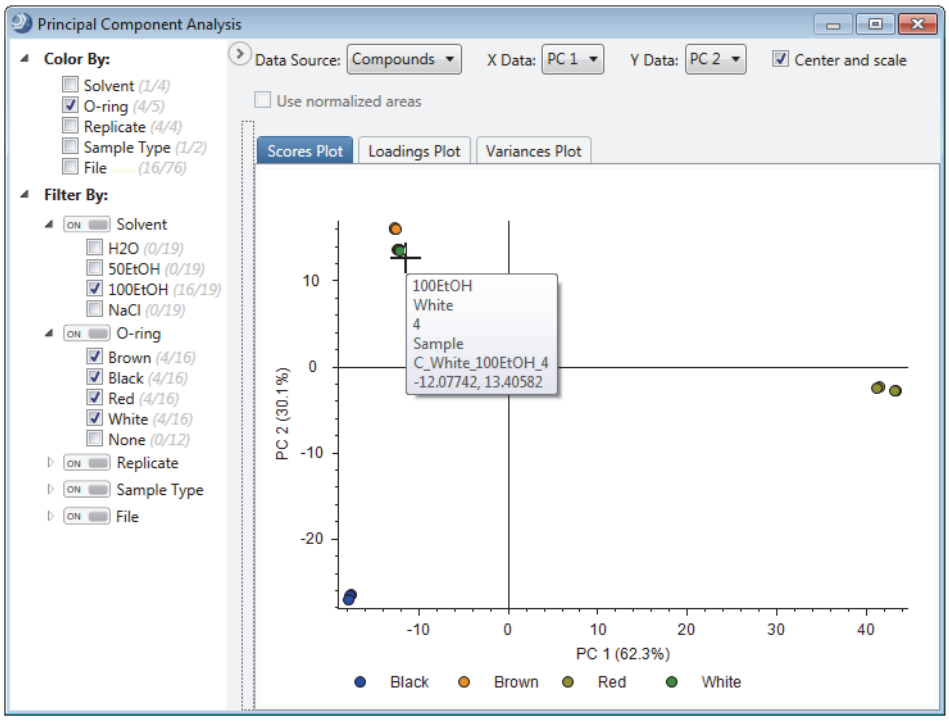
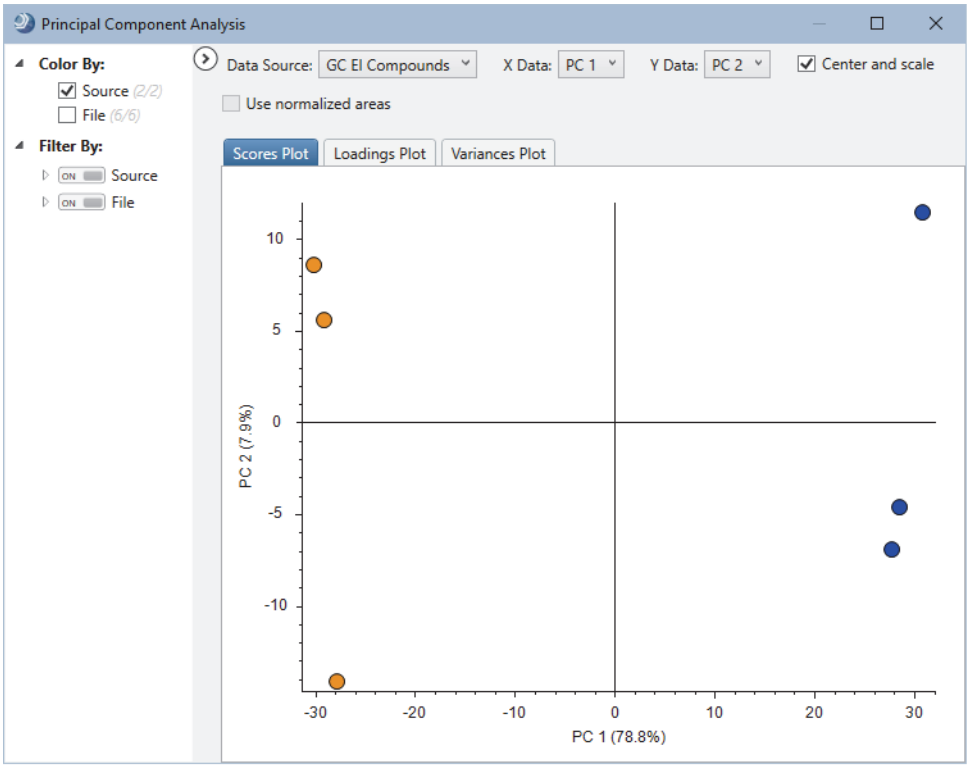


Figure 126 shows the scores plot for the compounds found in two sources of oregano. The principal components for the two groups are in opposite quadrants, which means the two groups are significantly different.

Figure 126. Scored plot for two sources of oregano



Interpret the loadings plot

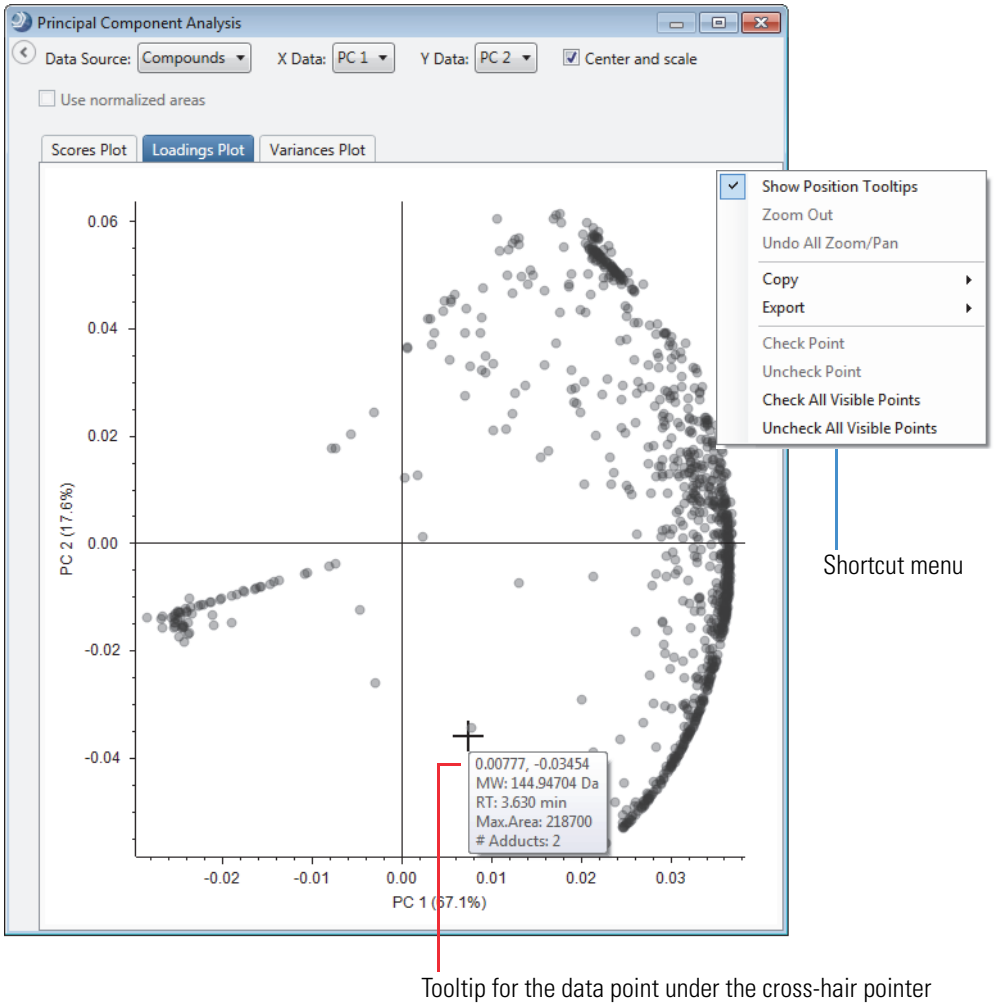
Use the loadings plot to interpret the relationship among the variables.

❖ To interpret the loadings plot

1. To determine the relative correlation between various data points, review their relative location in the plot.
   - Data points that are near each other are similar.
   - Data points that are on opposite sides of the origin have a negative correlation.
   - Data points in the corners of the plot have a strong contribution to both principal components—that is, these data points differentiate between groups.
2. Place the cross-hair cursor on a data point to display a tooltip information about the compound.

   For LC studies the tooltip displays the principal component coordinates, molecular weight, retention time, maximum peak area, and number of adduct ions. See Figure 127.

Figure 127. Loadings plot with its shortcut menu displayed (LC study)



Work interactively with the loadings plot

The Loadings Plot is interactive with the selected data source table—that is, double-clicking a data point in the loadings plot selects its row in the data source table and updates the other opened graphical views. In addition, checking data points (compounds, expected compounds, or features) in the Loadings Plot checks the corresponding data points in these interactive views—Differential Analysis, Partial Least Squares Discriminant Analysis, and Descriptive Statistics.

❖ To select a data point or check one or more data points in the Loadings Plot

- To select a data point, double-click it.

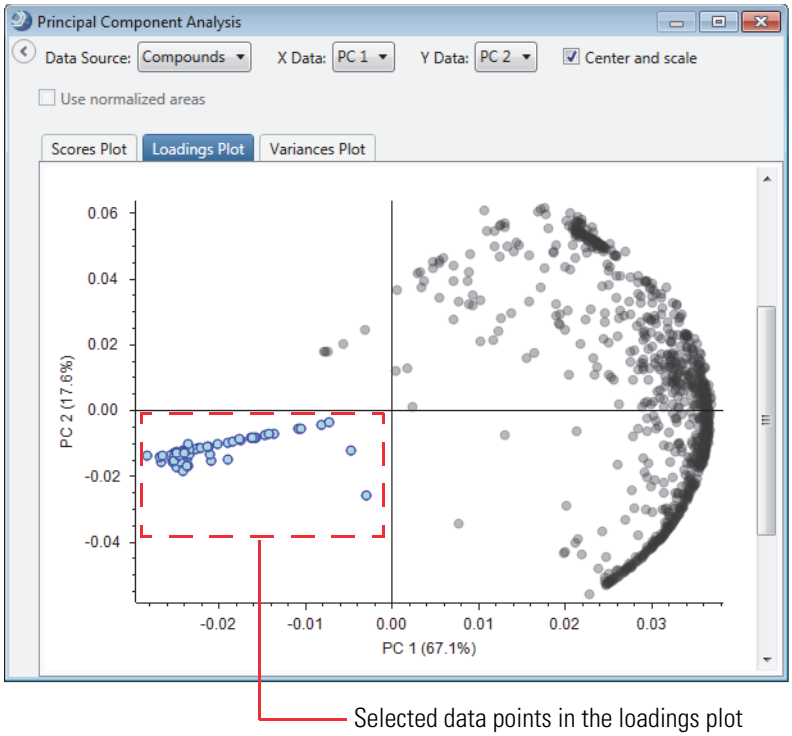
  The application highlights the corresponding row in the data source table and updates the other opened and interactive views.

- To check a single data point, right-click the point and choose **Check Point**.

- To check multiple points, drag the mouse pointer across a rectangular area of the plot to zoom in on that area, then right-click the plot and choose **Check All Visible Points**.

  The application selects the check boxes for the checked data points in the data source table and changes the color of the selected points to blue in the loadings plot. The color of the checked data points also changes to blue in the interactive views.

  Figure 128. Loadings plot with checked points shown in blue



- To clear all the selected check boxes in the result table, right-click the result table and choose **Uncheck All > In This Table**.

Interpret the variance plot

Use the variance plot to determine the relative differentiation between sample groups.

❖ To interpret the variance plot

Compare the contribution of the first two or three principal components to the cumulative variance.

For example, Figure 129 shows the variance plot for the compounds leached from red O-rings soaked either in water or an aqueous solution of sodium chloride.

Figure 130 shows the variance plot for the same type of O-rings soaked either in water or ethanol.

The PC1–PC3 components make up more of the cumulative variance when comparing the extraction strength of water to ethanol than when comparing water to a salt solution. From these results, you can infer that the extraction strengths of water and ethanol differ more than the extraction strengths of water and a salt solution.

Figure 129. Water versus an aqueous solution of sodium chloride (extraction strength)

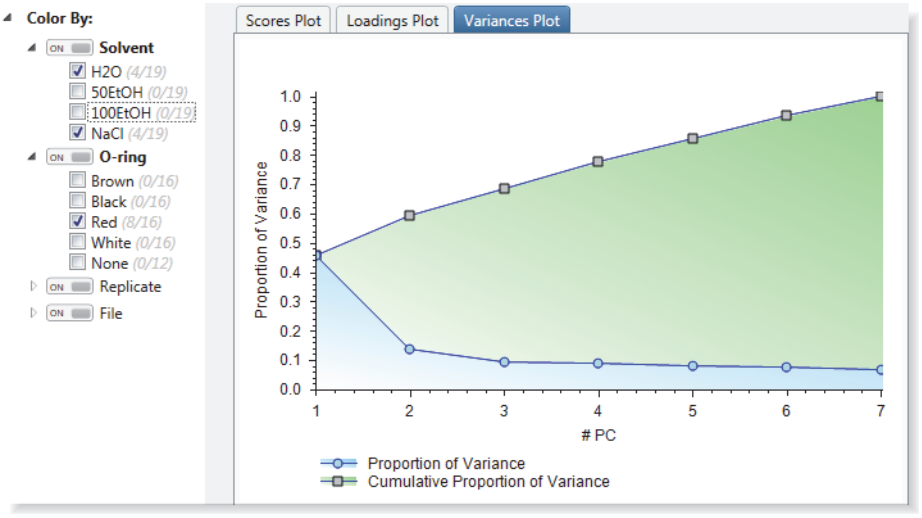
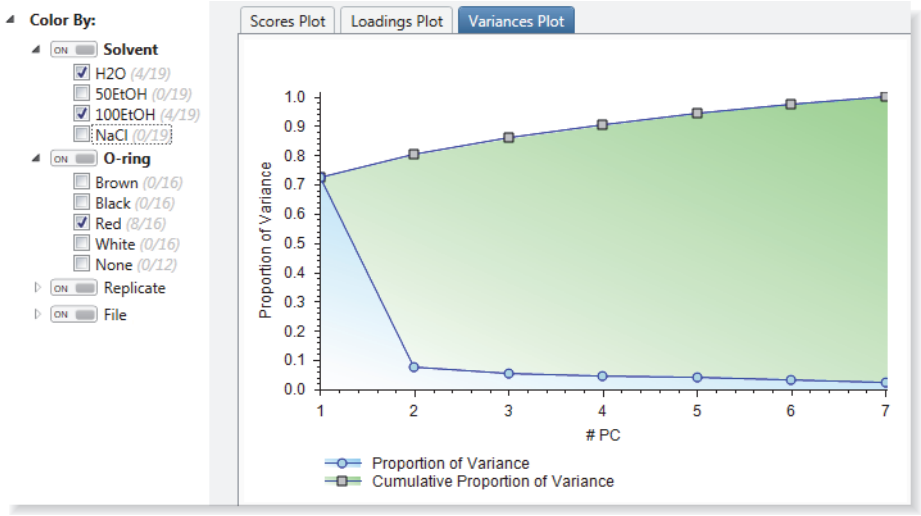


Figure 130. Water versus ethanol (extraction strength)



Principal Component Analysis view parameters

Table 111 describes the parameters in the Principal Component Analysis view.

Table 111. Principal Component Analysis parameters

Parameter	Description
Data Source	Specifies the source of the data. The selection list depends on the processing workflow. Selections: Compounds, Expected Compounds, and Merged Features
X Data	Specifies the principal component to plot on the *x* axis. Selections: PC1, PC2, PC3, PC4, or PC5
Y Data	Specifies the principal component to plot on the *y* axis. Selections: PC1, PC2, PC3, PC4, or PC5
Center and Scale	Centers and scales the data.
Use Normalized Areas	Uses the normalized data. Available if the processing workflow includes the Normalize Areas node.
Scores Plot page	Displays a plot of one principal component versus a second principal component.
Loadings Plot page	Displays the compounds in the selected table plotted against the selected principal components. This plot is interactive with the selected results table.
Variances Plot page	Displays the proportion and the cumulative proportion of the variance contributed by each principal component.

Descriptive Statistics view

Use the Descriptive Statistics view to visually compare the statistics of the peak areas for all compounds currently displayed in one of the following result tables as a box-and-whisker plot:

- Compounds
- Expected Compounds

A box-and-whisker plot displays the data for a variable as a rectangular box with a set of whiskers at each end. The line through the rectangle represents the median value in the data set. The lower portion of the rectangle represents the data points that fall within the second quartile and the upper portion represents the data points that fall within the third quartile. The circles that fall outside the fence whiskers are outliers.

The application uses the following equations to calculate the upper and lower fences:

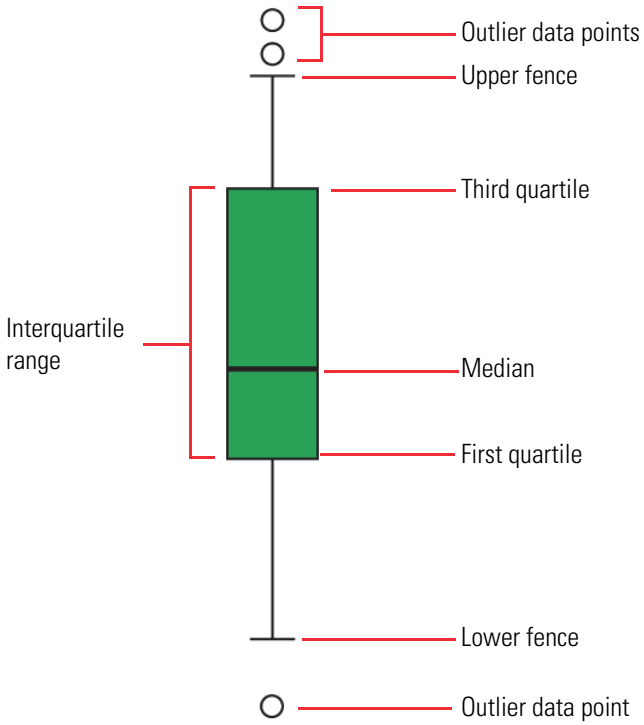
Interquartile range (IQR) = Quartile 3 (Q3) – Quartile 1 (Q1)

Upper fence = Q3 + IQR × 1.5

Lower fence = Q1 – IQR × 1.5

Note To calculate the quartiles, the application uses a method that is similar to the type 6 method in the R statistical computing software.

Figure 131. Box-and-whisker display of the data distribution



By default, the graph displays the data for all the samples and duplicates the grouping on the Grouping and Ratios page of the analysis. Each group appears in a different color. The legend shows the colors of the sample groups.

Use the Group By check boxes in the collapsible pane to change the grouping. Use the Filter By check boxes to remove samples from the plot.

For more information about the shortcut menu commands, see "Copy or save graphical views for publication."

Table 112. Common tasks for the Descriptive Statistics view

Task	Procedure
Copy or save the data as an image.	1. Right-click the plot and choose **Show Legend**. 2. Right-click the plot and choose **Copy > Image** to copy an image to the Clipboard. –or– Right-click the plot, choose **Export > Image As**, and select an image type to save the data to an image file.
Copy or save the data as editable text.	Right-click the plot and choose **Copy > Data** to copy the text to the Clipboard. You can paste this text to Notepad, an Excel spreadsheet, and so on. The data appears in a columnar format. –or– Right-click the plot and choose **Export > Data As** to save the data to a text file. The file contains two data sets. The first set consists of these columns from left to right: Groups, Name, Minimum Value, Maximum Value, Std. Deviation, Mean, Median, Q1 Value, Q2 Value, and Q3 Value. The second set lists the outlier data points and consists of these columns from left to right: Groups, Name, and Outlier.
View the entry in the result table for an outlier data point.	In the plot, double-click the data point.
Select the check box for an outlier data point.	In the plot, right-click the data point and choose **Check Point**. In the result table, the check box is selected for the corresponding compound or expected compound.
Export the outlier data points to a spreadsheet.	1. In the view, zoom in on the outlier points so that they are the only visible points on the screen. 2. Right-click the plot and choose **Check All Visible Points** to select the rows for these outliers in the compounds table. 3. In the compounds table, sort the checked rows by the variable of interest. For example, sort the rows by molecular weight, retention time, or both. 4. Right-click the compounds table and choose **Export > Export to Excel**. 5. In the Export to Excel dialog box, select a folder and name the file, select the **Checked Items Only** check box, and click **Export**.

Table 113 describes the components of the Descriptive Statistics view.

Table 113. Descriptive Statistics view parameters

Parameter	Description
Data Source	Specifies the result table for the source data. Selections: Compounds or Expected Compounds
Log-transform Data	Determines whether the data appears in a linear scale or the $\log_{10}$ scale. Selecting this check box transforms the area counts to the $\log_{10}$ scale.
Use Normalized Areas	Select to display normalized chromatographic peak areas. Available when the processing workflow includes the Normalize Areas node.
Graph	
x axis	Displays the name of the sample group.
y axis	Displays the area in a linear scale or in a $\log_{10}$ scale.
Outlier data points	The circles represent outlier points. When the Show Position Tooltips command is enabled, placing the cursor over a data point displays the following information: MW, RT, Max. Area, and #Adducts.
Rectangle	The rectangles represent the second and third quartiles for the data set. When the Show Position Tooltips command is enabled, placing the cursor over the rectangle displays the following information: filename, group, maximum value (including the outliers), 3^{rd} quartile, median, 1^{st} quartile, minimum value (including the outliers).
Legend	By default, the legend is hidden. Choosing Show Legend from the shortcut menu displays the legend. The legend shows the group colors.

Differential Analysis view

Use the Differential Analysis view to display a volcano plot of the differential analysis performed during data processing or to run a new differential analysis.

For details about working with the Differential Analysis view, see the following topics:

- Review the initial differential analysis
- Change the analysis settings for a differential analysis
- Run a new differential analysis
- Differential Analysis view parameters and shortcut menu commands

Review the initial differential analysis

❖ **To open the Differential Analysis view and review the initial analysis**

1. Open the result file for an analysis that included at least two raw data files.
2. In the menu bar, choose **View > Differential Analysis**.

   If the processing workflow included the Differential Analysis node, the Differential Analysis view opens with the differential analysis from data processing. The ratios in the Comparison list match the ratios on the Grouping and Ratios Summary page of the Summaries view. The initial p-value setting is 0.05 ($-\log_{10}$ 0.05 = 1.3) and the initial Log_2 Fold change setting is 1 (a ratio of 2 to 1). Depending on the setting for the Log_{10} Transform parameter in the Differential Analysis node, the *y*-axis scale spans the p-value range (0–1) or the $-\log_{10}$ p-value range ($-\log_{10}$ 0 = Infinity, $-\log_{10}$ 1 = 0).
3. To show the legend, right-click the plot and choose **Show Legend**.

   The data points are color-coded, as defined by the legend.

   Figure 132 shows a comparison between two extraction solvents—water and an aqueous solution of 50% ethanol.

Figure 132. Differential Analysis view with the analysis run during data processing (LC study)

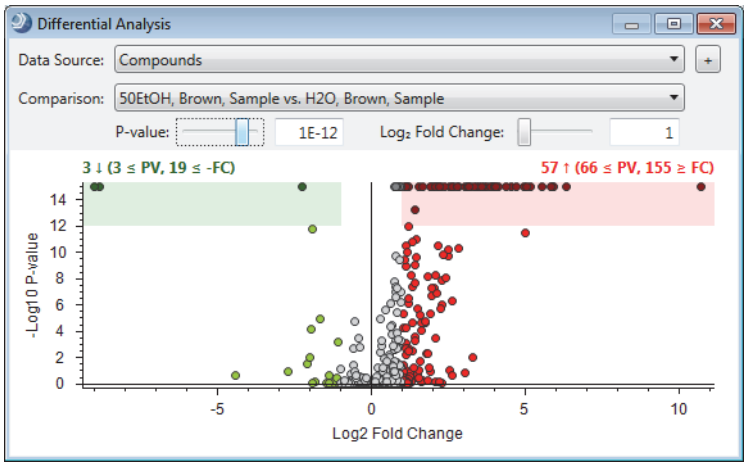
Change the analysis settings for a differential analysis

❖ **To change the analysis displayed in the volcano plot**

- Select a different ratio from the Comparison list. This changes the data points in the plot.
- Change the p-value setting by dragging the slider. This changes the *y*-axis range of the shaded areas.

Figure 133 shows the effect of changing the p-value setting.

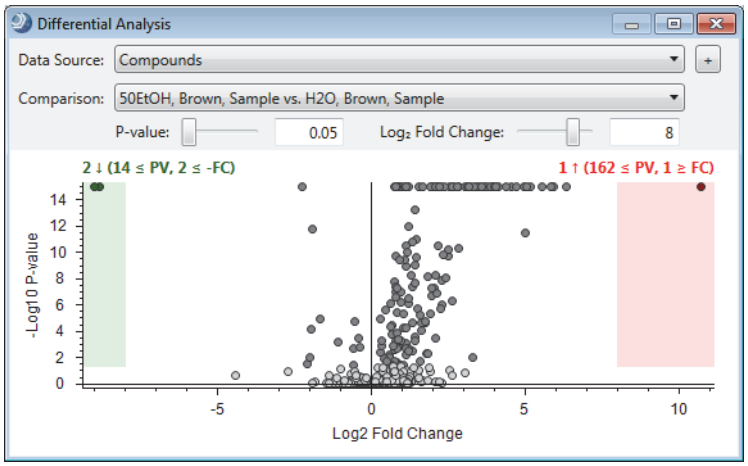
Figure 133. P-value decreased from 0.05 to 1E–12



- Change the fold change setting by dragging the slider. This changes the *x*-axis range of the shaded areas.

Figure 134 shows the effect of changing the Log_2 Fold Change setting.

Figure 134. Fold change increased from 1 to 8



Run a new differential analysis

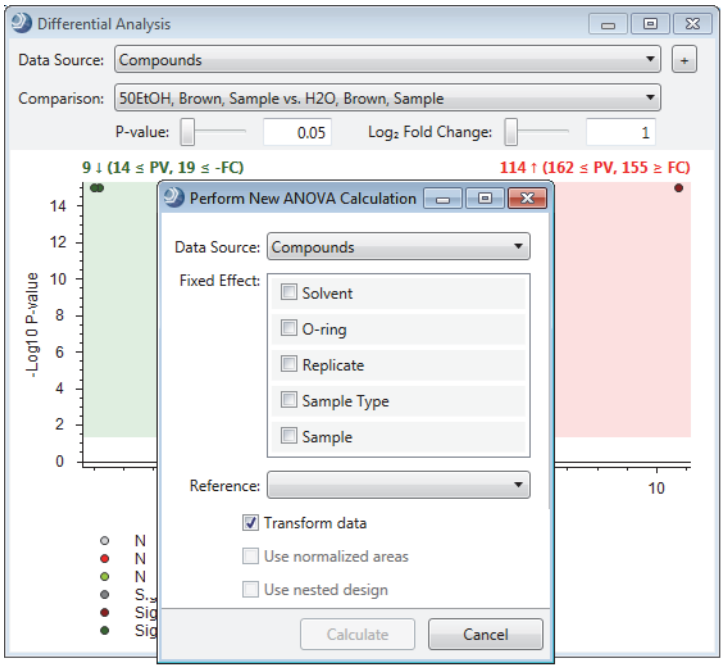
Use the Perform New ANOVA Calculation dialog box to set up and compare different ratios than those on the Grouping and Ratios page of the analysis.

❖ To run a new differential analysis

1. In the Differential Analysis view, click the **Perform New ANOVA Calculation** icon, , to the right of the Data Source box.

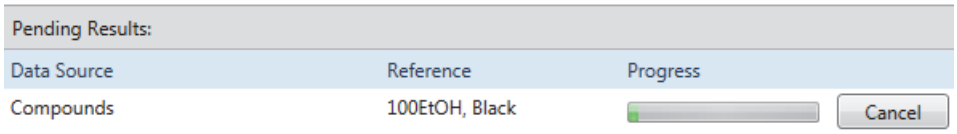
   The Perform New ANOVA Calculation dialog box opens.

   Figure 135. Perform New ANOVA Calculation dialog box in front of the Differential Analysis view



2. In the Data Source list, select a different result table if applicable.
3. In the Fixed Effect area, select one or more variables to create new sample groups.
4. In the Reference list, select one of the new sample groups as the denominator for the group ratios.
5. (Optional) To transform the data to the $\log_{10}$ scale, select the **Transform Data** check box.
6. (Optional) To normalize the chromatographic peak areas, select the **Use Normalized Areas** check box. This check box is available if the processing workflow included the Normalize Areas node.
7. (Optional) To calculate p-values for a nested design, select the **Use Nested Design** check box. This check box is available if the original analysis included a biological study factor and nested sample groups.
8. Click **Calculate**.

The Perform New ANOVA Calculation dialog box closes, and the Pending Results area appears at the bottom of the view. The Pending Results area displays the data source (result table), the reference group, and the progress of the new calculation.



When the calculation is complete, the new ratio (*sample group* vs. *reference group*) appears in the Comparison list.

9. To view the analysis, select the data source in the Data Source list and the new ratio in the Comparison list.

   The volcano plot updates with the selected analysis.

Differential Analysis view parameters and shortcut menu commands

Table 114 describes the parameters in the Differential Analysis view.

Table 114. Differential Analysis view parameters (Sheet 1 of 2)

Parameter	Description
Data Source	Specifies the result table for the source data. Selections: Compounds or Expected Compounds table
Perform New ANOVA Calculation	Opens the Perform New ANOVA Calculation dialog box for setting up a new differential analysis.
Comparison	Specifies the ratio for comparison. Selections: Generated ratios on the Grouping and Ratios page of the analysis and any new analyses that you have run and saved To save the differential analyses run in the Differential Analysis view, save the result file.
P-value	Specifies the p-value for the null hypothesis. Use the slider to change the value in the corresponding box. Default: 0.05 ($-\log_{10} 0.05 = 1.3$)

Table 114. Differential Analysis view parameters (Sheet 2 of 2)

Parameter	Description
Log_2 Fold Change	Specifies the fold change (ratio in the log base 2 scale) between the sample group and the reference group. This value creates an upper and lower threshold for each group ratio. Use the slider to change the value in the corresponding box. Data points that fall outside the upper and lower thresholds are in the shaded regions. Default: 1 (two-fold change)
Graph	
x axis	Displays the log_2 fold change.
y axis	Displays the p-value in a linear scale or in a $-log_{10}$ scale.
Analysis summaries	The summaries display the number of data points with a p-value above the statistical significance level and a fold change outside the empirical threshold.
Shaded regions	The region shaded in red identifies the data points that are significantly different (populations differ based on the p-value setting) and that fall outside the lower fold change threshold. The region shaded in green identifies the data points that are significantly different (populations differ based on the p-value setting) and that fall outside the upper fold change threshold.
Legend	By default, the legend is hidden. Choosing Show Legend from the shortcut menu displays the legend. The legend contains color-coded circles for these conditions: • Nonsignificant and does not meet FC (fold change) threshold • Nonsignificant and greater than upper FC threshold • Nonsignificant and less than lower FC threshold • Significant and does not meet FC threshold • Significant and greater than upper FC threshold • Significant and less than lower FC threshold

Table 115 describes the shortcut menu commands for the Differential Analysis view.

Table 115. Shortcut menu commands for the Differential Analysis view (Sheet 1 of 2)

Command	Description
Show Position Tooltips	Displays information about the compound.
Zoom Out	Undoes the last zoom.
Undo All Zoom/Pan	Zooms out to the full plot range.

Table 115. Shortcut menu commands for the Differential Analysis view (Sheet 2 of 2)

Command	Description
Copy and Export commands	See "Export spectral data to a new or existing mzVault library."
Show Legend	Displays the legend for the color-coded data points.
Note The color-coded data points (circles) represent compounds in the selected data source. Selecting a data point turns it blue and selects the check box for the corresponding compound in the data source table.	
Check Point	To activate this command, point to a data point. Selects the data point in the view and the check box for the corresponding compound in the data source table.
Uncheck Point	To activate this command, point to a selected compound. Returns the data point to its original color clears the corresponding check box in the data source table.
Check All Visible Points	Selects all the visible data points.
Uncheck All Visible Points	Clears the check boxes for all the visible data points.
Check All Up-Regulated Points	Selects all the data points in the pink-shaded region of the plot.
Check All Down-Regulated Points	Selects all the data points in the green-shaded region of the plot.

Partial Least Squares Discriminant Analysis view

Use the Partial Least Squares Discriminant Analysis view to determine whether two groups are different and to identify the variables that contribute to that difference.

See these topics:

- Identify a set of compounds to discriminate groups
- Partial Least Squares-Discriminant Analysis view parameters

Identify a set of compounds to discriminate groups

❖ **To determine a set of compounds that you can use to tell two groups apart**

1. Open a result file from an analysis with study factors.
2. From the menu bar, choose **View > Partial Least Squares - Discriminant Analysis**.

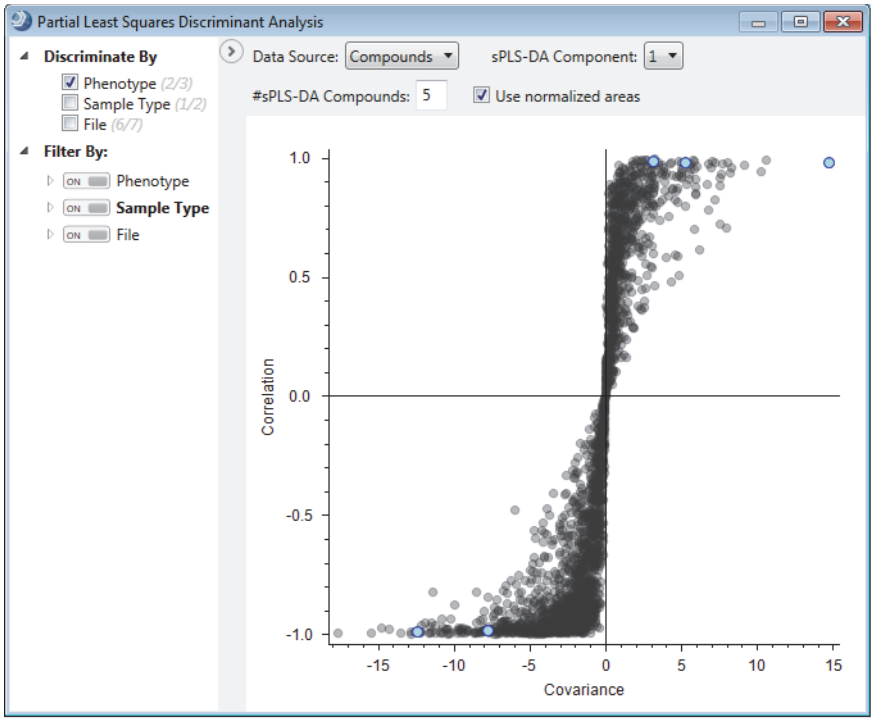
The Partial Least Squares Discriminant Analysis view opens to the right of the tabbed result tables.

3. In the collapsible pane on the left, under Discriminate By, select the study factors that you want to discriminate by.
4. On the right above the plot, select the data source from the Data Source list.
5. In the #sPLS-DA Compounds box, type the number of compounds that you want to use to differentiate the selected study factors.
6. To update the plot, click anywhere in the plot.

   The orange circles represent the discriminating compounds.
7. Right-click the plot and choose **Check All sPLS-DA Points**.

   The application selects the check boxes of the corresponding compounds in the selected data source. The blue circles represent the checked discriminating compounds.

Figure 136. PLS-DA view with five checked discriminating compounds (LC study)



8. To view the list of compounds that you can use to differentiate the selected experimental variables, set up a result filter to display only the checked compounds in the selected result table.

Partial Least Squares-Discriminant Analysis view parameters

Table 116 describes the parameters in the Partial Least Squares - Discriminant Analysis view.

Table 116. Partial Least Squares - Discriminant Analysis view parameters

Parameter	Description
Data Source	Specifies the result table for the source data. Selections: Compounds table or Expected Compounds table
sPLS-DA Component	Specifies the analysis component. Selection: 1 to 6
#sPLS-DA Compounds	Specifies the number of compounds that when used together can discriminate between the values for the study variables selected under Discriminate By.
Use Normalized Areas	Uses the normalized areas in the result file. Available when the processing workflow includes the Normalize Areas node.

KEGG Pathways view

Use the KEGG Pathways view to display the reaction pathways for a mapped compound. You can map compounds in the following compounds tables: Compounds table and Expected Compounds table.

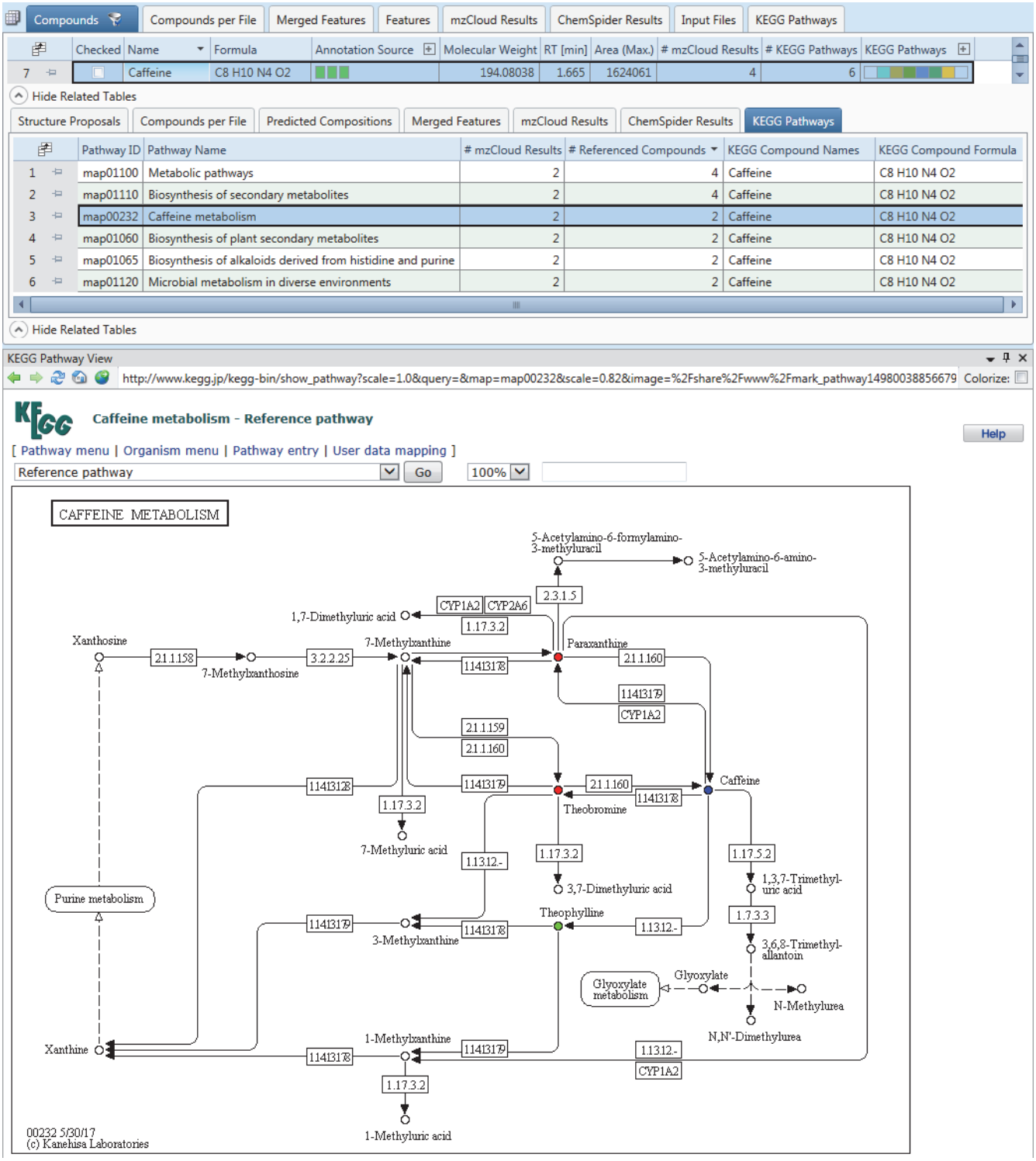
❖ To view the KEGG pathways for a compound

1. Open a result file that contains mapped KEGG pathways—that is, a result file from an analysis that included the Map to KEGG Pathways node.
2. In the main compounds table, select a compound.
3. Below the main compounds table, click **Show Related Tables** to show the related tables.
4. In the related tables pane, click the **KEGG Pathways** tab to make it the active result table.
5. In the KEGG Pathways table, select the pathway that you want to view.
6. In the menu bar, choose **View > KEGG Pathways**.

   The selected KEGG pathway opens. The blue circle indicates the selected compound in the KEGG pathway. The red circles indicate related compounds that were not found in the mzCloud database. The green circles indicate related compounds that were found in the mzCloud database.

Figure 137 shows the selections of caffeine in the Compounds table and caffeine metabolism in the KEGG Pathways table. The related Compounds tables shows the compounds related to caffeine, which appear as red circles in the pathway diagram.

Figure 137. Caffeine metabolism pathway where caffeine appears as a blue circle (LC study)



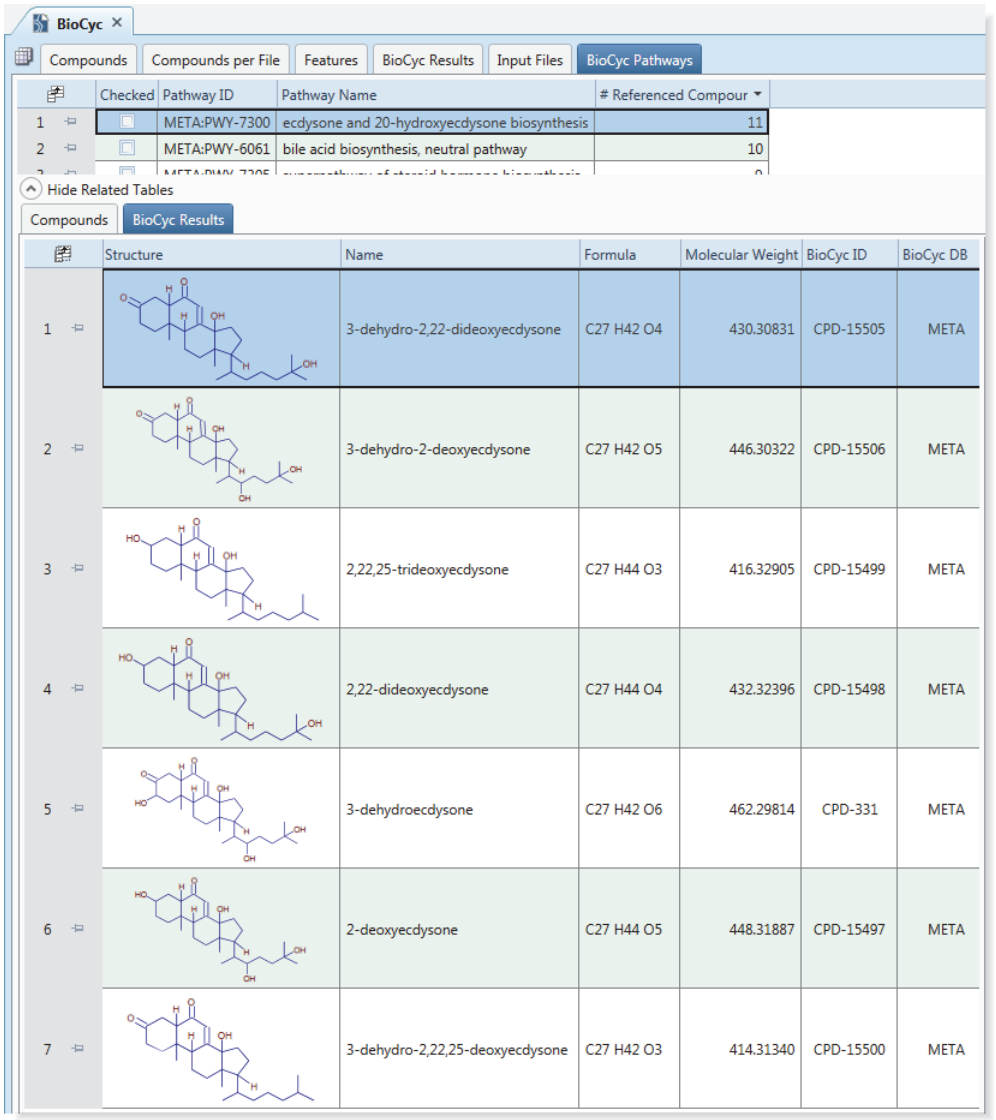
BioCyc Pathways view

When the processing workflow for a result file includes the Map to BioCyc Pathways node, use the BioCyc Pathways view to display the mapped pathways for a selected compound.

❖ To view the BioCyc Pathways for a compound

1. Open a result file for an analysis that maps the detected compounds to their BioCyc pathways.
2. In the main table pane, click the **BioCyc Pathways** tab.
3. Select a pathway of interest.
4. Below the BioCyc Pathways table, click **Show Related Tables**.
5. Click the **BioCyc Results** tab.
6. In the BioCyc Results table, select a compound of interest.

Figure 138. BioCyc Results table for the selected pathway



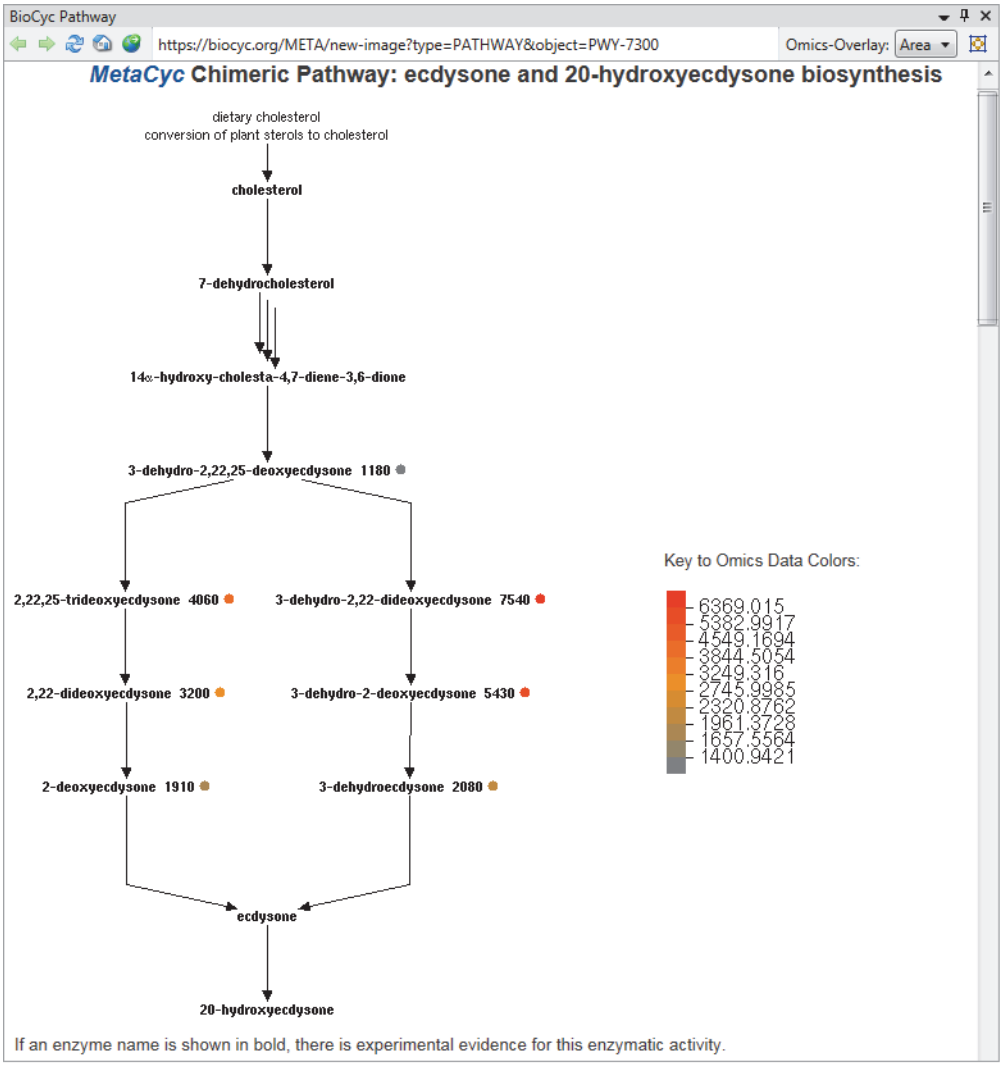
7. From the application menu bar, choose **View > BioCyc Pathways**.

   The BioCyc Pathways view opens to the right of the result tables.

8. In the Omics-Overlay list, select **Area**.

   Figure 139 shows a BioCyc pathway with an Area overlay.

Figure 139. BioCyc Pathways view with an area overlay



Metabolika Pathways view

Use the Metabolika Pathways view to display the mapped pathways for a selected compound.

❖ To view a mapped pathway for a compound

1. Open a result file from an analysis that included the Map to Metabolika Pathways node.
2. In the Compounds table, select the compound.
3. Click **Show Related Tables**.
4. In the Related Tables pane, click the **Metabolika Pathways** tab.
5. Select the pathway that you want to view.
6. From the application menu bar, choose **View > Metabolika Pathways**.

   The view opens to the right of the Compounds table and displays the selected pathway. The structure for the selected compound is blue, the structures for other detected compounds are red, and the structures for undetected compounds in the pathway are black.
7. To overlay a data source, select the source from the Overlay Data Source list and type or select a cell size from **6** to **30** pixels in width in the Overlay Cell Size box.

   The data source selections depend on the processing workflow, but always include the annotation source, chromatographic peak area, or Metabolika pathways graphic.

Retention Time Corrections view

When the processing workflow for a result file includes the Align Retention Times node and the analysis includes more than one input file, use the Retention Time Correction view to inspect the regression curves for the alignment features (the $m/z \times$ RT).

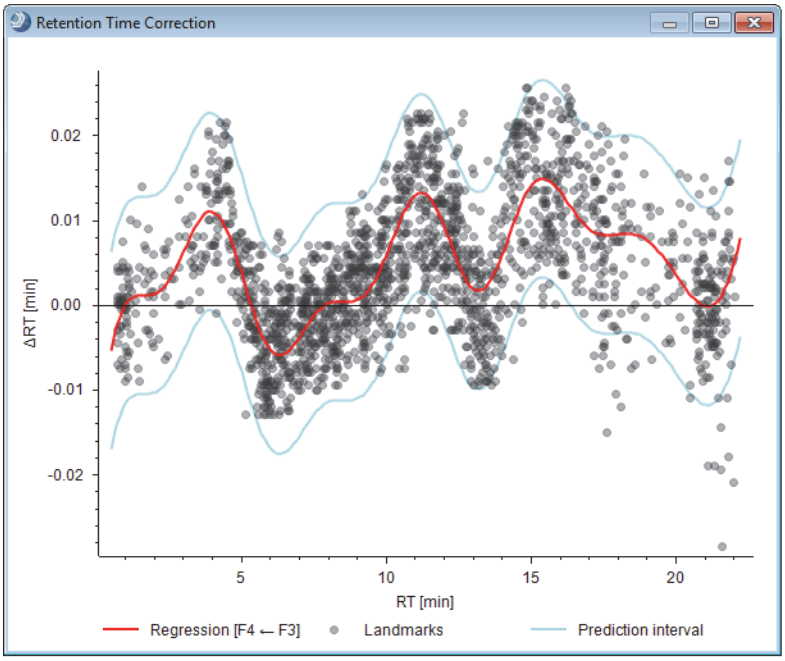
❖ To open the Retention Time Corrections view

1. Open a result file for an analysis with multiple input files.
2. In the menu bar, choose **View > Retention Time Corrections**.

   In the default layout, the Retention Time Correction view opens to the right of the tabbed result tables. Because you need to select a row in the Input Files table, the view is empty.
3. In the main result tables, click the **Input Files** tab.
4. Do the following, as applicable:

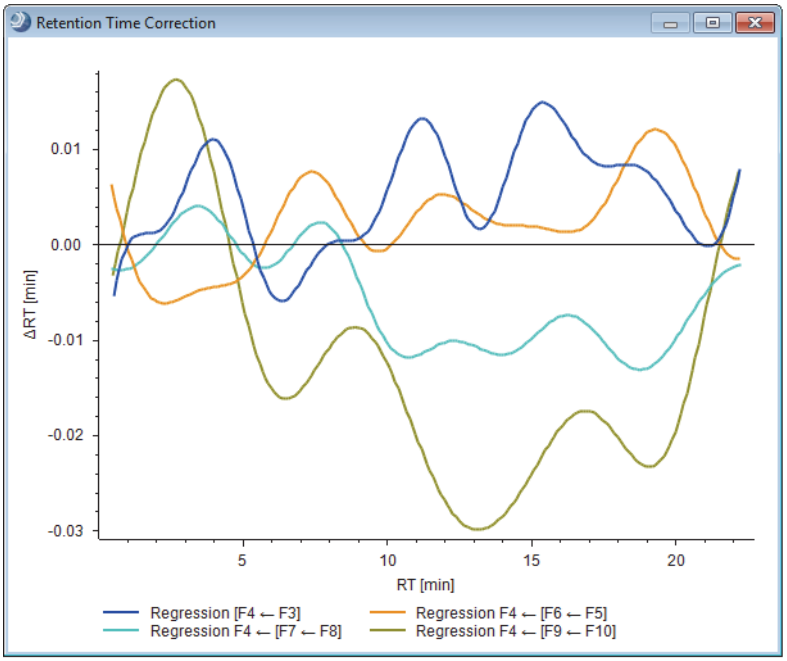
   - To view the regression curve for one input file as well as the prediction interval for the landmark features in the file, select one input file.

Figure 140. Retention Time Correction view with the regression curve for one input file



- To view overlaid regression curves for multiple input files, select multiple input files.

Figure 141. Retention Time Correction view with regression curves for multiple input files



Compound Area Corrections view

When the processing workflow for a result file includes a QC corrections node and the analysis includes samples with the sample type assignment of Quality Control, use the Compound Area Corrections view to inspect the corrected peak areas for each compound in the compounds table.

For information about acquiring a set of raw data files with interspersed quality control samples, see "Using quality control samples to compensate for batch effects."

❖ To open the Compound Area Correction view

1. Open a result file for an analysis with batch normalization—that is, an analysis that includes QC samples and a processing workflow with a QC correction node.
2. In the compounds table, select one or more compounds.
3. From the menu bar, choose **View > Compound Area Corrections**.

   In the default layout, the Compound Area Correction view opens to the right of the tabbed result tables. The Compound Area Correction view displays a scatter plot of the areas for the selected compound on the *y* axis against the acquisition time for each input file on the *x* axis.

   The legend below the plot describes the data point symbols and the regression curve or curves.

   The Apply QC Correction node generates two regression lines: a blue curve for the original areas and an orange curve for the corrected areas.

Table 117 describes the data point symbols. The legend is not static. If a compound does not include any gap-filled QC samples, the legend does not include the diamond symbols for that compound.

Table 117. Compound Area Corrections view legend (Sheet 1 of 2)

Data point symbol	Description
QC samples	
(▲) Blue triangle	Original area for the QC sample
(△) Orange triangle	Corrected area for the QC sample
(◆) Blue diamond	Original area for a gap-filled QC sample
(◇) Orange diamond	Corrected area for a gap-filled QC sample
Non-QC samples	
(●) Blue circle	Original area for a non-QC sample
(○) Orange circle	Corrected area for a non-QC sample

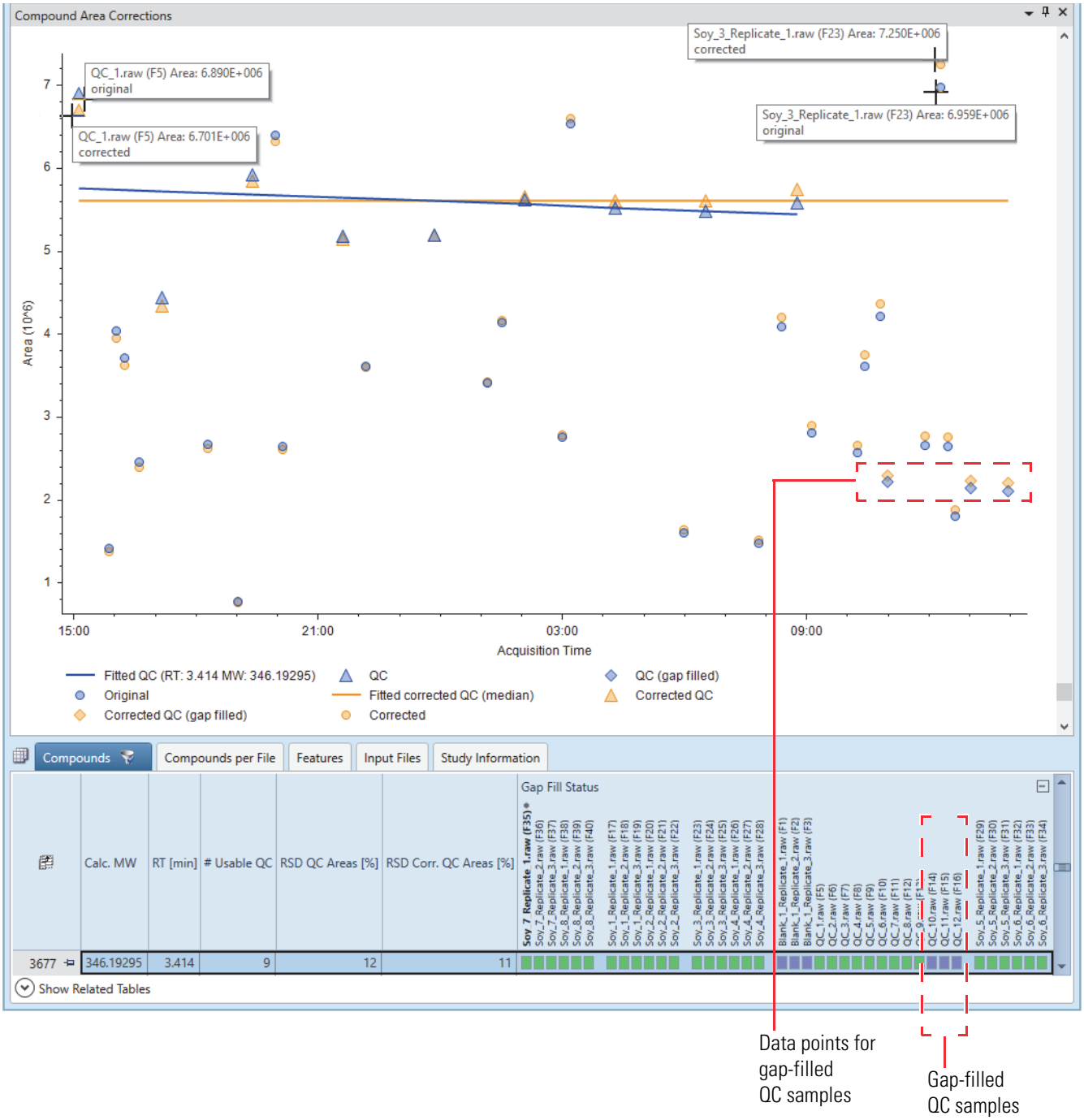
Table 117. Compound Area Corrections view legend (Sheet 2 of 2)

Data point symbol	Description
Regression lines from a processing workflow with the Apply QC Correction node	
Blue line across the time axis	Regression curve for the corrected original compound areas in the QC samples
Orange line across the time axis	Regression curve for the corrected compound areas in the QC samples
Regression line from a processing workflow with the Apply SERRF QC node (LC studies only)	
Orange line across the time axis	Regression curve for the corrected compound areas in the QC samples The Apply QC SERRF Correction node generates only one regression line.

Pointing to a data point (circle, triangle, or diamond) displays a tooltip with the input file name, the compound area, and the status—original or corrected.

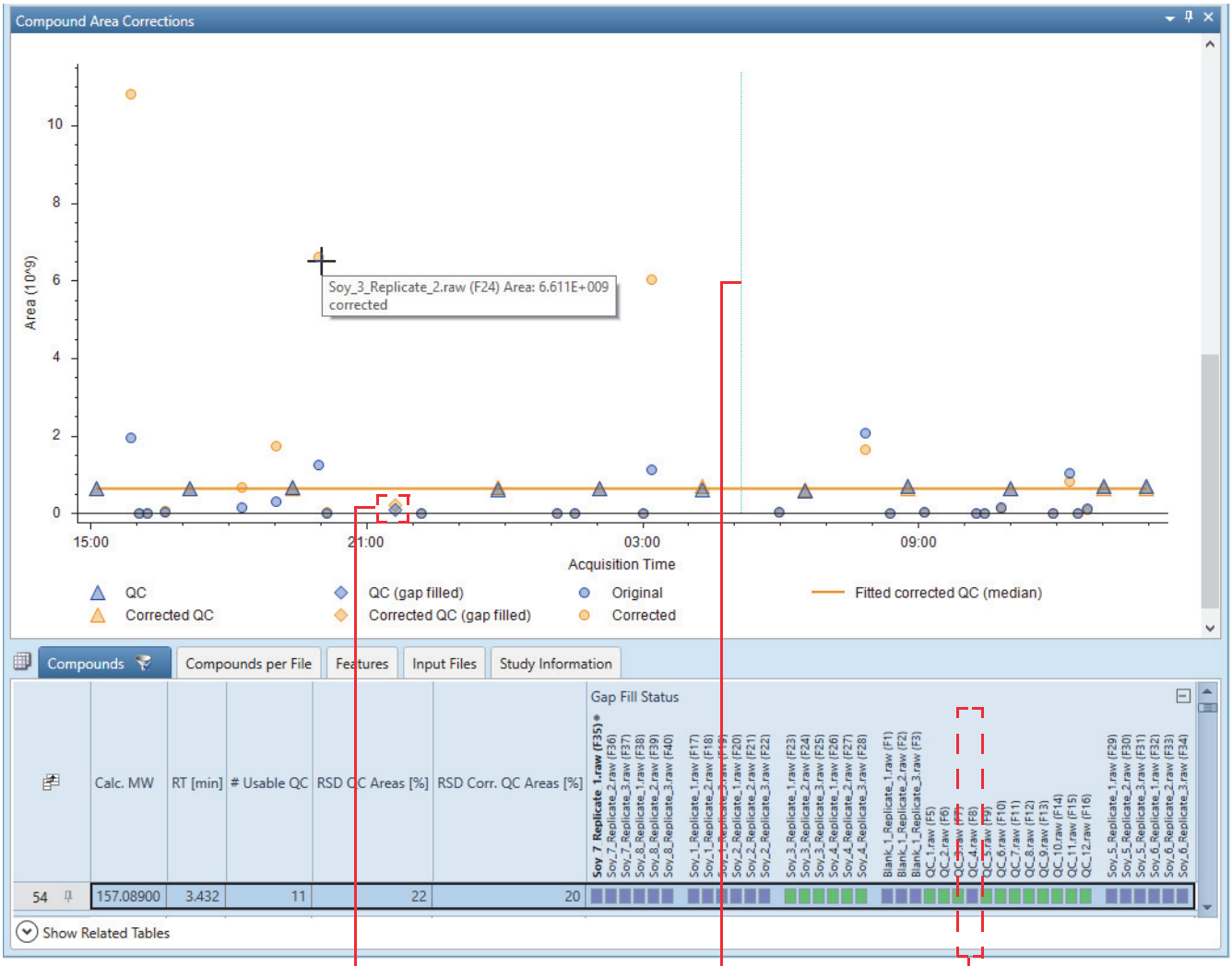
Figure 142 shows the Compound Area Corrections view for a compound with 12 QC samples. The chromatographic peak area for three of the QC samples is gap-filled.

Figure 142. Compound Area Corrections view for an analysis with the Apply QC Correction node, 12 QC samples, and a compound with three gap-filled QC samples



For an LC study, if you use the Apply SERRF QC Correction node and the analysis includes input files from more than one batch, a blue vertical line separates the batches in the plot. Figure 143 shows an analysis with the Apply AC Correction node for a set of input files from two batches.

Figure 143. Compound Area Corrections view (Apply SERRF QC node for LC studies))

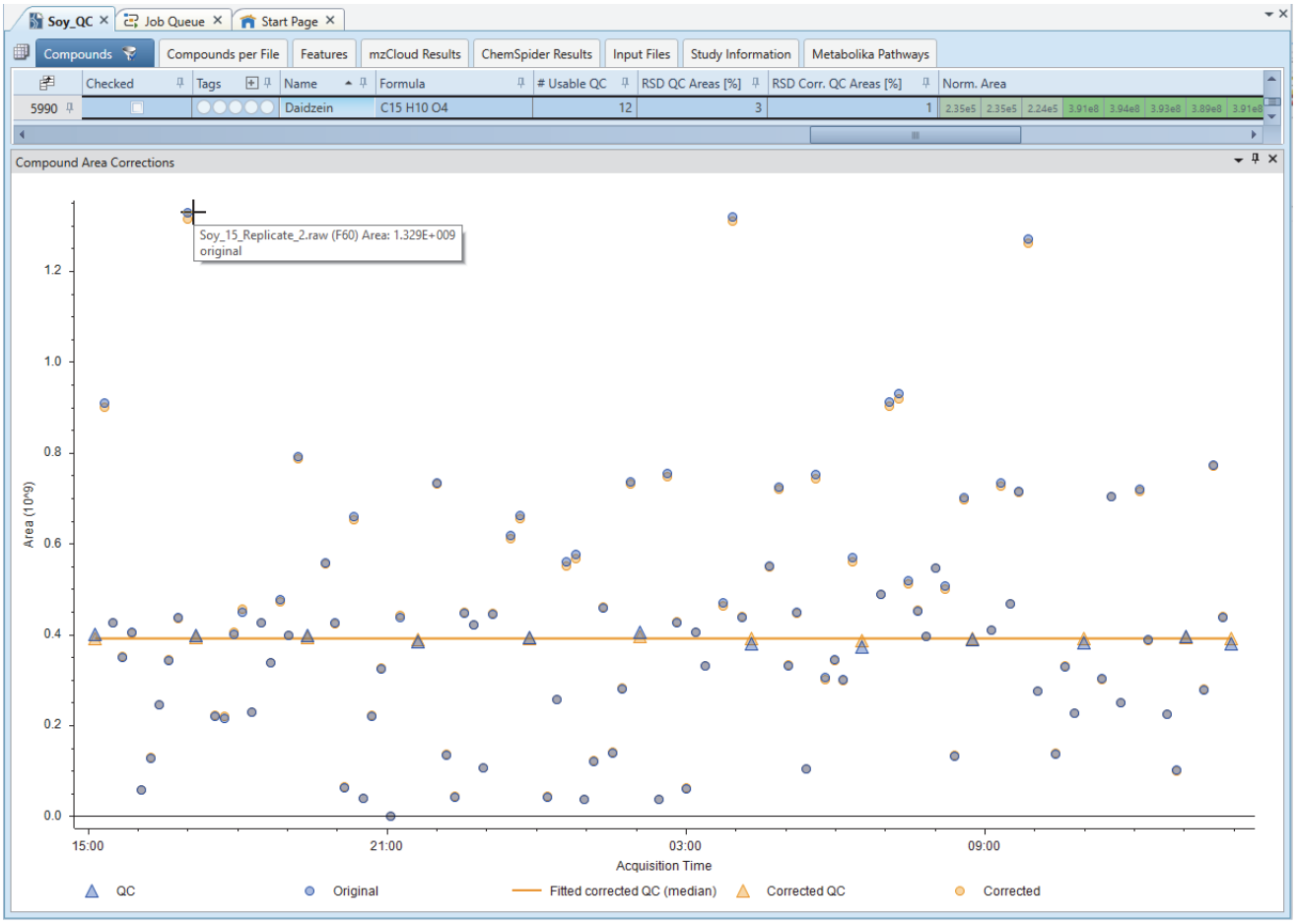


Data points for gap-filled QC samples

Demarcation line for the two batches

Gap-filled QC sample

Figure 144. Compound Area Corrections view for a selected compound (daidzein)



Hierarchical Clustering Analysis view

Use the Hierarchical Cluster Analysis view to visualize the correlation between detected compounds and selected samples in a two-dimensional array of color-coded rectangles (heat map) where each rectangle represents the relative amount (by area) of a specific compound in a specific sample.

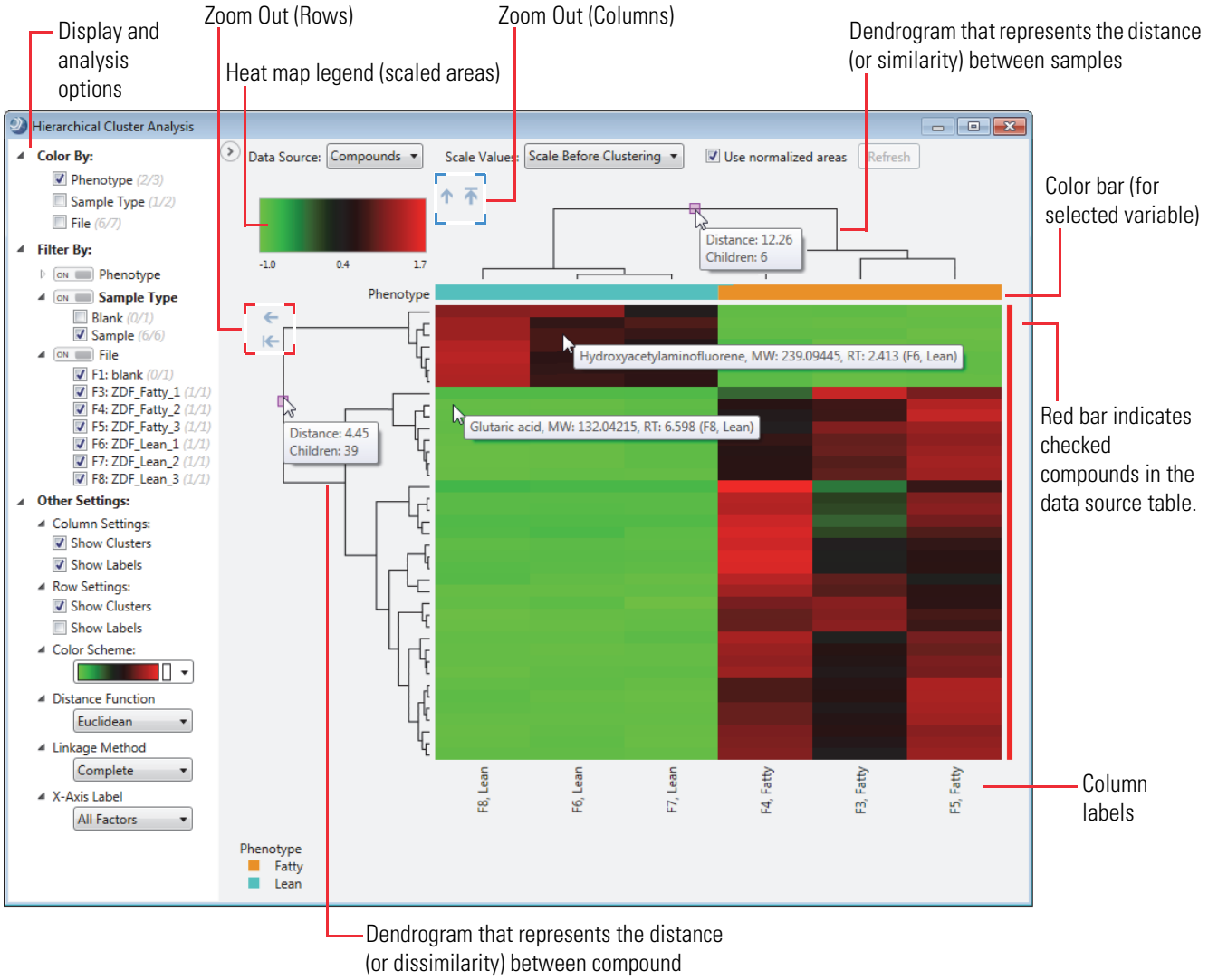
The application uses an agglomerative (bottom-up) approach to find the similarities between samples and compounds. Initially, the hierarchical cluster analysis assigns each compound to its own singleton cluster. The analysis then proceeds iteratively, at each stage joining the two most similar clusters into a new cluster, continuing until there is one overall cluster represented by a dendrogram.

The dendrogram to the left of the heat map represents the distance (or dissimilarity) between the compound clusters. The width of each node is proportional to the distance (or dissimilarity) between two compounds at the lowest level or two compound clusters at the higher levels. The dendrogram above the heat map represents the distance (or similarity) between samples. The height of each node is proportional to the distances (or similarity) between two samples at the lowest level or two sample clusters at the higher levels.

Pointing to a dendrogram node displays the distance between clusters, and pointing to a heat map cell displays the compound and sample information.

By default, under Filter By, all the input files are selected, and under Other Settings, the Show Labels check box for the compound labels is clear.

Figure 145. Hierarchical cluster analysis for the compounds detected in six samples from lean and fat ZDF rats (LC studies)



To determine how to cluster the data, the application provides a choice of commonly used distance functions and linkage methods (see Table 120 and Table 121).

Note The Heat Map supports clustering for 2 to 2000 compounds.

To set up a hierarchical clustering analysis and work interactively with the heat map's cells, see these topics:

- Set up a hierarchical clustering analysis
- Work interactively with the heat map grid
- Hierarchical Cluster Analysis view parameters

Set up a hierarchical clustering analysis

❖ To set up the hierarchical clustering analysis

1. Filter the result table that you want to use as the data source. The analysis uses the only visible compounds in the table.

   Note When you apply a filter that displays only the checked compounds in the selected result table, a red bar appears to the right of the heat map. If only a subset of the compounds is checked, the bar is discontinuous, with red indicating a checked compound and gray indicating an unchecked compound.

2. In the Data Source list, select the data source.

   The Compounds table is the data source for untargeted analyses, and the Expected Compounds table is the data source for targeted analysis. For a combination analysis that generates a Compounds table and an Expected Compounds table, you can select either table as the data source.

3. In the Scale Values list, select whether to scale the heat map data before or after clustering or not at all.

4. To normalize the areas for the compounds, select the **Use Normalized Areas** check box.

5. In the left pane, under Filter By, select the check boxes for the samples to include in the analysis.

   By default, all the sample files are selected.

   Note By default, under Other Settings, the following check boxes are selected:

   Column Settings: Show Clusters and Show Labels—Displays a dendrogram above the heat map and sample labels below the heat map.

   Row Settings: Show Clusters—Displays a dendrogram to the left of the heat map.

6. In the left pane, under Other Settings, select these analysis options:
   - Under Distance Function, select how the analysis determines the distance between the data points, where the data points are files (columns) or compounds (rows) (Table 120).
   - Under Linkage Method, select how the analysis performs the clustering analysis (Table 121).
7. In the left pane, select these labeling options:
   - Under Color By, select whether to display color bars above the heat map to visually differentiate the samples by their study factor variables.
   - Under Other Settings > Row Settings, select whether to display the compound labels.

     Selecting the Show Labels check box under Row Settings displays the compound labels to the right of the heat map.
   - Under Other Settings > X-Axis Label, select the label for the sample columns.
8. To run the analysis, click **Refresh**.

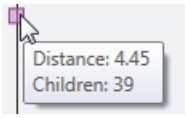
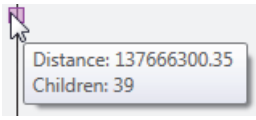
Work interactively with the heat map grid

After you run a hierarchical heat map analysis, you can enlarge the heat map, zoom in and out on the heat map, and point to specific cells in the heat map for more information.

Table 118. Common tasks for the heat map grid (Sheet 1 of 2)

Task	Procedure
Enlarge the heat map.	To increase the heat map width, drag its left or right edge. To increase its height, drag its top or bottom edge.
Zoom in on an area of the heat map.	Drag the pointer across the rectangular area of the heat map.
Zoom out of an enlarged area of the heat map by using the shortcut menu commands.	Right-click the heat map and choose one of the following: **Zoom Out Column**, **Zoom Out Row**, **Undo All Column Zoom**, or **Undo All Row Zoom**.
Zoom out of an enlarged area of the heat map by using the zoom icons.	To zoom out of a row selection, click the **Zoom Out Row** icon,  , or the **Undo All Row Zoom** icon,  , below the heat map legend. To zoom out of a column selection, click the **Zoom Out Column** icon,  , or the **Undo All Column Zoom** icon,  , to the right of the heat map legend.

Table 118. Common tasks for the heat map grid (Sheet 2 of 2)

Task	Procedure
View information about a heat map cell.	Point to the cell. The tooltip displays the compound's name (if available), its MW, RT, file ID, and the study factor value (if available).
View the distance value for a dendrogram node.	Point to the node. The tooltip displays the distance value. For an analysis where the chromatographic peak areas are scaled before clustering, the distance values are scaled.  For an analysis where the chromatographic peaks areas are not scaled or are scaled after clustering, the distance values are not scaled. 

Hierarchical Cluster Analysis view parameters

Table 119 describes the parameters in the Hierarchical Clustering Analysis view.

Table 119. Hierarchical Clustering Analysis view parameters (Sheet 1 of 3)

Parameter	Description
Button	
Refresh	Runs the hierarchical clustering analysis on the compounds displayed in the selected data source (result table) and the samples selected in the left pane under Filter By.
Parameters in the right pane	
Data Source	Specifies the result table for the source data. Selections: Compounds table or Expected Compounds table

Table 119. Hierarchical Clustering Analysis view parameters (Sheet 2 of 3)

Parameter	Description
Scale Values	Specifies if and when to perform a z-score transformation on the data points: • None—The application does not scale the data. The heat map legend displays a scale in area counts, and the dendrogram nodes display the distance in area counts. • Scale After Clustering— Applies a z-score transformation after performing the hierarchical clustering. The heat map legend displays the range of the scaled values, and the dendrogram nodes display the distance in area counts. • Scale Before Clustering—Applies a z-score transformation before performing the hierarchical clustering. The heat map legend displays the range of the scaled values, and the dendrogram nodes display the scaled distance values.
Use Normalized Areas	When selected, normalizes the chromatographic peak areas for the selected compounds before running the analysis.
Parameters in the left pane	
Color By	
Displays the selected color bars for the selected variables above the heat map.	
Filter By	
By default, all the check boxes—except for the Blank sample type—are selected. Clearing a check box removes the corresponding item from the analysis.	
Other Settings	
Column Settings	
Show Clusters	When selected, displays the dendrogram for the samples above the heat map; that is, this selection displays the dendrogram for the items selected under Filter By.
Show Labels	When selected, displays the labels across the bottom of the heat map for the items selected under Filter By. The X-Axis Label parameter at the bottom of the left pane provides labeling options.
Row Settings	
Show Clusters	When selected, displays the dendrogram for the compounds to the left of the heat map.
Show Labels	When selected, displays the labels across the bottom of the heat map for the items selected under Filter By. The X-Axis Label parameter at the bottom of the left pane provides labeling options.

Table 119. Hierarchical Clustering Analysis view parameters (Sheet 3 of 3)

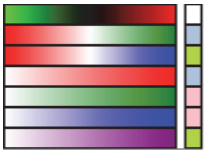
Parameter	Description
Color Schemes	Specifies the color scheme for the heat map. Default: • Available values  • Missing values ▯ white Selection: Available values Missing values 
Distance Function	Specifies the distance function to use for calculating the distance between data points (see Table 120). Default: Euclidean
Linkage Method	Specifies the method to use for hierarchical clustering (see Table 121). Default: Complete
X-Axis Label	Specifies the labels for the sample columns. Selections: All Factors, Selected Factors, File ID, Full File Name, and Sample Name

Table 120. Distance functions (Sheet 1 of 2)

Distance function	Description
Euclidean	Computes the Euclidean distance between two data vectors, which is the geometric distance in the multidimensional space.
Manhattan	Computes the city-block (Manhattan) distance between two vectors. The Manhattan distance between two data items is the sum of the differences of their corresponding components. In most cases, the Manhattan distance measure yields results similar to the simple Euclidean distance. However, the effect of outliers is dampened because the distances are not squared.
Maximum	Computes the maximum distance on any one of the dimensions between two vectors. Use this function to define two objects as different if they differ in any one of the dimensions.

Table 120. Distance functions (Sheet 2 of 2)

Distance function	Description
Pearson	Computes the Pearson product-moment correlation, which is a measure for the shape similarity between two clusters.
Squared Euclidean	Computes the squared Euclidean distance between two data vectors. The Euclidean Squared distance metric uses the same equation as the Euclidean distance metric, but it does not take the square root.

Table 121. Linkage methods

Linkage method	Description
Average	Computes the distance between two clusters as the average distance between all pairs of objects in the two different clusters.
Centroid	Computes the distance between two clusters as the difference between centroids. The centroid of a cluster is the average point in the multidimensional space.
Complete	Computes the distance between two clusters as the greatest distance between any two objects in the different clusters (furthest neighbors).
Median	Computes the distance between two clusters as the difference between centroids, using the size of each cluster as a weighting factor.
Single	Computes the distance between two clusters as the distance of the two closest objects (nearest neighbors) in the clusters.
WARD	Computes the distance between two clusters using Ward's method, which uses an analysis of variance approach to evaluate the distances between clusters. The smaller the increase in the total within-group sum of squares as a result of joining two clusters, the closer they are. The within-group sum of squares of a cluster is defined as the sum of the squares of the distance between all objects in the cluster and the centroid of the cluster. Ward's method tends to produce compact groups of well-distributed size.
Weighted Average	Computes the distance between two clusters as the average distance between all pairs of objects in the two different clusters, using the size of each cluster as a weighting factor.

mzLogic Analysis view

You can use the mzLogic Analysis view in two ways:

- To run an mzLogic analysis for a data set that was processed with a workflow that did not include the Apply mzLogic node
- To update an older analysis with new similarity results from the mzCloud spectral database

Note The application does not save the results from this mzLogic analysis to the result file; however, you can add suitable candidates to the Structure Proposals table for a compound and apply FISh scoring.

The ranking score provided by an mzLogic analysis is not a probability score. It is only a measure of how similar a putative structure is to closely matching structures in the mzCloud spectral database.

To run and review an mzLogic Analysis, see these topics:

- Perform an mzLogic analysis
- Review the results of an mzLogic analysis
- mzLogic Analysis view parameters

Perform an mzLogic analysis

❖ **To perform an mzLogic analysis**

1. Open a result file from an untargeted analysis.
2. Select a compound in the Compounds table.
3. From the application menu bar, choose **View > mzLogic Analysis**.

   The mzLogic Analysis view opens to the right of the Compounds table. If the selected result file does not include results from an identity search, the Candidates area is empty. Otherwise, the Candidates area contains candidates from the identity search nodes.
4. To add candidates from the ChemSpider database, click **ChemSpider** and run a search.
5. To run forward and reverse similarity searches on the candidates, click **mzCloud Similarity**.

   If the application finds similar structures in the mzCloud database, it populates the Similar Structures from mzCloud area and the Calculate Score button becomes available. The structure tiles in this area include an mzCloud Match score and a Coverage value at the top and a formula and delta mass value at the bottom.
6. To display an mzLogic score for each candidate, click **Calculate Score**.

Review the results of an mzLogic analysis

❖ **To review the results of an mzLogic analysis**

1. In the mzLogic Analysis view, open the Similar Structures from mzCloud area.
2. In the Candidates area, click a candidate to select it.

   In the Similar Structures from mzCloud area, the matching portions of the similar structures are highlighted in blue.

mzLogic Analysis view parameters

Table 122. mzLogic Analysis view parameters (Sheet 1 of 2)

Parameter	Description
ChemSpider	Opens the ChemSpider Search dialog box. See "Find a structure in the ChemSpider database."
mzCloud Similarity	Runs a forward and reverse mzCloud similarity search.
Calculate Score	Calculates the mzLogic scores for the available candidates. Available when the Candidates and Similar Structures from mzCloud areas are populated.
Back	Returns the focus to the previously selected compound in the Compounds table. Available when the Auto Refresh check box is clear and you select a different compound in the Compounds table.
Refresh	Refreshes the Candidates area when you select another compound. Available when the Auto refresh check box is clear.
Auto refresh	Select so that when you select another compound, the application automatically refreshes the Candidates area.
Size	Controls the size of the structure tiles in the Candidates area. Default: Medium Selection: Small, Medium, or Large

Table 122. mzLogic Analysis view parameters (Sheet 2 of 2)

Parameter	Description
Candidates area	Displays structure candidates as tiles. The structure candidates are provided by identity searches during data processing or a separate ChemSpider search from the result file. If the identity searches find duplicate structures, the application consolidates them. Right-clicking a tile displays a shortcut menu with the following commands: • Add to Structure Proposals—Adds the selected structure to the Structure Proposals table for the selected compound. • Add to Structure Proposals and Apply FISh Scoring—Opens the Settings dialog box for applying the FISh scoring algorithm. Then, runs the FISh scoring algorithm and adds the structure and FISh Coverage score to the Structure Proposals table for the selected compound.
Similar Structures from mzCloud area	Displays the results of the mzCloud similarity search for the selected compound. Selecting a candidate highlights the maximum common substructure in blue for the similar structures.
Sort By	Sorts the similar structures by the selected parameter. Default: mzCloud Match Selection: mzCloud Match, Forward Coverage, or Reverse Coverage

FISh Scoring Queue view

Use the FISh Scoring Queue view to display the progress of FISh scoring.

❖ To submit compounds to the FISh Scoring Queue view

1. Open a result file.
2. From the menu bar, choose **View > FISh Scoring Queue**.

   The FISh Scoring Queue opens to the right of the result tables.
3. Start the FISh scoring process as follows:
   - For compounds with assigned structures, go to step 4.
   - For compounds without assigned structures, go to step 5.

4. For compounds with assigned structures, do the following:
   a. To open the Settings dialog box, do one of the following:
      - In the compounds table (Compounds table or Expected Compounds table), right-click a compound and choose **Apply FISh Scoring**.
      - In any of the related search results tables, right-click a compound and choose **Add to Structure Proposals and Apply FISh Scoring**.
      - In a Structure Proposals table, right-click a compound and choose either **Apply FISh Scoring to Selected** or **Apply FISh Scoring to All**.
   b. In the Settings dialog box, make the appropriate selections and click **OK**.

      FISh scoring begins.
5. For compounds without assigned structures, do the following:
   a. To open the Compound Annotation Editor dialog box, do one of the following:
      - In the compounds table (Compounds table or Expected Compounds table), right-click a compound and choose **Edit Compound Annotations**.
      - In a Structure Proposals table, double-click a compound.
   b. Enter the structure by opening a structure file, drawing the structure, or running a ChemSpider search.
   c. Click the **FISh Scoring** tab.
   d. Make the appropriate selections for the FISh scoring algorithm.
   e. At the bottom of the dialog box, select the **Apply FISh Scoring** check box and click **Save**.

   FISh scoring begins.

Descriptive information for the result tables

For general information about opening result files and working with the result tables, see Chapter 8, "Review the analysis results."

Note The Statistical Methods table is new in the Compound Discoverer 3.3 application.

For information about specific result tables, see the following topics:

- Common result tables
- Expected Compounds result tables
- Compound detection result tables
- Compound Identification result tables
- Pathway Mapping result tables
- Compound Scoring tables
- Statistical Methods table
- Differential analysis columns
- Descriptive statistics columns
- QC Correction columns
- Annotations Source column in a compounds table
- Peak Rating columns
- Peak quality factor (PQF) columns in the result tables

Common result tables

For information about the result tables that are independent of the analysis type, see these topics:

- Adducts table
- Chromatogram Peaks table

- File Alignments table
- FISh Trace Fragments table
- Input Files table
- Manual Peaks table
- Merged Features table
- Specialized Traces table
- Study Information table
- Structure Proposals table

Adducts table

Use the Adducts table to view the list of adducts in the Adducts library. By default, the Adducts table is hidden. See "Show or hide result tables."

Chromatogram Peaks table

Use the Chromatogram Peaks table to view information about the quality of the chromatographic peak for a specific feature or a specific expected feature. The Chromatogram Peaks table displays information about the chromatographic peak for the feature or expected feature that you selected in the related table.

Table 123 describes the columns in the Chromatogram Peaks table.

Table 123. Chromatogram Peaks table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Area	Displays the integrated peak area.
Apex m/z	Displays the *m/z* value of the mass spectral peak at the chromatogram peak apex.
Apex RT [min]	Displays the retention time of the chromatogram peak apex.
Apex Intensity	Displays the intensity at the chromatogram peak apex.
Left RT [min]	Displays the start point for the chromatographic peak.
Right RT [min]	Displays the end point for the chromatographic peak.

Table 123. Chromatogram Peaks table (Sheet 2 of 2)

Column	Description
Isotope Number (hidden)	(For chromatographic peaks detected by the Detect Compounds node in an LC study) Displays the index number for the isotopic mass spectrum peak that the application used to create the XIC. The Detect Compounds node creates an XIC trace for each isotope. (For chromatographic peaks found by the Find Expected Compounds node in an LC study) Always displays a value of 0, as the Find Expected Compounds node creates only one filtered XIC trace for each ion. The Find Expected Compounds node creates the filtered XIC trace by summing the intensity of all the mass spectrum peaks that match the theoretical isotope pattern. When even only one required isotope is missing, the intensity of the XIC drops down to 0.
Peak Model	Displays the peak model for the chromatographic peak and includes information about the width and symmetry of the peak.

File Alignments table

For LC studies, use the File Alignments table to check the alignment process for each input file.

The retention time alignment node creates the File Alignments table. See "Align Retention Times node."

Table 124 describes the columns in the File Alignments table.

Table 124. File Alignments table

Column	Description
Study File ID	Displays the study file ID (F#) of the sample where the algorithm has corrected the measured retention time of the detected features against a set of features from the reference file.
Ref. File ID	Displays the study file ID (F#) of the input file that the analysis used as the reference file.
Kind	Displays the parameter that the algorithm used in the regression model. Retention time (RT) is the current regression model.
Description	Displays a description of the alignment process. • For the original Align Retention Times node, this column displays the alignment model. • For the Align Retention Times (ChromAlign) node, this column displays the following statement—Mapped to Reference File. If you did not select a reference input file for the node's Reference File parameter, the node automatically selects the first sample file (assigned the Sample Type of Sample) in the Files for Analysis area.
#Landmarks	For the original Align Retention Times node, this column displays the number of features that the analysis used to align the specified file to the reference file. For the Align Retentions Times (ChromAlign) node, this column displays the value 0 (zero), as this node does not use landmarks to align the features across the input files.
RMSE	Displays the estimated error for the corrected retention times of the features in the selected input file as the root-mean-square error.

FISh Trace Fragments table

Use the FISh Trace Fragments table to view the structures and the summed intensities of the expected fragment ions.

The Create FISh Trace node creates the FISh Trace Fragments table when the Individual Traces parameter for this node is set to True. See "Create FISh Trace node."

Table 125 describes the columns in the FISh Trace Fragments table.

Table 125. FISh Trace Fragments table

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Parent Compound	Displays the selected compound in the Create FISh Traces node.
Formula	Displays the elemental composition of the fragment ion.
Ion	Displays the ion description.
m/z	Displays the mass-to-charge ratio of the ion.
TIC	Displays the total ion current for the fragment ion.
Mode	Displays the fragmentation mode.
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID (F#) of the input file.
Structure	Displays the ion's molecular structure.

Input Files table

Use the Input Files table, which is common to all processing workflows, to view information about the input file set (Xcalibur RAW files) that the application processed to produce the result file.

For a result file from an analysis of multiple input files from an LC/MS acquisition sequence, use the related File Alignments table to check the chromatographic alignment of the features in the input files.

Table 126 describes the information displayed in the Input Files table.

Table 126. Input Files table

Column	Description
Alignment Score	For the Align Retention Times (ChromAlign) node, displays the alignment score (0.000 to 1.000).
Creation Date	Displays the acquisition time stamp from the data system.
File Name	Displays the file name of the input file.
Instrument Hardware (hidden)	Displays the hardware version of the Thermo Scientific mass spectrometer or analog detector used to acquire the raw data file.
Instrument Name	Displays the mass spectrometer type used to acquire the raw data file.
Max. Mass [Da]	Displays the maximum mass that the analysis processed.
Min. Mass [Da]	Displays the minimum mass that the analysis processed.
RT Range [min]	Displays the data acquisition time for the raw data file.
Software Revision	Displays the software version of the instrument control software used to acquire the raw data file.
Ref. File ID	For LC studies, this column displays the reference file that the retention time alignment algorithm used.
Sample Type	Displays the sample type.
Study File ID	Displays the file identification number (F#) assigned by the Compound Discoverer application.
Study factor columns	Each study factor column displays the study factor value (item).

Manual Peaks table

Use the Manual Peaks table to view information about the manual peaks that you add to the result file.

The Manual Peaks table is a main table. It is also related to the main Specialized Traces table. To create this table, you must add a manual peak to a specialized trace. See "Manually integrate chromatographic peaks."

Table 127 describes the columns in the Manual Peaks table.

Table 127. Manual Peaks table

Column	Description
Trace Type	Displays the trace type. The trace type can be any of the specialized traces, including Analog, UV, PDA, TIC, BPC, XIC, Pattern Trace, or FISh Trace.
Area	Displays the chromatographic peak area.
Left RT [min]	Displays the start point of the chromatographic peak.
Right RT [min]	Displays the end point of the chromatographic peak.
Study File ID	Displays the study file ID (F#) of the input file.

Merged Features table

Use the Merged Features table to view ion conflicts between the Features and Expected Features tables. Also use the Merged Features table to correlate the chromatographic peaks detected by an analog detector to the chromatographic peaks detected by the mass spectrometer.

The Merge Features Node adds the Merged Features table to the result file. The Merged Features table has the following primary related tables: Expected Compounds, Expected Compounds per File, Compounds, Compounds per File, and Manual Peaks.

Tip When you add the Merge Features node to the processing workflow, the Find Expected Compounds node and the Detect Compounds node automatically connect to it. The Merge Features node consolidates the chromatographic peaks from these two input nodes.

Table 128 describes the columns in the Merged Features table.

Table 128. Merged Features table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Name	Use this column to describe or name the found chromatographic peak. To name the chromatographic peak, type alphanumeric text in the Name table cell.
Apex m/z	Displays the area weighted average mass of all related features. $\frac{\sum m/z \times \text{Area}}{\sum m/z}$
RT [min]	Displays the area weighted average retention time of all related features (same *m/z* × RT dimensions within the specified tolerances). $\frac{\sum \text{RT} \times \text{Area}}{\sum \text{RT}}$
Max. Area	Displays the area of the largest chromatographic peak found in the data set for the current *m/z* × RT dimensions.
Ion Conflict Status	Indicates whether there is a conflict between the Detect Compounds and Find Expected Compounds nodes.
(■) Green	No conflict—Both nodes assigned the same ion to this chromatographic peak.
(■) Orange	Not found by the Detect Compounds node. Indicates that the expected compound might be in doubt because the Detect Compounds node did not detect it.
(■) Gray	Found only by 'Detect Compounds' node or 'Find Expected Compounds' node—Only the stated node found this ion.
(■) Red	Conflicting ions or Multiple ions per node—Either the two nodes assigned different ions or one of the nodes assigned more than one ion to this *m/z* value and retention time.

Table 128. Merged Features table (Sheet 2 of 2)

Column	Description
Detect Compounds	Indicates whether the Detect Compounds node found the current feature in each input file.
(□) Gray	No matches found
(■) Green	Single match found
(■) Orange	Multiple matches found
Find Expected Compounds	Indicates whether the Find Expected Compounds node found the current feature in each input file.
(□) Gray	No matches found
(■) Green	Single match found
(■) Orange	Multiple matches found
Max. Area	Displays the maximum area of all the features from both the Features per File table and the Expected Features table for this compound across the set of input files.
Max. Areas (for each input file)	For each input file, displays the maximum chromatographic peak area for the features with the same *m/z* × RT dimensions (within the specified tolerances) found by the Find Expected Compounds node, the Detect Compounds node, or both nodes.
Note The Differential Analysis node generates these columns: Group Areas, Ratio, and Log2 Fold Change. For information about these columns, see "Differential analysis columns."	
Comments	Use this column to store comments about the current feature (unique *m/z* × RT dimensions). This column accepts alphanumeric text and special characters.

Specialized Traces table

Use the Specialized Traces table to view traces created by the tracer nodes.

The Specialized Traces table lists the specialized traces that you requested in the processing workflow. For information about manually integrating chromatographic peaks in a specialized trace, see "Manually integrate chromatographic peaks."

For information about the Chromatograms view, see "Chromatograms view."

Tip To view a trace in the Chromatograms view, select the trace of interest in the Specialized Traces table.

Table 129 describes the columns in the Specialized Traces table.

Table 129. Specialized Traces table

Column	Description
Checked	Use this column to select the rows that you want to display in the results table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Study File ID	Displays the study file ID (F#) of the input file.
Trace/Detector Type	Displays the trace type generated during data processing. • Create Mass Trace node—TIC, BPC, or XIC • Create Analog Trace node—UV Trace, Total Scan, Spectrum Maximum, *Wavelength–Wavelength*, or Analog trace • Create FISh Trace node—FISh Trace • Create Pattern Trace node—Pattern Trace
Custom Label	Displays the text that you entered in the Custom Label box for the processing workflow node that generated the trace. You can edit the text in this column.
Description	Displays a description of the trace.
Spectrum File	Displays the file name of the raw data file that includes the trace.

Study Information table

Use the Study Information table to review the sample, groups, and ratios information for the set of processed input files.

Table 130 describes the columns in the Study Information table.

Table 130. Study Information table

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Sample	Displays sample identifier.
Study File ID	Displays the study file ID (F#) of the input file. See "Remove input files or update their location."
Sample Identifier	Displays the file name of the raw data file.
File Name	Displays the file name and file extension of the raw data file.
Sample Type	Displays the sample type that you selected for the raw data file.
CF: *study factor columns*	Displays the values of the named study variables.
Sample Group	Displays the sample group.
Replicate Group (hidden)	Displays the replicate groups for biological samples.
Ratios	Displays the ratios that include the raw data file.
Ratios (by Bio. Rep.) (hidden)	Displays the biological replicate ratios that include the raw data file.

Structure Proposals table

Use the Structure Proposals table to store custom structure proposals for the selected compound in the main compounds table (Expected Compounds table or Compounds table) on the result page.

For information about adding structure proposals to the table, see "Add or delete proposed structures for a compound."

Table 131 describes the columns in the Structure Proposals table.

Table 131. Structure Proposals table

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Structure	Displays the structure of the compound. See "Modify the result page layout for ease of use."
Name	Displays an application-generated name or a user-specified name for the compound. To edit this entry, click the table cell and type text in the box.
Formula	Displays the elemental composition formula of the compound.
Molecular Weight	Displays the molecular weight of the compound.
FISh Coverage	Displays the FISh coverage score that is based on the proposed structure. See "FISh scoring for proposed structures."
Comments	Displays an application-generated comment or a user-specified comment for the compound. To edit this entry, click the table cell and type text in the box.

Expected Compounds result tables

For information about the result tables for a targeted workflow with the Find Expected Compounds node, see these topics:

- Expected Compounds table
- Expected Compounds per File table
- Expected Features per File table
- Expected Formulas table
- Related Structures table
- Transformations table

Expected Compounds table

Use the Expected Compounds table to view information about the targeted compounds that the analysis finds. This result table contains all of the expected compounds that the analysis found in the input file set and groups these compound by formula, molecular weight, and retention time (unique formula × MW × RT).

The Group Expected Compounds node adds the Expected Compounds table to the result file.

Table 132 describes most of the columns in the main Compounds table and the first-level related Compounds tables. For information about the differential analysis, descriptive statistics, and quality control columns, see the applicable topic:

- Differential analysis columns

  Note The Differential Analysis node generates the following columns: Group Areas, Group CV[%], Ratio, Log2 Fold Change, P-value, and Adj. P-value.

- Descriptive statistics columns

  Note The Descriptive Statistics node generates the following columns: Min. Area, Q1 Area, Median Area, Q3 Area, Mean Area, Area SD, and Area CV [%].

- QC Correction columns

  Note The QC correction node generates the following columns: #Usable QC, RSD QC Areas [%], RSD Corr. QC Areas [%], and Norm. Area.

Table 132. Expected Compounds table columns in alphabetical order (Sheet 1 of 5)

Column	Node	Description
#Adducts (hidden)	Group Expected Compounds	Displays the number of adduct ions that the analysis found for the expected compound.
#BioCyc Pathways (hidden)	Map to BioCyc Pathways	Displays the number of BioCyc pathways that include the expected compound.
#ChemSpider Results	Search ChemSpider	Displays the number of matching compounds found by the ChemSpider search for the current composition or molecular weight. Use the related ChemSpider Results table to investigate the matching compounds.
#KEGG Pathways (hidden)	Map to KEGG Pathways	Displays the number of KEGG pathways that include the expected compound.
#Metabolika Pathways (hidden)	Map to Metabolika Pathways	Displays the number of Metabolika pathways that include the expected compound.
#mzCloud Results	Search mzCloud Node	Displays the number of matching compounds found by the mzCloud search for this molecular weight. Use the related mzCloud Results table to investigate the matching compounds.
#mzVault Results	Search mzVault	Displays the number of matching compounds found by the mzVault search for this molecular weight. Use the related mzCloud Results table to investigate the matching compounds.
#Spectra with MSn (n>2) Hit	Search mzCloud	Displays the number of spectra with MS level > 2 that match the mzCloud result for this compound. Available when the Search MSn Tree parameter in the Search mzCloud node is set to True. (The default setting in the templates provided with the application is True. The default setting in the Search mzCloud on the Workflow Nodes page is False.)
Annot. Δ Mass [Da] (hidden)	Group Expected Compounds	Displays the difference between the measured (observed in the spectrum) and theoretical molecular weight (calculated from the formula) of the compound in daltons.
Annot. Δ Mass [ppm]	Group Expected Compounds	Displays the difference between the measured (observed in the spectrum) and theoretical molecular weight (calculated from the formula) of the compound in ppm. An orange background indicates that the difference is greater than 5 ppm.

Table 132. Expected Compounds table columns in alphabetical order (Sheet 2 of 5)

Column	Node	Description
Annotation MW (hidden)	Group Expected Compounds	Displays the molecular weight of the assigned formula.
Area (hidden when the analysis includes study groups)	Group Expected Compounds	Displays the area for the compound (Formula × MW × RT) in each sample (input file).
Area (Max.)	Group Expected Compounds	Displays the area of the largest chromatographic peak for the compound (Formula × MW× RT) found in the sample set.
Background (hidden)	Mark Background Compounds	Displays a selected or clear check box that indicates whether the compound was also found in the Blank sample above the user-specified Sample/Blank or Blank/Sample level. • Selected—Indicates that the compound is a background compound. • Clear—Indicates that the compound is not a background compound.
BioCyc Pathways (hidden)	Map to BioCyc Pathways	Indicates the BioCyc pathways where the analysis found the expected compound.
Calc. MW	Group Expected Compounds	Displays the neutral mass, in daltons, retrieved from the leftmost isotopes (typically the monoisotopic isotope) of the related compounds per file table.
Checked	–	Use this column to select the rows that you want to display in the results table and in reports after you apply result filters.
Composition Change	Group Expected Compounds	Displays the composition change caused by any dealkylation or dearylation reaction, any of the user-specified transformation reactions, or both.
Dealkylated	Group Expected Compounds	When this column contains an X, the expected compound is the product of a dealkylation reaction.
FISh Coverage	FISh Scoring	Displays the FISh coverage score from the FISh Scoring node. See "FISh scoring for proposed structures."
Formula	Group Expected Compounds	Displays the elemental formula of the parent compound and the theoretical formulas for the dealkylation and transformation products.
Gap Status (hidden)	Group Expected Compounds	Indicates the gap status for the compound: (▢) Gray—Full Gap (■) Green—No Gap

Table 132. Expected Compounds table columns in alphabetical order (Sheet 3 of 5)

Column	Node	Description
Group Areas	Group Expected Compound	Displays the median chromatographic peak area for the compound in each study group. Available if the analysis included study groups.
KEGG Pathways (hidden)	Map to KEGG Pathways	Indicates the KEGG pathways where the analysis found the expected compound.
Mass List Matches	Search Mass Lists	Indicates the mass lists where the analysis found the expected compound. • (▢) Gray—No matches found • (▢) Green—Single match found • (▢) Orange—Multiple matches found
Metabolika Pathways (hidden)	Map to Metabolika Pathways	Indicates the Metabolika Pathways where the analysis found the expected compound.
MS Depth (hidden)	Group Expected Compounds	Displays the depth of the available MSn data for the compound. When the MS2 scans are not from an Identification Only sample, you can view them by selecting the rows for the compound in its related Expected Features table.
MS2	Group Expected Compounds	Indicates whether the analysis found data-dependent fragmentation scans for the compound. • (▢) Red—No MSn—There are no available MSn scans. • (▢) Green—ddMS2 for preferred ion—There is at least one data-dependent MS2 scan for the preferred adduct ion. • (▢) Blue—ddMS2 for other ion—There is at least one data-dependent MS2 scan, but the scans are not for the preferred adduct ion. • (▢)Orange—DIA only—Only data-independent [all ions fragmentation (AIF)] scans are available.
mzCloud Best Match	Search mzCloud	Displays the score for the best hit from the mzCloud mass spectrum database.
mzCloud Best Match Confidence	Search mzCloud	Displays the confidence value for the best hit from the mzCloud mass spectrum database. The confidence values addresses whether comparison spectra have enough spectral peaks to make a confident match.

Table 132. Expected Compounds table columns in alphabetical order (Sheet 4 of 5)

Column	Node	Description
mzCloud Best Sim. Match	Search mzCloud	Displays the best similarity match of the mzCloud results found for this compound. Available when you select a Similarity Search in the Search mzCloud node. By default, the Similarity Search parameter is set None in the node. The setting for this parameter varies in the various templates provided with the application. In the metabolomics templates, the Similarity Search is set to Confidence forward.
mzCloud Best Tree Match	Search mzCloud	Displays the best tree match in the mzCloud results found for this compound considering all the submitted spectra with MS level ≥ 2. Available when Search MSn Tree you set Search MSn Tree to True. 'mzCloud Best Tree Match' and '# Spectra with MSn (n>2) Hit' columns will be available when Search MSn Tree is set to 'True' in the Search mzCloud node
mzCloud Library Matches (hidden)	Search mzCloud	Indicates whether the search found matches in the selected libraries. • (▢) Gray—No matches found • (▢) Green—Single match found • (▢)Orange—Multiple matches found
mzVault Best Match	Search mzVault	Displays the score for the best hit from the mzVault mass spectrum library.
Name	Group Expected Compounds	Displays the user-specified compound name. To populate this cell, you can type a name or use the Edit Compound Annotation command.
Parent Compound	Group Expected Compounds	Displays the targeted compound.
For more information about the peak quality factors and the color-coded table cells, see "Chromatographic peak rating filter."		
Peak Rating	Group Expected Compounds	Displays the calculated peak rating for the compound.
PQF: FWHM2Base	Group Expected Compounds	Displays the calculated peak quality factor for the compound's chromatographic peak.
PQF: Jaggedness	Group Expected Compounds	Displays the calculated value for the jaggedness of the compound's chromatographic peak.

Table 132. Expected Compounds table columns in alphabetical order (Sheet 5 of 5)

Column	Node	Description
PQF: Modality	Group Expected Compounds	Displays the calculated value for the modality of the compound's chromatographic peak.
PQF: Zig-Zag Index	Group Expected Compounds	Displays the calculated value for the zig-zag index of the compound's chromatographic peak.
Reference Ion	Group Expected Compounds	Displays the most common ion for the expected compound across the input files.
RT [min]	Group Expected Compounds	Displays the weighted average of the retention times for the chromatographic peak in the input files.
RT Tolerance [min] (hidden)	Group Expected Compounds	Displays the retention time tolerance setting in the Group Expected Compounds node.
Structure (hidden)	–	Displays the structure of the compound from a custom annotation.
Tags	–	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Transformations	Group Expected Compounds	Displays the chemical transformation for the expected compounds that have undergone any of the user-specified transformations.

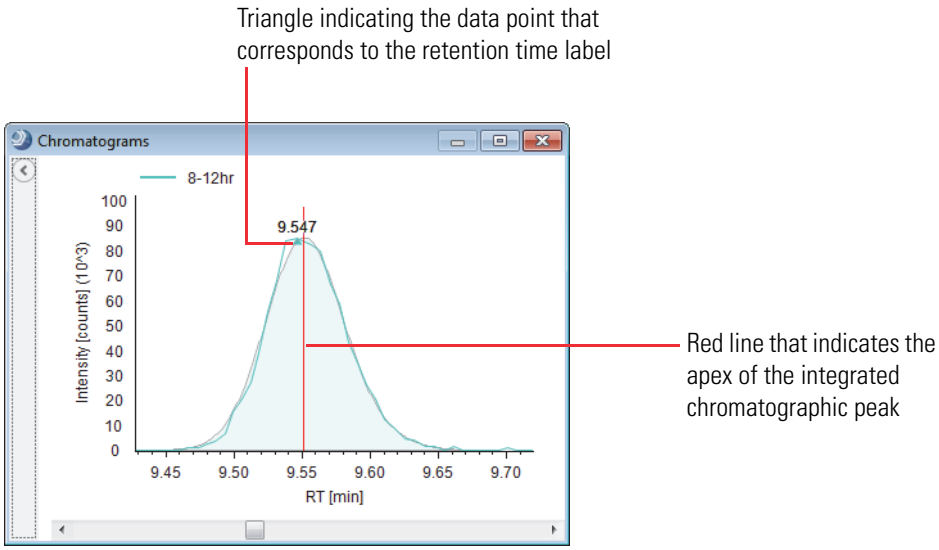
Expected Compounds per File table

Use the Expected Compounds per File table to review the expected compounds found in each input file. The uniqueness for each row is defined by the following expression:

Parent Compound × Formula × MW × Dealkylations and Transformations × RT

Clicking a row in the Expected Compounds per File table displays an XIC trace for the selected compound. The XIC trace is a summation of the related ion traces. The integrated peak area is shaded, the vertical red line indicates the chromatographic peak apex, and the triangle indicates the data point that corresponds to the retention time (RT) label. When the data has been chromatographically aligned (by using the Align Retention Times node), the RT values for the labeled data points might differ slightly from those for the closest MS1 scan in the spectral tree.

Figure 146. Expected compound trace for a single input file



The Find Expected Compounds node creates the Expected Compounds per File table. The primary tables related to this table are as follows: Expected Compounds, Input Files, Expected Formulas, Merged Features, Expected Features, and Related Structures.

Table 133 describes the columns in the Expected Compound per File table. By default, some of these columns are hidden.

Table 133. Expected Compounds per File table (Sheet 1 of 3)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Parent Compound	Displays the user-specified parent compound or compounds. You specify the parent compound or compounds in the Generate Expected Compounds node or nodes.
Formula	Displays the elemental formula of the expected compound.
Calc. MW	Displays the calculated molecular weight (MW) of the expected compound.
Dealkylated	Displays an X when the parent compound has undergone a dealkylation reaction.
Transformations	Displays the chemical transformations for the expected compound.

Table 133. Expected Compounds per File table (Sheet 2 of 3)

Column	Description
Composition Change	Displays the composition change caused by a dealkylation reaction, any of the user-specified transformation reactions, or both.
RT [min]	Displays the apex retention time (in minutes) of the largest chromatographic peak that the node found for the expected compound. The chromatographic peak is a composite peak of all of the ionic species (adduct ions) that the analysis found for the expected compound. The chromatographic peak area is the summed area of the adduct peaks.
FWHM [min]	Displays the width of the chromatographic peak at its half-height. Use this value to determine the best RT tolerance for peak grouping.
Best SFit [%]	Displays the best spectral fit value for the set of expected compound ions for the expected compound. The spectral fit value increases as the number of matching isotopes increases.
Best SD (hidden)	Displays the best spectral distance value between the theoretical and measured isotope pattern.
Max. #MI	Displays the maximum number of matching isotopes for any of the expected compound ions.
#Adducts	Displays the number of detected adducts. The analysis detects only the adduct ions that you specified for the Ions parameter in the Generate Expected Compounds node. With the default setting of [M+H]+1 only, the application finds only this one adduct ion species for each compound.
Area	Displays the summed chromatographic peak area for all of the expected compound ions (adducts) that make up the chromatographic peak. To display the table of expected compound ions for the expected compound, show the related tables and click the **Expected Features** tab.
Parent Area [%]	Displays the area of the selected component (Parent Compound × Formula × MW × Dealkylations and Transformations × RT) as a percentage of the total chromatographic peak area for the related components (Parent Compound × Formula × MW × Dealkylations and Transformations).

Table 133. Expected Compounds per File table (Sheet 3 of 3)

Column	Description
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID (F#) of the input file. You can filter the data by using this integer; for example, the following filter reduces the table to the expected compounds found in one input file: Study File ID is equal to F1, F2, F3...F11, and so on.

Expected Features per File table

Use the Expected Features per File table to review the expected features (chromatographic peaks with the same *m/z* × RT dimensions) that the analysis found for a compound in a specific input file.

The Find Expected Compounds node creates the Expected Features per File table.

Table 134 describes the columns in the Expected Features per File table.

Table 134. Expected Features per File table (Sheet 1 of 3)

Column	Description
#MI	Displays the number of matched isotopes for the ion.
Area	Displays the summed area of all the related peaks (same expected compound) in the current input file.
Charge	Displays the charge of the ion.
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
File ID (hidden)	Displays the integer that the application assigned to the input file.
FWHM [min]	Displays the width of the chromatographic peak at its half-height in minutes.
Intensity (hidden)	Displays the maximum intensity of all the related peaks per input file.
Ion	Displays the ionized form of the compound.
m/z	Displays the mass-to-charge ratio of the ion.
Molecular Weight	Displays the molecular weight of the monoisotopic neutral compound.

Table 134. Expected Features per File table (Sheet 2 of 3)

Column	Description
Parent Area [%]	Displays the chromatographic peak area of the current ion as a percentage of the total chromatographic peak area at the current retention time (within the specified tolerance) for the expected compound selected in the Expected Compounds per File table
For information about the peak quality factors, see "Peak quality factors."	
PQF: FWHM2B	Displays the calculated peak quality factor for the ratio of the peak width a half the maximum peak height versus the peak width at the base of the expected compound's chromatographic peak.
PQF: J	Displays the calculated peak quality factor for the jaggedness of the expected compound's chromatographic peak.
PQF: M	Displays the calculated peak quality factor for modality of the expected compound's chromatographic peak.
PQF: ZZI	Displays the calculated peak quality factor for the zigzag index of the expected compound's chromatographic peak.
PQFs Pass Thresholds	The settings for the PQF thresholds depend on the processing workflow. When the processing workflow includes only a targeted analysis, the PQF thresholds are hard-coded. The hard-coded values are as follows: • PQF:J (Jaggedness) ≤ 0.4 • PQF: ZZI (Zig-Zag Index) ≤ 0.25 • PQF: M (Modality) ≤ 0.9 When the processing workflow includes an untargeted analysis, the targeted analysis uses the user-specified thresholds in the Detect Compounds node.
RT [min]	Displays the chromatographic retention time of the ion.
SD (hidden)	Displays the spectral distance score.
SFit [%]	Displays the similarity score between the theoretical and measured isotope patterns as a percentage.
Study File ID	Displays the study file ID (F#) of the input file.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.

Table 134. Expected Features per File table (Sheet 3 of 3)

Column	Description
ΔMass [Da]	Displays the mass difference, in daltons, between the theoretical mass of the ion and the measured mass.
ΔMass [ppm]	Displays the mass difference, in ppm, between the theoretical mass of the ion and the measured mass.

Expected Formulas table

Use the Expected Formulas table to review the chemical formulas that the analysis found across the input file set. This table lists the theoretical compounds that the Generate Expected Compounds nodes predict by evaluating the effect of the user-specified dealkylation, dearylation, and transformation reactions on the user-specified parent compounds.

Clicking a row in the Expected Formulas table displays overlaid XIC traces for the selected expected compound, with one XIC trace for each input file where the compound is detected. Each XIC trace is a summation of the ion traces for the same neutral elemental composition (same molecular weight). By default, the Chromatograms view zooms in on the *x*-axis range of the detected peaks for the same expected compound.

The Find Expected Compounds Node creates the Expected Formulas table, which has the following primary related tables: Expected Compounds, Input Files, Expected Compounds per File, Related Structures, and Transformations.

For information about targeted processing workflows, see "Targeted processing workflows for expected compounds."

Table 135 describes the columns in the Expected Formulas table.

Table 135. Expected Formulas table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the results table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Order (related table)	When you select the Expected Formulas table that is related to the Transformations table, this column displays the order of the selected transformation.

Table 135. Expected Formulas table (Sheet 2 of 2)

Column	Description
Parent Compound	Displays the targeted compound.
Formula	Displays the elemental formula of the parent compounds and the theoretical formulas for the dealkylation and transformation products.
Molecular Weight	Displays the molecular weight (MW) of the expected compound. Expected compounds include the parent compounds and their theoretical dealkylation and transformation products.
Dealkylated	When this column contains an X, the expected compound is the product of a dealkylation reaction.
Transformations	Displays the chemical transformation for the expected compounds that have undergone any of the user-specified transformations.
Composition Change	Displays the composition change caused by any dealkylation or dearylation reaction, any of the user-specified transformation reactions, or both.
Area (Max.)	Displays the maximum summed chromatographic peak area for the expected formula in one of the input files. • When the result file contains data from only one input file, this area matches the summed chromatographic peak area for the expected formula. • When the result file contains data from more than one input file, this area comes from the input file with the largest summed chromatographic peak area for the expected formula.

Related Structures table

There is a Related Structures table for each feature in the Expected Features table and each compound in the Expected Compounds per File table. The Related Structures table shows the structure of the product compound generated by the dealkylation reaction.

❖ To open the Related Structures table

1. Open a result file from a targeted analysis (Find Expected Compounds node).
2. Select a row in one of these tables—Expected Features or Expected Compounds per File.
3. Click **Show Related Tables**.
4. Click the **Related Structures** tab.

Table 136 describes the columns in the Related Structures table.

Table 136. Related Structures table

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Parent Compound	Displays the user-specified parent compound or compounds.
Formula	Displays the chemical formula of the parent compound or the theoretical transformed compounds.
Molecular Weight	Displays the molecular weight (MW) of the parent compound or theoretical reaction product.
Dealkylated	Displays an X when the parent compound has undergone a dealkylation reaction.
Composition Change	Displays the composition change caused by any dealkylation reaction.
Structure	When a compound is the result of transformations that include a dealkylation step, this column displays the product of the dealkylation step. Otherwise, this column displays the structure of the parent compound.

Transformations table

Use the Transformations table to review the transformations for each formula in the Expected Formulas table.

Table 137 describes the columns in the Transformations table.

Table 137. Transformations table

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Name	Displays the name of the transformation.
Phase	Displays the Phase assignment for the transformation.
Leaving Group	Displays the leaving group for the transformation.
Arriving Group	Displays the arriving group for the transformation.
ΔMass [Da]	Displays the neutral mass shift for the transformation in daltons.
Order	Displays when the transformation was applied in the reaction pathway. Range: An integer from 1 to the user-specified maximum number of steps.

Compound detection result tables

For information about the result tables for the untargeted compound detection nodes (for LC/MS/MS data), see these topics, listed in alphabetical order:

- Compounds table (LC studies)
- Compounds per File table
- Features per File table
- Filled Gaps table
- Labeled Features table
- Labeled Compounds per File table
- Similar Compounds Related table

Compounds table (LC studies)

Use the Compounds table to review the unknown compounds found across the input file set.

The Group Compounds node creates the Compounds table.

Tip For information using the shortcut menu commands for the Compounds table, see "Shortcut menu commands for the result tables."

Tip Clicking a row in the Compounds table displays XIC traces for the selected unknown compound, with one XIC trace for each input file. Each XIC trace is the summation of all the related ion traces. The summed XIC trace is made up of the data points with the highest intensity at each time point.

To view the adduct ion traces for a compound detected in a specific input file, do the following:

1. Select the compound in the Compounds table.
2. In the first set of related tables for the selected compound, select the input file in the Compounds per File table.
3. In the second set of related tables (for the compound detected in the selected input file), open the Features table and select the adduct ion of interest.

Table 138 describes most of the columns in the main Compounds table and the first level related Compounds tables. For information about the differential analysis, descriptive statistics, and quality control columns, see the applicable topic:

- Differential analysis columns

  Note The Differential Analysis node generates the following columns: Group Areas, Group CV[%], Ratio, Log2 Fold Change, P-value, and Adj. P-value.

- Descriptive statistics columns

  Note The Descriptive Statistics node generates the following columns: Min. Area, Q1 Area, Median Area, Q3 Area, Mean Area, Area SD, and Area CV [%].

- QC Correction columns

  Note The QC correction node generates the following columns: #Usable QC, RSD QC Areas [%], RSD Corr. QC Areas [%], and Norm. Area.

Table 138. Compounds table columns listed in alphabetical order (Sheet 1 of 10)

Column	Node	Description
Symbol = first character		
#Adducts (hidden)	Group Compounds	Displays the number of adduct ions that the analysis found for the compound.
#BioCyc Pathways (hidden)	Map to BioCyc Pathways	Displays the number of BioCyc pathways that include the current compound.
#ChemSpider Results	Search ChemSpider	Displays the number of matching compounds found by the ChemSpider search for the current composition or molecular weight. Use the related ChemSpider Results table to investigate the matching compounds.
#KEGG Pathways (hidden)	Map to KEGG Pathways	Displays the number of KEGG pathways that include the current compound.
#Metabolika Pathways (hidden)	Map to Metabolika Pathways	Displays the number of Metabolika pathways that include the current compound.
#mzCloud Results	Search mzCloud Node	Displays the number of matching compounds found by the mzCloud search for the calculated molecular weight. Use the related mzCloud Results table to investigate the matching compounds.

Table 138. Compounds table columns listed in alphabetical order (Sheet 2 of 10)

Column	Node	Description
#mzVault Results	Search mzVault	Displays the number of matching compounds found by the mzVault search for this molecular weight. Use the related mzCloud Results table to investigate the matching compounds.
#Similarity Results (hidden)	Apply mzLogic	Displays the number of similarity results from the Apply mzLogic node.
#Spectra with MSn (n>2) Hit	Search mzCloud	Displays the number of spectra with MS level > 2 that match the mzCloud result for this compound. Available when the Search MSn Tree parameter in the Search mzCloud node is set to True. (The default setting in the templates provided with the application is True. The default setting in the Search mzCloud on the Workflow Nodes page is False.)
# Usable QC	Apply QC Correction	Displays the number of usable QC samples.
Annotation Source	Assign Compound Annotations	Indicates the match status for the selected compound from the search nodes in the processing workflow. The expanded column heading displays the annotation sources. The Assign Compound Annotations node determines the validity of the annotations from the Predict Compositions node and the search nodes in the processing workflow. Possible states for each annotation source: • (■) Green—Full Match—The current formula and structure annotations match the best available item from the particular source (online database or local mass list). • (■) Gray—No Results—Retrieved no data from the particular source. • (■) Orange—Not the Top Hit—Current compound annotation matches one of the hits, but not the top one. • (■) Orange—Partial Match—Only the formula for the current compound annotation matches the items retrieved from the particular source. • (■) Orange—Unused—Retrieved items from the particular source, but did not assign any annotations. • (■) Red—Invalid mass—The best available item from the particular source has a molecular weight that does not match the molecular weight of the compound within the specified mass tolerance. • (■) Red—No match—The particular source does not have an item that matches the current annotations for the compound.

Table 138. Compounds table columns listed in alphabetical order (Sheet 3 of 10)

Column	Node	Description
Annot. ΔMass [Da] (hidden)	Assign Compound Annotations	Displays the mass difference in daltons between the experimental mass and the annotated mass.
Annot. ΔMass [ppm}	Assign Compound Annotations	Displays the mass difference in ppm between the experimental mass and the annotated mass.
Annotation MW (hidden)	Assign Compound Annotations	Displays the molecular weight of the matched compound from the specified annotation source.
Area (one subcolumn for each input file) (hidden if the analysis includes study groups)	Group Compounds	Displays an area column for each input file. To display the areas for each input file, click the expand icon to the right of the column name.
Area (Max.)	Group Compounds	Displays the maximum chromatographic peak area from all of the input files for compounds with the same retention time and molecular weight (within the user-specified RT and mass tolerances).
Avg. Exchange	Analyze Labeled Compounds	Average number of atoms exchanged for compound detected in input file.
Background (hidden)	Mark Background Compounds	Displays a selected or clear check box that indicates whether the compound was also found in the Blank sample above the user-specified Sample/Blank or Blank/Sample level. • Selected—Indicates that the compound is a background compound. • Clear—Indicates that the compound is not a background compound.
BioCyc Pathways (hidden)	Map to BioCyc Pathways	Displays whether the current compound is present in the named pathway. To display the pathway names, click the expand icon to the right of the column name.
Calc. MW	Group Compounds	Displays the calculated molecular weight of the neutral compound.
Checked	Group Compounds	Selecting this check box specifies that the compound is a selected item.

Table 138. Compounds table columns listed in alphabetical order (Sheet 4 of 10)

Column	Node	Description
Class Coverage	Compound Class Scoring	Displays the class coverage score for the compound by individual compound classes. Expand the header to display the names of the compound class libraries. Color-coded cells: • Light green to dark green for values from 0.00 to 100.00 or gray • Gray / N/A means no MS2 spectra are available for the compound or there are 0 matched and 0 unmatched centroids in the MS2 spectra. At a value of 0.00, the node found no fragment structures or *m/z* values in common with items in the compound class library. At a value of 100%, the compound matches all the items in the compound class library. Scores range from 0.00 to 100.00
FISh Coverage (hidden)	N/A	Displays the FISh Coverage score for a custom annotation.
Formula	Assign Compound Annotations	Displays the predicted chemical formula for the neutral compound. For the analysis to predict and display a chemical formula for all compounds in the table, the processing workflow must include the Predict Compositions node and the Assign Compound Annotations node. When the processing workflow includes any of the search nodes, the Assign Compound Annotations node assigns the formula by using the specified priority for the data sources. The default priority for the data sources is (1) mzCloud Search, (2) Predicted Compositions, (3) Mass List Match, (4) ChemSpider Search.
You can use the Fill Gaps node or the Apply Missing Value Imputation node to fill gaps for missing chromatographic peaks. Both nodes generate a Gap Fill Status column and a Gap Status column; however, the indicators and tooltip descriptions for the two nodes differ.		
Gap Fill Status (hidden)	Fill Gaps	Indicates whether and how the analysis filled the gap. (■) Green—No Gap to Fill. (■) Blue—The analysis filled the gap in one of three ways: Filled by Spectrum Noise, Filled by Simulated Peak, or Filled by Trace Area.

Table 138. Compounds table columns listed in alphabetical order (Sheet 5 of 10)

Column	Node	Description
Gap Status (hidden)	Fill Gaps	Indicates whether chromatographic peak for the compound was completely missing or whether some of the user-specified ions were not detected. (■) Purple—Missing Ions—Indicates some missing ions (but not a full gap). (■) Gray—Full Gap—Indicates a full gap. (■) Green—No Gap—Indicates a compound without any gap.
Gap Fill Status (hidden)	Apply Missing Value Imputation	Indicates whether and how the analysis filled the gap. (■) Green—No Gap to Fill. (■) Orange—The analysis filled the gap in one of three ways: Imputed by Group Median, Imputed by Low Area Value, or Imputed by Random Forest.
Gap Status (hidden)	Apply Missing Value Imputation	Indicates whether chromatographic peak for the compound was missing. (■) Gray—Indicates a full gap. (■) Green—No Gap—Indicates a compound without any gap.
KEGG Pathways (hidden)	Map to KEGG Pathways	Displays whether the current compound is present in the named KEGG pathway. To display the pathway names, click the expand icon to the right of the column name.

Table 138. Compounds table columns listed in alphabetical order (Sheet 6 of 10)

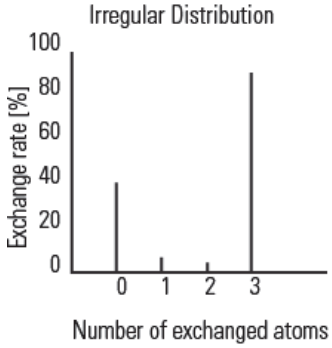
Column	Node	Description
Labeling Status (per file)	Analyze Labeled Compounds	The Analyze Labeled Compounds Node evaluates the measured isotope pattern versus the fitted isotope pattern (for the expected isotopologues) to determine the presence of contaminating masses. It also evaluates the distribution of the measured exchange rates for the expected isotopologues. These flags indicate the following states: • (■) Red—Contaminating Mass—The average exchange for the unlabeled sample is above the 0.1 threshold. • (■) Orange—Low Pattern Fit—The measured pattern significantly differs from the fitted pattern. The SFit value is below the threshold of 20%, the Fitted Coverage value is below the threshold of 60%, or the Measured Coverage value is below threshold of 60%. To review these values, see the "Labeled Features table." • (■) Blue—Irregular Exchange—The isotopologue exchange rates are discontinuous; for example, there is a significant valley in the exchange rates profile. This might indicate an incorrect analysis or a special type of kinetics. However, when this is the typical behavior expected for your experiments, consider changing the setting for Mark Irregular Exchanges in the Analyze Labeled Compounds node to False.  • (■) Green—No Warnings—The measured isotope patterns and the exchange rates are within acceptable limits. • (■) Gray—Compound was not detected in this sample.
Mass Defect	Calculate Mass Defect	Displays the calculated mass defect for the compound.

Table 138. Compounds table columns listed in alphabetical order (Sheet 7 of 10)

Column	Node	Description
Mass List Matches	Search Mass Lists	Indicates the match status for each mass list. • (■) Green—Single match found • (■) Orange—Multiple matches found • (■) Gray—No matches found Use the related Mass List Search Results table to investigate the matching compounds.
Metabolika Pathways (hidden)	Map to Metabolika Pathways	Displays whether the current compound is present in the named Metabolika pathways. To display the pathway names, click the expand icon to the right of the column name.
m/z	Group Compounds	Displays the *m/z* value of the leftmost isotope peak of the most common adduct ion of for this compound across the input files (area-weighted average)
MS Depth (hidden)	Group Compounds	Displays the maximum depth of the mass spectral tree that the analysis assigned to the compound. This column is not available when the input files do not have any fragmentation scans.
MS2	Group Compounds	Displays whether the analysis found data-dependent fragmentation scans for the compound. • (■) Red—No MSn—There are no available MSn scans. • (■) Green—ddMS2 for preferred ion—There is at least one data-dependent MS2 scan for the preferred adduct ion. • (■) Blue—ddMS2 for other ion—There is at least one data-dependent MS2 scan, but the scans are not for the preferred adduct ion. • (■) Orange—DIA only—Only data-independent [all ions fragmentation (AIF)] scans are available.
mzCloud Best Match	Search mzCloud	Displays the best match score (from 0 to 100) from the mzCloud identity search for the compound. Use the related mzCloud Results table to investigate the matching compounds.
mzCloud Best Match Confidence	Search mzCloud	Displays the confidence of the best match mzCloud result found for this compound.

Table 138. Compounds table columns listed in alphabetical order (Sheet 8 of 10)

Column	Node	Description
mzCloud Best Sim Match	Search mzCloud	Displays the best similarity score from the mzCloud similarity search for the compound. Available when the Similarity Search parameter for the Search mzCloud node is set to Similarity Forward or Similarity Reverse. Use the related mzCloud Results table to investigate the matching compounds.
mzCloud Best Tree Match	Search mzCloud	Displays the best tree match in the mzCloud results found for this compound considering all the submitted spectra with MS level ≥ 2.
mzCloud Library Matches (hidden)	Search mzCloud	Indicates the match status for the compound in the selected mzCloud databases. Possible states for each database: • (■) Green—Single match found • (■) Gray—No matches found • (■) Red—Multiple matches found
mzVault Best Match	Search mzVault	Displays the best match score from the mzVault identity search for the compound. Use the related mzVault Results table to investigate the matching compounds.
Name	Group Compounds	When the processing workflow includes a search node, this column displays the compound name from the best match in the searched databases.
Norm. Areas	Normalize Areas	Displays the normalized peak areas for the compound in each input file.
Pattern Matches	Pattern Scoring	Displays a filled rectangle when the compound matches the specified isotope pattern. The color of the filled rectangle has no specific meaning. Use the related Matched Patterns table to investigate the matched isotope pattern.
Peak Rating	Group Compounds	Displays the calculated peak rating for the compound.
PQF: FWHM2Base	Group Compounds	Displays the calculated peak quality factor for the ratio of the peak width a half the maximum peak height versus the peak width at the base of the detected compound's chromatographic peak.
PQF: Jaggedness	Group Compounds	Displays the calculated peak quality factor for the jaggedness of the detected compound's chromatographic peak.

Table 138. Compounds table columns listed in alphabetical order (Sheet 9 of 10)

Column	Node	Description
PQF: Modality	Group Compounds	Displays the calculated peak quality factor for modality of the detected compound's chromatographic peak.
PQF: Zig-Zag Index	Group Compounds	Displays the calculated peak quality factor for the zig-zag index of the detected compound's chromatographic peak.
QC Fill Status (hidden)	Apply QC Correction	Indicates the status for each QC sample. Possible states: • (■) Green—Filled by re-detected peak • (■) Gray—N/A • (■) Orange—Filled by matching ion • (■) Blue—Filled by simulated peak
Rel. Exchange [%]	Analyze Labeled Compounds	Average exchange relative to the maximum exchange rate. 100 × Average Exchange/Max. Exchange
Reference Ion	Group Compounds	Displays the most common adduct ion for this compound across the input files
RT [min]	Group Compounds	Displays the retention time of the chromatographic peak for the compound.
RT Tolerance [min] (hidden)	Group Compounds	Displays the retention time tolerance specified in the Group Compounds node.
Structure (hidden)	Group Compounds or structure proposal	Displays the structure of the compound. The structure field is populated, the searches return a structure, or you edit the annotations.
Tags	–	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
The following three columns appear in the related Compounds table for the main KEGG Pathways table. Each column contains an ordered list for the same KEGG compounds—that is, the first item in the KEGG Compound IDs column corresponds to the first item in the KEGG Compound Names column and the first item in the KEGG Compound Formula column, and so on.		
KEGG Compound IDs	Map to KEGG Pathways	Displays a list of the KEGG compound IDs in ascending order from left to right.
KEGG Compound Names	Map to KEGG Pathways	Displays a list of the KEGG compound names.
KEGG Compound Formulas	Map to KEGG Pathways	Displays a list of the KEGG compound formulas.

Table 138. Compounds table columns listed in alphabetical order (Sheet 10 of 10)

Column	Node	Description
The following two columns appear in the related Compounds table for the main KEGG Pathways table and the search results tables.		
Max. ΔMass [Da]		Displays the maximum mass difference between the measured mass for the compound in the Compounds table and the theoretical mass of the compound, in daltons.
Max. ΔMass [ppm]		Displays the maximum mass difference between the measured mass for the compound in the Compounds table and the theoretical mass of the compound, in parts per million.
This column appears in related Compounds table for the main mzCloud Search Result table.		
Scan Number	Search mzCloud	Displays the scan number of the scan that matches the reference scan in the mzCloud database.
This column appears in the related Compounds table for the main mzVault Results table.		
ΔRT [min]	Search mzVault	Displays the difference between the measured retention time of the compound and the retention time of the mzVault library entry in minute.

Compounds per File table

Use the Compounds per File table to review the compounds detected in each input file.

Table 139 describes the columns in the Compounds per File table.

Table 139. Compounds per File table (Sheet 1 of 2)

Column	Description
#Adducts	Displays the number of adduct ions.
Area (All Ions) (hidden)	Displays the chromatographic peak area in counts * minutes for the summed peaks of all the adduct ions in this input file.
Area (Reference Ion)	Displays the chromatographic peak area in counts * minutes in the XIC trace for the most common adduct ion across the input files.
Calc. MW	Displays the calculated molecular weight of the neutral compound.
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters. Clear: False or Selected: True
File ID (hidden)	Displays the study file ID.

Table 139. Compounds per File table (Sheet 2 of 2)

Column	Description
FWHM [min]	Displays the width of the chromatographic peak at its half-height. Use this value to determine the best RT tolerance for peak grouping.
Intensity (Max.) (hidden)	Displays the chromatographic peak height at the apex in intensity counts.
Max #MI	Displays the number of matching isotope peaks.
Reference Ion	Displays the ion definition of the reference ion.
RT [min]	Displays the retention time at the chromatographic peak apex for the reference ion (displayed in the Reference Ion column) in this input file.
Study File ID (hidden)	Displays the study file ID.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.

Related Topics

- Shortcut menu commands for the result tables
- Show or hide table columns

Features per File table

Use the Features per File table to review the features detected in the input files.

The Detect Compounds Node adds the Features per File table to the result file.

Table 140 describes the columns in the Features per File table.

Table 140. Features per File table (Sheet 1 of 3)

Column	Description
# Good Peaks (hidden)	Number of chromatograms peaks (one or more for each isotopic ion for the feature) that pass the peak quality factor thresholds specified in the Detect Compounds node under Isotope Pattern Detection.
#MI	Displays the number of matching isotopes for the unknown compound ion.
# Poor Peaks (hidden)	Displays the number of chromatographic peaks that do not pass the peak quality factor thresholds specified in the Detect Compounds node under Isotope Pattern Detection.

Table 140. Features per File table (Sheet 2 of 3)

Column	Description
Area	Displays the area of the reference isotopic chromatographic peak for this feature in this input file.
Charge	Displays the charge on the ion.
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
File ID	Displays the integer that the application assigned to the input file.
FWHM [min]	Displays the peak width at its half-height in minutes.
Intensity (hidden)	Displays the intensity of the ion.
Ion	Displays the ion definition of the molecular ion adduct.
m/z	Displays the mass-to-charge ratio of the ion.
Molecular Weight	Displays the neutral mass of the unknown ion based on the measured *m/z* value (in daltons).
Parent Area [%]	Displays the chromatographic peak area of the current peak as a percentage of the total chromatographic peak area for the parent compound (which is the compound selected in the Compounds per File table) per input file.
PQF: FWHM2B	Displays the calculated peak quality factor for the ratio of the peak width a half the maximum peak height versus the peak width at the base of the detected feature's chromatographic peak.
PQF: Jaggedness	Displays the calculated peak quality factor for the jaggedness of the detected feature's chromatographic peak.
PQF: Modality	Displays the calculated peak quality factor for modality of the detected feature's chromatographic peak.
PQF: Zig-Zag Index	Displays the calculated peak quality factor for the zig-zag index of the detected feature's chromatographic peak.
Processing Node No (hidden)	Displays the number of the workflow node in the processing workflow. These numbers are hidden in the Workflow Tree area on the Workflows page of an analysis if you kept the default selection of Hide Node Numbers on the Workflow Editor Settings view of the Configuration page.

Table 140. Features per File table (Sheet 3 of 3)

Column	Description
Ref. Isotope Idx (hidden)	Displays the isotope index of the reference peak (most intense isotope) that the analysis used to create the XIC trace and report the chromatographic peak area for this feature. The isotope index is 0, 1, 2, and so on where 0 equals the A0 isotope in the isotope pattern. Available when the Use Most Intense Isotope parameter is set to True in the Detect Compounds node.
Ref. m/z (hidden)	Displays the mass of the reference peak (*m/z* value of the most intense isotope) used to create the XIC trace and report the chromatographic peak area for this feature. Available when the Use Most Intense Isotope Only parameter is set to True.
RT [min]	Displays the retention time in minutes of the chromatographic peak that contains the unknown compound ion.
Study File ID	Displays the study file ID (F#) of the input file.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.

Filled Gaps table

For LC studies, use the Filled Gaps table to review the chromatographic peaks (Full Gap or Missing Ion) that the Fill Gaps node finds. The Filled Gaps table is a related table for the compound that you select in the Compounds table.

By default, the Filled Gaps table is hidden. To display the table, click the **Select Table Visibility** icon, , select the **Filled Gaps** check box, and click **OK**.

Table 141 describes the columns in the Filled Gaps table.

Table 141. Filled Gaps table (Sheet 1 of 3)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Ion Description	Displays a description of the adduct where M is the neutral compound.
Charge	Displays the charge of the ion.

Table 141. Filled Gaps table (Sheet 2 of 3)

Column	Description
Exp. m/z	Displays the *m/z* value for the adduct ion found in the other input files. This value is based on the adduct type and the compound's molecular weight.
Exp. RT [min]	Displays the average retention time of the adduct ion found in the other input files.
Exp. Left RT [min]	Displays the average peak start time of the detected chromatographic peaks for the adduct ion in all the input files included in the analysis.
Exp. Right RT [min]	Displays the average peak end time of the detected chromatographic peaks for the adduct ion in all the input files included in the analysis.
Exp. FWHM [min]	Displays the average peak width at the peak's half height (full width at half maximum) for the adduct ion in all the input files included in the analysis.
Area	Displays the area of the chromatographic peak found by the Fill Gaps node.
Fill Status	Indicates the gap status for the chromatographic peak detected or redrawn by the Fill Gaps node are as follows: • (■) Green (Filled by Re-detected Peak)—The chromatographic peak was detected with the PPD algorithm (set to a lower threshold than in the Detect Compounds node). • (■) Green (Filled by Matching Ion)—The gap was replaced with a chromatographic peak for a matching ion. • (■) Blue (Filled by Spectrum Noise)—The gap was replaced with a chromatographic peak based on the spectrum noise level. • (■) Blue (Filled by Simulated Peak)—The gap was replaced with a chromatographic peak that was simulated with a Gaussian fit algorithm. • (■) Blue (Filled by Trace Area)—The gap was filled by the trace area. The trace area is the area under the curve within the retention time range defined by the chromatographic peak detected in other files for analysis. The analysis uses the retention time at the peak apex and the start and end points for the detected chromatographic peak to determine the area under the curve for missing peaks.

Table 141. Filled Gaps table (Sheet 3 of 3)

Column	Description
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID (F#) of the input file.

Labeled Features table

Table 142 describes the columns in the Labeled Features table. The labeled features are the labeled adduct ions.

Table 142. Labeled Features table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Ion	Displays the ion definition of the molecular ion adduct.
Charge	Displays the charge on the ion.
Molecular Weight	Displays the molecular weight of the unknown compound.
m/z	Displays the mass-to-charge ratio of the ion.
RT [min]	Displays the retention time in minutes of the chromatographic peak that contains the unknown compound ion.
FWHM [min]	Displays the width of the chromatographic peak for the adduct ion at its half-height in minutes.
Intensity (hidden)	Displays the intensity of the ion.
Area	Displays the area of the chromatographic peak that contains the unknown compound ion.
Parent Area [%]	Displays the chromatographic peak area of the current peak as a percentage of the total chromatographic peak area for the parent compound (compound selected in the Compounds per File table) per input file.
Max. Exchange	Displays the maximum number of atoms considered for isotopologue evaluation.
Avg. Exchange	Displays the average number of atoms exchanged for the ion.
Rel. Exchange [%]	Displays the relative number of atoms exchanged versus the maximum number of exchangeable atoms for the feature's elemental composition.

Table 142. Labeled Features table (Sheet 2 of 2)

Column	Description
Exchange Rate [%]	Displays the exchange rate for individual isotopologues.
#MI	Displays the number of matching isotopes for the unknown compound ion.
SFit [%]	Displays the spectral similarity score between the measured and theoretical isotope pattern.
Fitted Cov. [%]	Displays the how well the intensities of the fitted isotope pattern match those of the theoretical isotope pattern.
Measured Cov. [%]	Displays the how well the intensities of the measured isotope pattern match those of the theoretical isotope pattern.
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID (F#) of the input file.

Labeled Compounds per File table

Table 143 describes the columns in the Labeled Compounds per File table. The related table displays details about the selected compound in the higher-level table. To view the compound name for a component in the main Labeled Compound per File table, open its related Compounds table.

Table 143. Labeled Compounds per File table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Molecular Weight	Displays the molecular weight of the unknown compound.
RT [min]	Displays the retention time in minutes of the chromatographic peak that contains the unknown compound ion.
FWHM	Displays the width of the chromatographic peak for the adduct ion at its half-height in minutes.
Max. #MI	Displays the maximum number of matching isotope peaks.
#Adducts	Displays the number of adducts (features).
Area	Displays the area of the chromatographic peak that contains the unknown compound ion.

Table 143. Labeled Compounds per File table (Sheet 2 of 2)

Column	Description
Max. Exchange	Shows the maximum number of exchangeable atoms that the analysis considered.
Avg. Exchange	Displays the average number of atoms exchanged for the ion.
Rel. Exchange [%]	Displays the relative number of atoms exchanged versus the maximum number of exchangeable atoms.
Status	The Analyze Labeled Compounds Node evaluates the measured isotope pattern versus the fitted isotope pattern (for the expected isotopologues) to determine the presence of contaminating masses. It also evaluates the distribution of the measured exchange rates for the expected isotopologues. For information about the status flags, see "Labeling Status (per file)."
Exchange Rate [%]	Displays the contribution of individual isotopologues to the final measured pattern.
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID (F#) of the input file.

Similar Compounds Related table

Use the Similar Compounds table to review the compounds that the application connected to a selected compound in the Compounds table.

The Similar Compounds table is generated by the Generate Molecular Networks node. See "Generate Molecular Networks node."

Table 144 describes the columns in the Similar Compounds table.

Table 144. Similar Compounds table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.

Table 144. Similar Compounds table (Sheet 2 of 2)

Column	Description
Direction	Displays the direction in which the transformation was applied, and defines which compound is a substrate and which is a product. Forward—The selected compound acts as a substrate to which the transformation was applied. The connected similar compound is a product of the transformation. Reverse—The selected compound is a product of the transformation. The connected similar compound acts as a substrate to which the transformation was applied.
Mass Shift [Da]	Displays the difference between the measured molecular weights of the two compounds.
Composition Change	Displays the difference between the elemental compositions of the two compounds.
Transformations	Displays the name of assigned transformation pathway—that is, this column lists the names of the individual steps. Displays "Isomer" when the elemental composition of the substrate and product compounds are identical.
Transformation Mass [Da]	Displays the total theoretical mass of the assigned transformation steps in Daltons.
# Fragments	Displays the number of fragments available for the selected compound.
MSn Score	Displays the final spectral similarity score between the two compounds as the average of the forward and reverse coverages.
Forward Cov. [%]	Displays the relative number of matched centroids in the product compound's MSn spectra.
Forward Matches	Displays the number of matched centroids in the product compound's MSn spectra.
Reverse Cov. [%]	Displays the relative number of matched centroids in the substrate compound's MSn spectra.
Reverse Matches	Number of matched centroids in the substrate compound's MSn spectra.

Compound Identification result tables

For information about the result tables for the compound identification workflow nodes, see these topics:

- ChemSpider Results table
- Mass List Search Results table
- mzCloud Results table
- mzCloud Results Hits table
- mzVault Results table
- mzVault Results Hits table
- Predicted Compositions table

ChemSpider Results table

Use the ChemSpider Results table to review the compounds found in the ChemSpider databases. The Search ChemSpider Node creates the ChemSpider Results table.

❖ **To open the ChemSpider information for a specific ChemSpider hit**

Click the link in the CSID column.

The ChemSpider web page for the selected hit opens in your default web browser.

Table 145 describes the columns in the ChemSpider Results table.

Table 145. ChemSpider Results table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Name	Displays the name of the compound hit in the ChemSpider database.
Structure	Displays the molecular structure of the compound.
Formula	Displays the chemical formula of the compound.
Molecular Weight	Displays the molecular weight of the compound to five decimal places.
CSID	Displays the ChemSpider identification number.

Table 145. ChemSpider Results table (Sheet 2 of 2)

Column	Description
#References	Displays the number of references for the compound in the ChemSpider database.
Additional hidden columns	
SMILES (hidden)	Displays the compound's molecular structure by using short ASCII strings. SMILES stands for simplified molecular input line entry system.
InChi (hidden)	Displays the international chemical identifier for the compound.
#Data Sources (hidden)	Displays the number of ChemSpider data sources that include the compound.
#PubMed References (hidden)	Displays the number of PubMed references for the compound. You can use a PubMed reference to access the scientific literature.
#RSC (hidden)	Displays the number of Royal Society of Chemistry references for the compound.
Additional columns in the related ChemSpider Results table	
Compound Match	Indicates the match status between the current item and the assigned compound annotation. (■) Green—Full Match (■) Orange—Partial Match (■) Red—No Match
ΔMass [Da]	Displays the mass difference in daltons between the search mass and the mass of the matching compound in the ChemSpider database.
ΔMass [ppm]	Displays the mass difference in ppm between the search mass and the mass of the matching compound in the ChemSpider database.
SFit[%]	Displays the spectral similarity score from the Apply Spectral Distance node.

Mass List Search Results table

Use the Mass List Search Results table to review the compounds in the selected mass lists that match the compounds detected by the Detect Compounds node.

The Search Mass Lists Node creates the Mass List Search Results table.

The main Mass List Search Results table displays all of the compounds in the selected mass lists that match the compounds detected by the untargeted analysis. The related Mass List Search Results table lists information about the compound selected in the main Compounds table.

Table 146 describes the columns in the Mass List Search Results table.

Table 146. Mass List Search Results table (Sheet 1 of 2)

Column	Description
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Formula	Displays the elemental composition of the compound in the mass list.
Molecular Weight	Displays the molecular weight of the compound in the mass list.
RT [min]	Displays the chromatographic retention time (when available) of the compound in the mass list.
Structure	Displays the structure (when available) of the compound in the mass list.
Name	Displays the name of the compound in the mass list.
Miscellaneous annotations	These columns display additional information about the compound in the mass list.
Reference List Name	Displays the name of the mass list that contains the matching compound.
Additional columns in the related Mass List Search Results table	
Compound Match (LC studies only)	Indicates the match status between the current item and the assigned compound annotation. • (■) Green—Full Match • (■) Orange—Partial Match • (■) Red—No Match
Max. ΔMass [Da]	Displays the maximum mass difference between the measured mass for the compound in the Compounds table and the theoretical mass of the compound, in daltons.

Table 146. Mass List Search Results table (Sheet 2 of 2)

Column	Description
Max. ΔMass [ppm]	Displays the maximum mass difference between the measured mass for the compound in the Compounds table and the theoretical mass of the compound, in parts per million.
SFit[%] (LC studies only)	Displays the spectral similarity score from the Apply Spectral Distance node.

mzCloud Results table

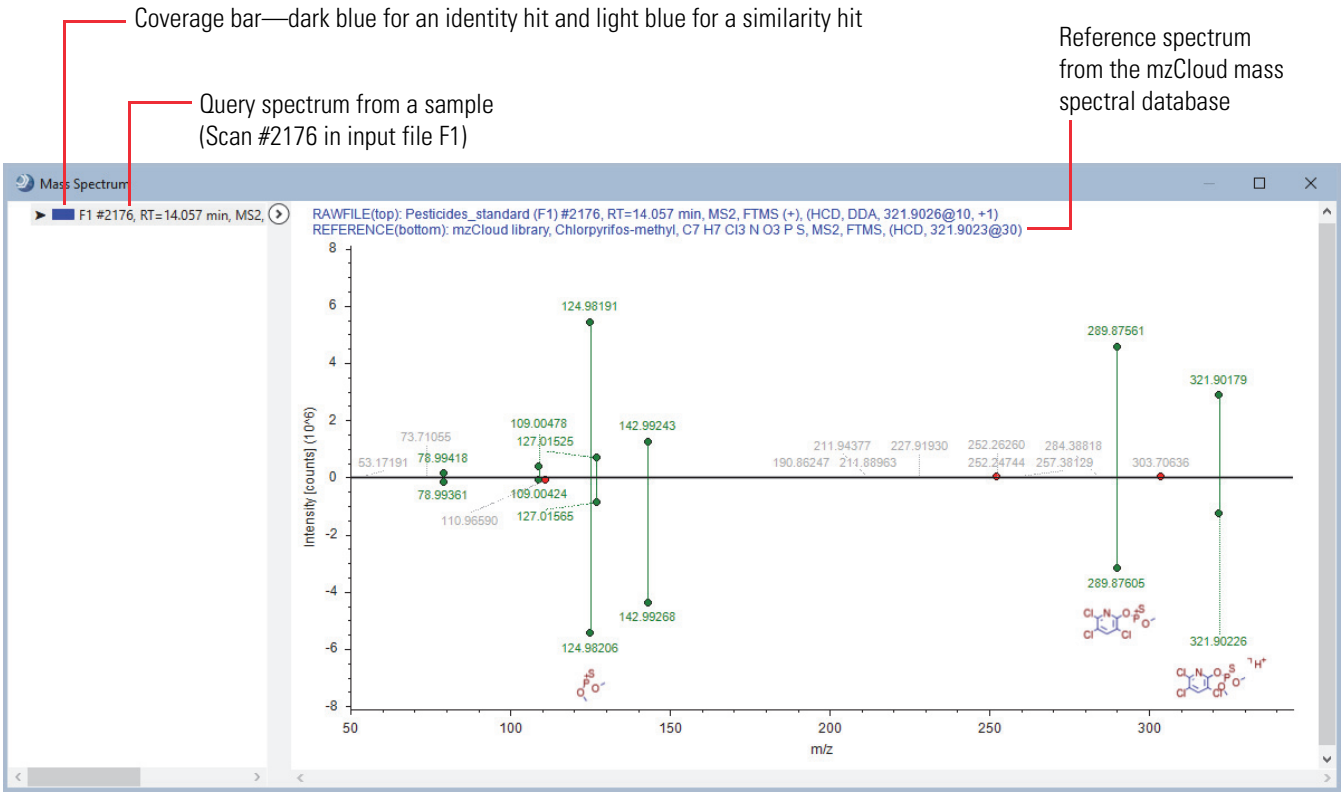
Use the mzCloud Results table to view the results of an mzCloud search.

The Search mzCloud Node creates the mzCloud Results table.

Selecting a row in the mzCloud Results table displays a mirror plot with the selected fragmentation scan on the top and the matched reference scan from the mzCloud database on the bottom. The centroids for the matching fragments are displayed as green sticks with a green circle at the end. Red circles on the *x*-axis indicate the *m/z* values of the missing fragments.

In the collapsible spectrum tree pane to the left of the spectrum plot, the coverage bars indicate whether the matching library spectrum is from an identity hit or a similarity hit.

Figure 147. Mirror plot with annotations for a matching spectrum in the mzCloud Results table



Tip To automatically annotate the matching fragments in the mirror plot, you must set the following advanced parameter in the Search mzCloud node to True—Annotate Matching Fragments. By default, this parameter is hidden and set to False.

Figure 148. Mass Spectrum view with an annotated mirror plot

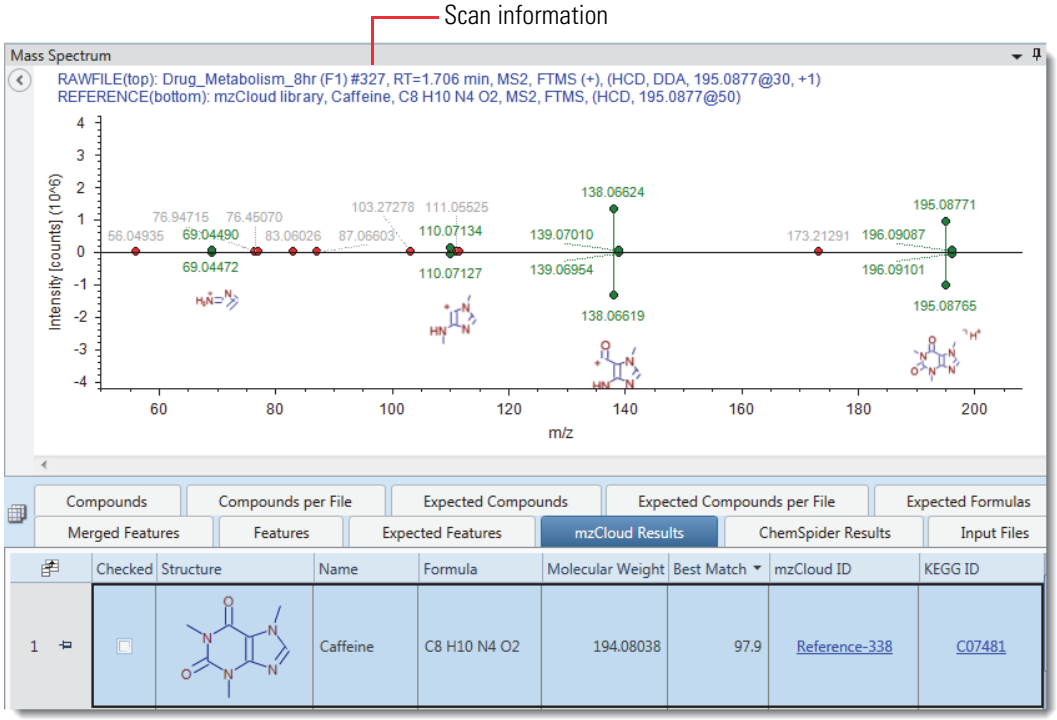


Table 147 describes the columns in the mzCloud Results table.

Table 147. mzCloud Results table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Structure	Displays the structure of the matching compound.
Name	Displays the compound name in the mzCloud database.
Formula	Displays the elemental composition formula of the matching compound.
Molecular Weight	Displays the molecular weight of the matching compound.
Best Match	Displays the match value (0 to 100%) between the best fragmentation scan for a compound (across the input files) and the matching mzCloud spectrum (mzCloud ID). The related Compounds table lists the scan number of the best fragmentation scan.

Table 147. mzCloud Results table (Sheet 2 of 2)

Column	Description
Best Sim. Match	Displays the best match score for a library spectrum to a fragmentation scan across the input files. The related Compounds tables lists the scan number of the similar fragmentation scan.
mzCloud ID	Displays the mzCloud ID (*Database-Number*) for the matching compound. Clicking this link opens the mzCloud database to the matching compound's reference spectrum.
KEGG ID	Displays the KEGG ID for the compound in the KEGG database.
Compound Class	Displays the mzCloud compound classes that include the compound.
mzCloud Library	Displays the name of the database where the search found the matching spectrum.
Additional columns in the related mzCloud Results table	
Compound Match	Indicates the match status between the current item and the assigned compound annotation. For color-coding information, see "Annotations Source column in a compounds table."
ΔMass [Da]	Displays the difference between the theoretical mass of the matching compound and the observed mass of the unknown compound in daltons.
ΔMass [ppm]	Displays the difference between the theoretical mass of the matching compound and the observed mass of the unknown compound in parts per million.
Match	Displays the match value (0–100%) between the specified scan number from the input files and the matching spectrum in the mzCloud database.

mzCloud Results Hits table

The mzCloud Results Hits table is a related table for the mzCloud Results table.

Table 148 describes the columns in the mzCloud Results Hits table.

Table 148. mzCloud Results Hit table (Sheet 1 of 2)

Column	Description
Confidence	Displays the confidence of the match.
Intensity Threshold	Displays the relative intensity threshold for the search spectrum.
Library Spectrum ID	Displays the spectrum ID of the library spectrum.

Table 148. mzCloud Results Hit table (Sheet 2 of 2)

Column	Description
Match	Displays the match quality of this search spectrum to the library spectrum.
Name	Displays the compound name in the mzCloud database.
Scan #	Displays the scan number from the input files that contains the best matching fragmentation spectrum.
Tree Match	Displays the tree match value (0–100%) between the specified scan number from the input files and the matching spectrum in the mzCloud database.
Type	Displays the match type: Identity or Similarity.

mzVault Results table

Use the mzVault Results table to review the results of an mzVault search.

The Search mzVault node creates the mzVault table.

Table 149 describes the columns in the mzVault Results table.

Table 149. mzVault Results table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to label the entries with custom tags that you created by using the Custom Tags Filter view. You can filter the result table on these tags.
Structure	Displays the structure of the matching compound.
# Related Compounds	Displays the number of unknown compounds with the same putative elemental composition but different retention times.
mzVault ID	Displays the ID number of the matching compound in the mzVault library.
Name	Displays the name of the matching compound.
Formula	Displays the elemental composition formula of the matching compound.
Molecular Weight	Displays the molecular weight of the matching compound.
Best Match	Displays the match value (0–100%) between the best fragmentation scan for a compound (across the input files) and the matching mzVault spectrum. The related Compounds table lists the scan number of the best fragmentation scan.

Table 149. mzVault Results table (Sheet 2 of 2)

Column	Description
mzVault Library	Displays the name of the mzVault library where the analysis found a matching compound.
ChemSpider ID	Displays the ChemSpider ID number for the matching compound. Clicking this link opens the ChemSpider database to the compound's record.
Compound Class	Displays the mzVault compound class that includes the compound.
mzCloud ID	Displays the mzCloud ID for the matching compound in the mzCloud database. Clicking this link opens the mzCloud database to the compound's record.
KEGG ID	Displays the KEGG ID for the matching compound in the KEGG database. Clicking this link opens the KEGG database to the compound's record.
Additional columns in the related mzVault Results table	
Compound Match	Indicates the match status between the current item and the assigned compound annotation. For color-coding information, see "Annotations Source column in a compounds table."
ΔMass [Da]	Displays the difference between the theoretical mass of the matching compound and the observed mass of the unknown compound in daltons.
ΔMass [ppm]	Displays the difference between the theoretical mass of the matching compound and the observed mass of the unknown compound in parts per million.
Scan Number	Displays the scan number from the input files that contains the best matching spectrum.
Match	Displays the match value (0–100%) between the specified scan number from the input files and the matching spectrum in the mzVault database.

mzVault Results Hits table

The mzVault Results Hits table is a related table for the mzVault Results table.

Table 150 describes the columns in the mzVault Results Hits table.

Table 150. mzVault Results Hit table

Column	Description
Intensity Threshold	Displays the relative intensity threshold for the search spectrum.
Match	Displays the match quality of this search spectrum to the library spectrum.
Name	Displays the compound name in the mzVault library file.
Scan #	Displays the scan number from the input files that contains the best matching fragmentation spectrum.

Predicted Compositions table

Each compound in the Compounds table has a related Predicted Compositions table.

Use the Predicted Compositions table to review the possible chemical formulas for the selected compound in the Compounds table. The Predicted Compositions tables lists the possible chemical formulas based on the compound's molecular weight.

The Predict Compositions Node creates the Predicted Compositions table.

Table 151 describes the columns in the Predicted Compositions result table.

Table 151. Predicted Compositions table (Sheet 1 of 3)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Compound Match	Displays whether the predicted composition matches the currently assigned compound annotation. (▮) Red—No Match (▮) Green—Full Match
Formula	Displays the predicted elemental composition.
Molecular Weight	Displays the molecular weight.

Table 151. Predicted Compositions table (Sheet 2 of 3)

Column	Description
ΔMass [Da]	Displays the difference between the theoretical mass and the measured mass in daltons.
ΔMass [ppm]	Displays the difference between the theoretical mass and the measured mass in ppm.
RDBE	Displays the rings and double bonds equivalent value for the predicted composition.
H/C	Displays the ratio of hydrogen to carbon atoms in the predicted composition.
Rank	Displays the rank order of each composition.
#Matched Iso.	Displays the number of matching isotopes.
#Missed Iso.	Displays the number of isotopes that were missing in the measured isotope pattern as compared to the theoretical pattern for the predicted composition.
#Matched Fragments	When the Use Fragments Matching algorithm is turned on in the Predict Compositions node, this column displays the number of centroids (*m/z* values) in the best MS2 scan that match possible fragments (mass values from a subset of the elemental compositions in the predicted composition).
SFit [%]	Displays the spectral similarity score between the theoretical and the measured isotope pattern as a percentage. The SFit [%] score = (1–SD) × 100
SD (hidden)	Displays the spectral distance score. A lower SD score corresponds to a higher SFit [%] score. Range: 0 to 1
Pattern Cov. (%)	Displays the summed intensity of the matching isotope peaks in the measured MS1 spectrum relative to the summed intensity of the theoretical isotope pattern. Provides a quantitative measure of how well the measured isotope pattern matches the theoretical isotope pattern. **Note** Because the base peak (leftmost peak) is typically responsible for most of the pattern intensity, even a small decrease in the percent coverage might be important. For example, a missing peak for an isotope with two ^{13}C atoms might cause only a small decrease in the summed intensity of the measured isotope pattern.

Table 151. Predicted Compositions table (Sheet 3 of 3)

Column	Description
MS Cov. (%)	Displays the summed intensity of matching isotope peaks in the measured pattern relative to the summed intensity of all the peaks in the measured pattern.
	IMPORTANT Low values for all of the candidates might indicate an overlapping pattern rather than a lack of good matches.
MSMS Cov. (%)	Displays the summed intensity of the matched fragment peaks relative to the summed intensity of all the fragment peaks in the selected fragmentation scan.
	Note Low values for all of the candidates might indicate a contaminating compound within the isolation window for the fragmentation scan.

Pathway Mapping result tables

For information about the result tables for the Pathway Mapping nodes, see these topics:

- BioCyc Pathways table
- BioCyc Results table
- KEGG Pathways table
- Metabolika Pathways table
- Metabolika Results table

BioCyc Pathways table

Use the BioCyc Pathways table to review all the mapped pathways in the result file.

The Map to BioCyc Pathways node creates the BioCyc Pathways table. The columns that are available in the main BioCyc Pathways table and the related BioCyc Pathways table depend on which nodes provide data to the Map to BioCyc Pathways node.

In an LC processing workflow, the Group Compounds node, the Group Expected Compounds node, or both nodes connect to the Map to BioCyc Pathways node. And the Map to BioCyc Pathways node connects to the Apply Spectral Distance node and the Apply mzLogic node when the processing workflow includes these nodes. The Group Compounds node creates the Compounds table, and the Group Expected Compound node creates the Expected Compounds table.

For more information, see "BioCyc Pathways view."

Table 152 describes the columns in the BioCyc Pathways main table. The BioCyc Pathways table lists all the BioCyc pathways that include at least one of the compounds in the main compounds table.

Table 152. BioCyc Pathways table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags.
Pathway Name	Displays the names of the mapped Metabolika pathways that include matching structures (by formula, mass, or both) for at least one compound in the Compounds table.
#Mapped Compounds	Displays the number of detected compounds (in the Compounds table) mapped onto the BioCyc pathway.
#Mapped Expected Compounds	Displays the number of expected compounds (in the Expected Compounds table) mapped onto the BioCyc pathway.
#Matched Compounds	Displays the number of compounds in the pathway that map to the Compounds table.
#Matched Expected Compounds	Displays the number of compounds in the pathway that map to the Expected Compounds table.
Total #Matched Compounds	Displays the number compounds in the pathway that map to the Compounds table, the Expected Compounds table, or both tables.
#Compounds in Pathway	Displays the total number of compounds in the pathway.

Table 152. BioCyc Pathways table (Sheet 2 of 2)

Column	Description
Additional columns in a BioCyc Pathways table for a compound in the main compounds table	
BioCyc Compound IDs (related table)	Displays BioCyc compound ID.
BioCyc Compound Names (related table)	Displays the BioCyc compound name.
BioCyc Compound Formula (related table)	Displays the BioCyc compound formula.

BioCyc Results table

Use the BioCyc Results table to review the compounds found in the mapped BioCyc database.

The Map to BioCyc Pathways node creates the BioCyc Results table.

Table 153 describes the columns in the BioCyc Results table.

Table 153. BioCyc Results table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Structure	Displays the molecular structure of the compound.
Name	Displays the compound name in the BioCyc database.
Formula	Displays the chemical formula of the compound.
Molecular Weight	Displays the molecular weight of the compound to five decimal places.
Additional columns in the related BioCyc Results table for a compound	
Compound Match	Indicates the match status between the current item and the assigned compound annotation.
Max. ΔMass [Da]	Displays the maximum mass difference between the measured mass for the compound in the Compounds table and the theoretical mass of the compound, in daltons.
Max. ΔMass [ppm]	Displays the maximum mass difference between the measured mass for the compound in the Compounds table and the theoretical mass of the compound, in parts per million.

Table 153. BioCyc Results table (Sheet 2 of 2)

Column	Description
BioCyc ID	Displays the BioCyc identification number for the compound.
BioCyc DB	Displays the name of the BioCyc database that mapped the compound.
mzLogic Score (LC studies)	Displays the mzLogic score provided by the Apply mzLogic node.
SFit[%] (LC studies)	Displays the spectral similarity score from the Apply Spectral Distance node.

KEGG Pathways table

Use the main KEGG Pathways table to review all of the mapped pathways that include compounds detected across the input file set.

The Map to KEGG Pathways Node creates the KEGG Pathways table.

Table 154 describes the columns in the main KEGG Pathways table and the KEGG Pathways table for a compound. The KEGG Pathways table lists all the KEGG pathways that include at least one of the compounds detected by the untargeted search.

Table 154. KEGG Pathways table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Pathway ID	Displays the identification number of the mapped KEGG pathway.
Pathway Name	Displays the name of the mapped KEGG pathway that includes at least one compound in the Compounds table.
#Referenced Compounds (LC studies)	Displays the number of detected compounds in the Compounds table that are referenced in the identified KEGG pathway. Available when the workflow includes the Group Compounds node.
#Referenced Expected Compounds (LC studies)	Displays the number of compounds in the Expected Compounds table that are referenced in the identified KEGG pathway. Available when the workflow includes the Group Expected Compounds node.

Table 154. KEGG Pathways table (Sheet 2 of 2)

Column	Description
#Identified Compounds (LC studies)	Displays the number of different KEGG compound IDs identified for the compounds in the Compounds table. Available when the workflow includes the Group Compounds node.
#Identified Expected Compounds (LC studies)	Displays the number of different KEGG compound IDs identified for the compounds in the Expected Compounds table. Available when the workflow includes the Group Expected Compounds node.
#All Identifications	Displays the number of unique identifications for all compound categories (for the compounds in the Expected Compounds table and the Compounds table) related to a specific pathway. Available when the workflow includes the Group Expected Compounds node and the Group Compounds node
#mzCloud Results (LC studies)	Displays the number of compounds in the identified KEGG pathway that the mzCloud search identified. Available when the workflow includes the Search mzCloud node.
Additional columns in the KEGG Pathways table for a compound in a main compounds table	
KEGG Compound IDs	Displays a list of the KEGG compound IDs in ascending order from left to right.
KEGG Compound Names	Displays a list of the KEGG compound names.
KEGG Compound Formulas	Displays a list of the KEGG compound formulas.
Max. ΔMass [Da]	Displays the maximum mass difference between the measured mass for the compound in the compounds table and the theoretical mass of the compound, in daltons.
Max. ΔMass [ppm]	Displays the maximum mass difference between the measured mass for the compound in the compounds table and the theoretical mass of the compound, in parts per million.

Metabolika Pathways table

Use the main Metabolika Pathways table to review all of the mapped pathways that include compounds detected across the input file set. Use the related Metabolika Pathways tables to review the results for specific compounds.

The Map to Metabolika Pathways node creates the Metabolika Pathways table.

Table 155 describes the columns in the Metabolika Pathways table. The main Metabolika Pathways table lists all the Metabolika pathways that include at least one of the compounds in any of the main compounds tables (Compounds table, Expected Compounds table, or both). The related table displays the search results for the selected compound in the main compounds table.

Table 155. Metabolika Pathways table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags.
Pathway Name	Displays the names of the mapped Metabolika pathways that include matching structures (by formula, mass, or both) for at least one compound in the Compounds table.
#Mapped Compounds	Displays the number of detected compounds (in the Compounds table) mapped onto the Metabolika pathway.
#Mapped Expected Compounds	Displays the number of expected compounds (in the Expected Compounds table) mapped onto the Metabolika pathway.
#Matched Compounds	Displays the number of compounds in the pathway that map to the Compounds table.
#Matched Expected Compounds	Displays the number of compounds in the pathway that map to the Expected Compounds table.
Total #Matched Compounds	Displays the number compounds in the pathway that map to the Compounds table, the Expected Compounds table, or both tables.
#Compounds in Pathway	Displays the total number of compounds in the pathway.
Additional columns in a Metabolika Pathways table for a compound in the main compounds table	
Metabolika Compound IDs (related table)	Displays Metabolika compound ID.

Table 155. Metabolika Pathways table (Sheet 2 of 2)

Column	Description
Metabolika Compound Names (related table)	Displays the Metabolika compound name.
Metabolika Compound Formula (related table)	Displays the Metabolika compound formula.

Metabolika Results table

Use the Metabolika results table for a specific compound to review the match between the putative compound in your experimental data and the mapped compounds. This table is empty when the compound in the main compounds table has zero associated Metabolika pathways.

The Map to Metabolika Pathways node creates the Metabolika Results table.

Table 156 describes the columns in the Metabolika Results table.

Table 156. Metabolika Results table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Structure	Displays the molecular structure of the compound.
Name	Displays the compound name in the Metabolika database.
Formula	Displays the chemical formula of the compound.
Molecular Weight	Displays the molecular weight of the compound to five decimal places.
Compound Match	Displays whether the Metabolika pathway structure is a full or partial match for the selected compound. (■)—Full Match (■)—Partial Match (■)—No Match Available for compounds in the Compounds table from an LC study.

Table 156. Metabolika Results table (Sheet 2 of 2)

Column	Description
mzLogic Score	Displays the normalized score from the Apply mzLogic node for the structure based on the mzCloud similarity matches (Apply mzLogic node). Available for compounds in the Compounds table when the processing workflow includes the Apply mzLogic node.
Original mzLogic Score (hidden)	Displays the score from the Apply mzLogic node for the structure based on the mzCloud similarity matches. Available for compounds in the Compounds table when the processing workflow includes the Apply mzLogic node.
Max. ΔMass [Da]	Displays the maximum mass difference between the measured mass for the compound in the compounds table and the theoretical mass of the compound, in daltons.
Max. ΔMass [ppm]	Displays the maximum mass difference between the measured mass for the compound in the compounds table and the theoretical mass of the compound, in parts per million.
SFit[%]	Displays the spectral similarity score from the Apply Spectral Distance node. Available when the processing workflow includes the Apply Spectral Distance node.

Compound Scoring tables

For information about the result tables for the unknown compound scoring nodes, see these topics:

- Compound Class Matches table
- Matched Patterns table
- Neutral Losses table

Compound Class Matches table

The Compound Class Matches table is related to the Compounds table. Use the Compound Class Matches table to review the compounds classes that match the compound selected in the Compounds table.

The Compound Class Scoring node adds the Class Coverage column to the Compounds table and creates the Compound Class Matches table, which is related to the Compounds table.

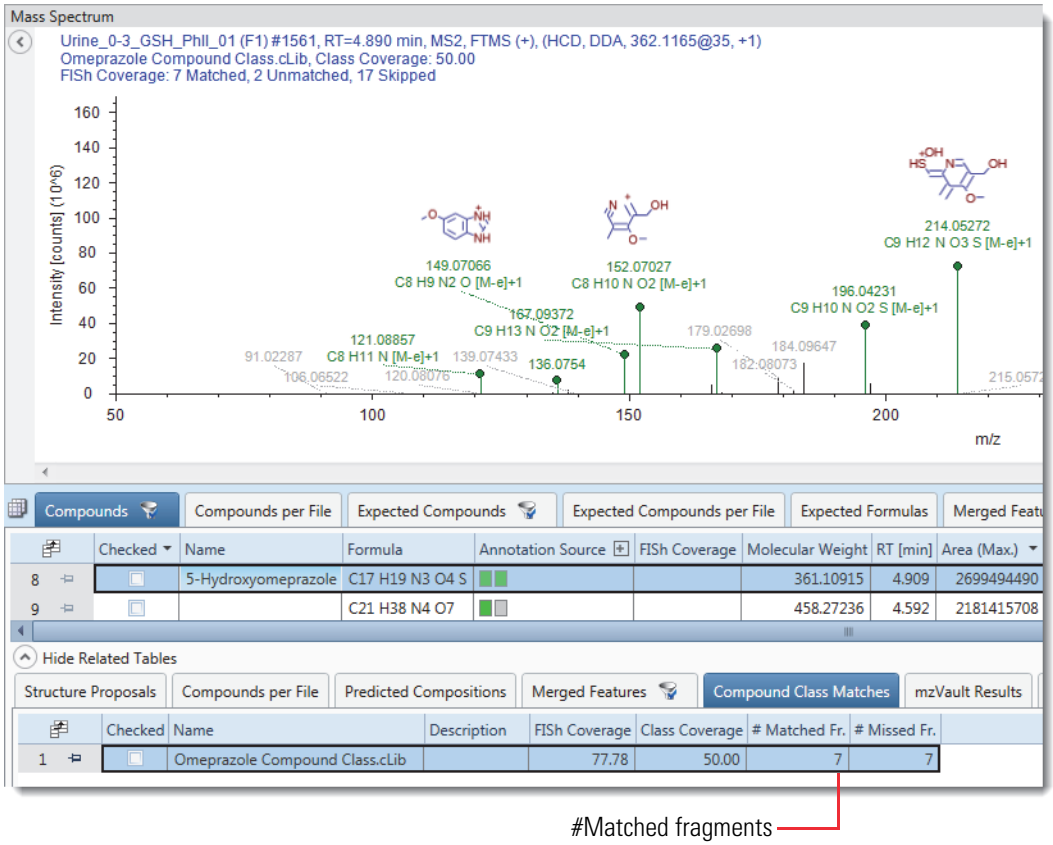
Table 157 describes the columns in the Compound Class Matches table.

Table 157. Compound Class Matches table

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Name	Displays the name of the library that contains the matching structure.
Description	Displays the user-specified description of the library.
FISh Coverage	Displays the FISh coverage score (see "FISh scoring for proposed structures.").
Class Coverage	Displays the number of matching centroids in the best fragmentation scan divided by the total number of fragments in the selected compound class libraries.
# Matched Fr.	Displays the number of library fragments that match the centroids in the best fragmentation scan for a compound.
# Missed Fr.	Displays the number of library fragments that do not match the centroids in the best fragmentation scan for a compound.

Figure 149 shows an annotated fragmentation scan of a detected compound. By comparing the *m/z* values of the centroids in the fragmentation scan against a compound class library with 11 structures, the application annotated 6 centroids in the fragmentation scan with matching structures from the library. The legend in the Mass Spectrum view lists the search library, the Class Coverage score, and the FISh Coverage score.

Figure 149. Fragmentation scan and compound class match result for a detected compound



Matched Patterns table

The Matched Patterns table is related to the Compounds table. Use the Matched Patterns table to review how well the isotopic pattern matches the compound selected in the Compounds table.

The Pattern Scoring node adds the Matched Patterns table to the result file.

Table 158 describes the columns in the Matched Patterns table.

Table 158. Matched Patterns table (Sheet 1 of 2)

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."
Name	Displays the name or chemical formula of the compound.

Table 158. Matched Patterns table (Sheet 2 of 2)

Column	Description
SFit [%]	Displays the spectral fit for the isotope pattern to the chemical formula.
SD	Displays the spectral distance score.
Pattern Coverage [%]	Displays the summed intensity of the matching isotope peaks in the measured MS1 spectrum relative to the summed intensity of the theoretical isotope pattern. Provides a quantitative measure of how well the measured isotope pattern matches the theoretical isotope pattern.
	Note Because the base peak (leftmost peak) is typically responsible for most of the pattern intensity, even a small decrease in the percent coverage might be important. For example, a missing peak for an isotope with two ^{13}C atoms might cause only a small decrease in the summed intensity of the measured isotope pattern.
#Matched Iso.	Displays the number of matching isotopes for the unknown compound.
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID (F#) of the input file.

Neutral Losses table

When the processing workflow for an analysis includes the Search Neutral Losses node, the result file includes the main Neutral Losses table and a related Neutral Losses table for each detected compound.

For more information, see Neutral loss detection and visualization.

Table 159 describes the columns in the main and related Neutral Losses tables.

Table 159. Neutral Losses table (Sheet 1 of 2)

Column	Description
Main table	
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Tags	Use this column to add custom tags to the result table items. You can filter the result table by these tags. See "Custom color-coded tags for result table entries."

Table 159. Neutral Losses table (Sheet 2 of 2)

Column	Description
Name	Displays the name of the neutral loss fragment. This name corresponds to the name of the neutral loss in the Neutral Losses view.
Formula	Displays the formula of the neutral loss fragment.
Molecular Weight	Displays the molecular weight of the neutral formula.
#Compounds	Displays the number of compounds where the application detected the specified neutral loss in their fragmentation spectra.
Related table for a specific compound	
Name	Displays the name of the neutral loss.
Formula	Displays the elemental composition of the neutral loss.
Molecular weight	Displays the neutral loss shift, in daltons, between the precursor ion and the fragment ion produced by the specified neutral loss.
#Compounds	Displays the number of compounds where the application detected the named neutral loss in their fragmentation scans.
Scan#	Displays the scan number where the application detected the specified neutral loss.
Precursor Mass	Displays the mass of the precursor ion that underwent the specified neutral loss.
Charge	Displays the charge of the fragment produced by the specified neutral loss.
Expected Mass	Displays the expected mass (*m/z* value) of the fragment produced by the specified neutral loss.
ΔMass [Da]	Displays the difference between the mass of the expected fragment produced by the specified neutral loss to the experimental mass of the fragment in the specified fragmentation scan, in daltons.
ΔMass [ppm]	Displays the difference between the mass of the expected fragment produced by the specified neutral loss to the experimental mass of the fragment in the specified fragmentation scan, in parts per million.

Statistical Methods table

For LC studies, when the analysis includes any of the following nodes, the analysis result includes the Statistical Methods table:

- Align Retention Times (ChromAlign) node
- Group Compounds node
- Fill Gaps node
- Apply Missing Value Imputation node
- QC Correction nodes
- Normalize Area node
- Differential Analysis node

Table 160 describes the columns in the Statistical Methods table.

Table 160. Statistical Methods table

Column	Description
Checked	Use this column to select the rows that you want to display in the result table and in reports after you apply result filters.
Method Description	Displays a description of the statistical methodology.
Node ID	Displays identification number for the workflow node in the processing workflow.
Node Name	Displays the name of the processing workflow node that applied the specified statistical methodology.
Node Workflow ID	Displays the identification number of the workflow node.
Processing Step	Displays the processing step where the analysis applied the specified statistical methodology.

Differential analysis columns

When the analysis includes sample groups and group ratios and the processing workflow includes the Differential Analysis node, the following columns appear in the Compounds table and the Expected Compounds table:

- Group Areas
- Group CV(%)
- Ratio
- Log2 Fold Change

- P-value
- Adj. P-value.

In addition, the following columns appear in the Merged Features table, Group Areas, Ratio, and Log2 Fold Change. The background colors of the table cells provide visual information about the numeric values in these columns.

Table 161 describes the columns from a differential analysis.

Table 161. Differential analysis columns (Sheet 1 of 3)

Column	Description
Group Areas	Displays the median chromatographic peak area for the compound in the sample group. To display the group names, click the expand icon to the right of the column heading. When the compound is not found, the cells have a gray background. The Differential Analysis node bins the group areas in the current result file on the Log10 scale, with one bin for each order of magnitude (1e4, 1e5, 1e6, and so on), and uses a different background color for each bin. The values in the lowest bin have a pale-yellow background. The values in the highest bin have a green background. Color-coding: • Lowest values: • Highest values: **Note** When a result table includes the Group Areas column, the Area column is hidden, by default.
Group CV(%)	Displays the coefficient of variation for the groups. Groups with a high degree of variation (20% or greater) have a red background. Color-coding: (20) Values equal to or greater than 20 have a red background. (5) Values from 0 to 19 have a white background.

Table 161. Differential analysis columns (Sheet 2 of 3)

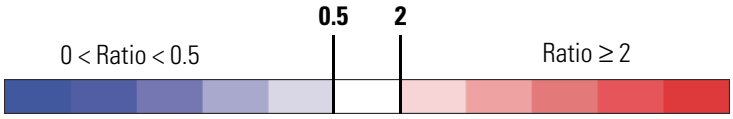
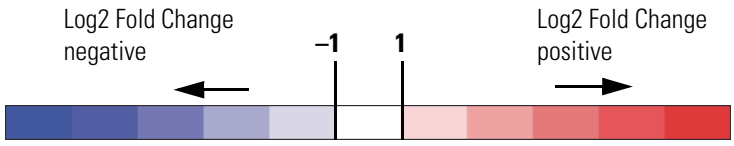
Column	Description
Ratio	Displays the area ratio or ratios for the generated ratios. A ratio of 0 (0/X) has a dark purple background (0.000). An undefined ratio (X/0) (labeled as Infinity) has an orange background (Infinity). The cells for compounds with defined ratios greater than 0 have the following background colors: • Compounds with ratios between 0 and 0.5 are divided into five equal bins. The background color for the table cells is a progressively darker blue hue as the ratio approaches zero. • Compounds with ratios greater than 2 are divided into five equal bins. The background color for the tables cells is a progressively darker red hue as the ratio increases. 
Log2 Fold Change	Displays the fold change (ratio) in the log base 2 scale. A log2 fold change of Infinity has an orange background (Infinity). When the ratio is 0 (0/X) or –Infinity in the Log2 format, the background color is a dark purple (–Infinity). The cells for compounds with log2 fold change values between – infinity and infinity have the following background colors: • Compounds with log2 fold change values more negative than –1.00 are divided into five equal bins. The background color for the table cells is a progressively darker blue hue as the value becomes more negative. • Compounds with log2 fold change values greater than 1.00 are divided into five equal bins. The background color for the table cells is a progressively darker red hue as the value increases. 

Table 161. Differential analysis columns (Sheet 3 of 3)

Column	Description
P-value	Displays the p-value for the sample group calculated by running the Tukey HSD test (post hoc) after an analysis of variance (ANOVA) test. The p-value is a number between 0 and 1. Given the following hypotheses: • Null hypothesis—There is no difference between the sample groups for the variable tested. • Alternate hypothesis—There is a difference between the sample groups for the variable tested. You can interpret the p-value as follows: • A low p-value means that you can reject the null hypothesis with a low probability of error that the alternate hypothesis is true. • A high p-value means that you can accept the null hypothesis with a low probability of error that the alternate hypothesis is true.
Adj. P-Value	(Differential Analysis node) Displays the adjusted p-value. The application adjusts p-values in cases of multiple testing. Multiple testing of a null hypothesis leads to higher probabilities of rejecting this null hypothesis by chance, and therefore the application corrects the whole set of hypotheses (for example, all detected compounds) as a function of the set size (for example, a set of 10 000 compounds has a stronger correction than one of only 1000). The application performs this correction by using the Benjamini-Hochberg algorithm for the false discovery rate.
P-value and Adj. P-value	Color-binning for p-values and adjusted p-values: • 1–0.05 [ ] Red • 0.05–0.01 [ ] Orange • 0.01–0.005 [ ] Yellow • 0.005–0.001 [ ] Yellow green • <0.001 [ ] Green

Descriptive statistics columns

The Descriptive Statistics post-processing node adds the columns described in Table 162 to the compounds tables (Compounds table and Expected Compounds table). The descriptive statistics columns are hidden by default.

Table 162. Descriptive statistics columns

Column	Description
Min. Area	Displays the minimum peak area for the compound in the sample set.
Q1 Area	Displays the lower boundary of the first quartile (25%) area for the compound in the sample set.
Median Area	Displays the median area for the compound (MW × RT) in the sample set.
Q3 Area	Displays the upper boundary of the third quartile (75%) area for this compound in the sample set.
Mean Area	Displays the calculated average area for the compound (MW × RT) in the sample set.
Area SD	Displays the standard deviation of the peak areas for the compound (MW × RT) in the sample set.
Area CV [%]	Displays the coefficient of variation of the area for the compound (MW × RT) in the sample set.

QC Correction columns

Table 163 describes the columns that the Apply QC Correction node (in combination with QC samples) adds to the various compounds tables.

Table 163. QC correction columns (Sheet 1 of 2)

Column	Description
Norm. Area (hidden)	Displays the normalized areas of the QC corrected compounds per input file. When a compound does not pass any of the QC correction filters, the area cell for the compound is empty. You can view the uncorrected chromatographic peak area for the compound in the corresponding Areas column.
# Usable QC	Displays the number of usable QC samples. See "Using quality control samples to compensate for batch effects."

Table 163. QC correction columns (Sheet 2 of 2)

Column	Description
RSD QC Areas [%]	Displays the relative standard deviation of the peak areas for the compound across the QC samples before area correction.
RSD Corr. QC Areas [%]	Displays the relative standard deviation of the peak areas for the compound across the QC samples after area correction.
QC Fill Status	Displays a status rectangle for each QC sample. Possible states: (■) Green—Filled by re-detected peak (■) Gray—N/A (■) Orange—Filled by matching ion (■) Blue—Filled by simulated peak

Annotations Source column in a compounds table

The Annot. Source column in the Compounds table for an LC study indicates the match status for each compound from the search nodes in the processing workflow. The expanded column heading displays the annotation sources.

For LC data, the Assign Compound Annotations node determines the validity of the annotations from the annotation sources that are selected in the Assign Annotations node when the processing workflow includes these annotation sources. You can select up to six compound identification and pathway mapping sources in the Assign Annotations node

The Annot. Source column indicates the match status for the selected compound from the compound identification nodes and pathway mapping node in the processing workflow. The expanded column heading displays the annotation sources.

Tip To sort by the annotation source, do the following:

1. Click the expand icon to display the vertical headings of the subordinate columns.
2. Select the heading of the subordinate column that you want to sort by.

   The selected subordinate column heading appears in bold text with an asterisk at the top of the vertical text.
3. Click the **Annot. Source** column heading to sort the table rows.

Table 164. Match states from the annotation source nodes in a processing workflow

Possible states	Meaning
(■) Green—Full Match	The current formula and structure annotations match the best available item from the particular source (online database or local mass list).
■ Gray—No Results	Retrieved no data from the particular source.
■ Orange—Not the Top Hit	Current compound annotation matches one of the hits, but not the top one.
■ Orange—Partial Match	Only the formula for the current compound annotation matches the items retrieved from the particular source.
■ Orange—Unused	Retrieved items from the particular source, but did not assign any annotations.
■ Red—Invalid mass	The best available item from the particular source has a molecular weight that does not match the molecular weight of the compound within the specified mass tolerance.
■ Red—No match	The particular source does not have an item that matches the current annotations for the compound.

Peak Rating columns

For information about how the Compound Discoverer application calculates the peak rating for a chromatographic peak, see "Chromatographic peak rating filter."

An analysis that includes the following workflow nodes generates a Peak Rating column in each of the following result tables.

- The Group Compounds node generates the Peak Rating column in the Compounds table.
- The Group Expected Compounds node generates the Peak Rating column in the Expected Compounds table.
- The Differential Analysis node generates the (recalculated) Peak Rating column in the GC CI Compounds table.

Table 165. Color-coding in the Peak Rating data column

Color	Calculated peak rating (0 to 10)
Gray	N/A
Orange	0 to 2.5
Yellow	>2.5 to 5.0
Yellow green	>5.0 to 7.5
Green	> 7.5 to 10.0

Peak quality factor (PQF) columns in the result tables

For information about how the Compound Discoverer application calculates the peak quality factors for a chromatographic peak, see "Peak quality factors."

The following result tables include PQF columns:

- Compounds table
- Compounds per File table
- Features per File table
- Expected Compounds table
- Expected Features per File table

Table 166. Color-coding for the four peak quality factors

	Peak Quality Factors			
Color	**FWHM to base**	**Jaggedness**	**Modality**	**Zig-Zag Index**
Gray	N/A	N/A	N/A	N/A
Dark Green	0.0 to 0.8	0.0 to 0.1	0.0 to 0.02	0 to 0.05
Yellow	0.8 to 0.9	0.1 to 0.4	0.02 to 0.3	0.05 to 0.2
Orange	0.9 to 1.0	0.4 to 1.0	0.3 to 1.0	0.2 to 1.0

11

Create and print reports

The following topics describe how to create, preview, and print reports:

- Reporting workflow
- Generate a report with an existing report template
- Create new report templates
- Edit existing report templates
- Reference information for the report template page
- Select the paper type, print width, page orientation, and watermark for a report template
- Preview and print a report

When you open a report template for editing, it opens as a tabbed page with a workspace area on the left. You can use the standard report templates provided with the application or you can create your own custom report templates.

Note The following reporting features are new in the Compound Discoverer 3.3 application:

- The name of the study and the file name of the result file (analysis result)—By default, these items appear in the upper-middle of the page header section and cover-page section of the report.
- mzCloud mirror plot—You can now add an mzCloud mirror plot to a report template. See "Add mzCloud mirror plots to a report template."

Reporting workflow

The following flowchart shows the reporting workflow (Figure 150 and Figure 151).

Figure 150. Reporting workflow (page 1)

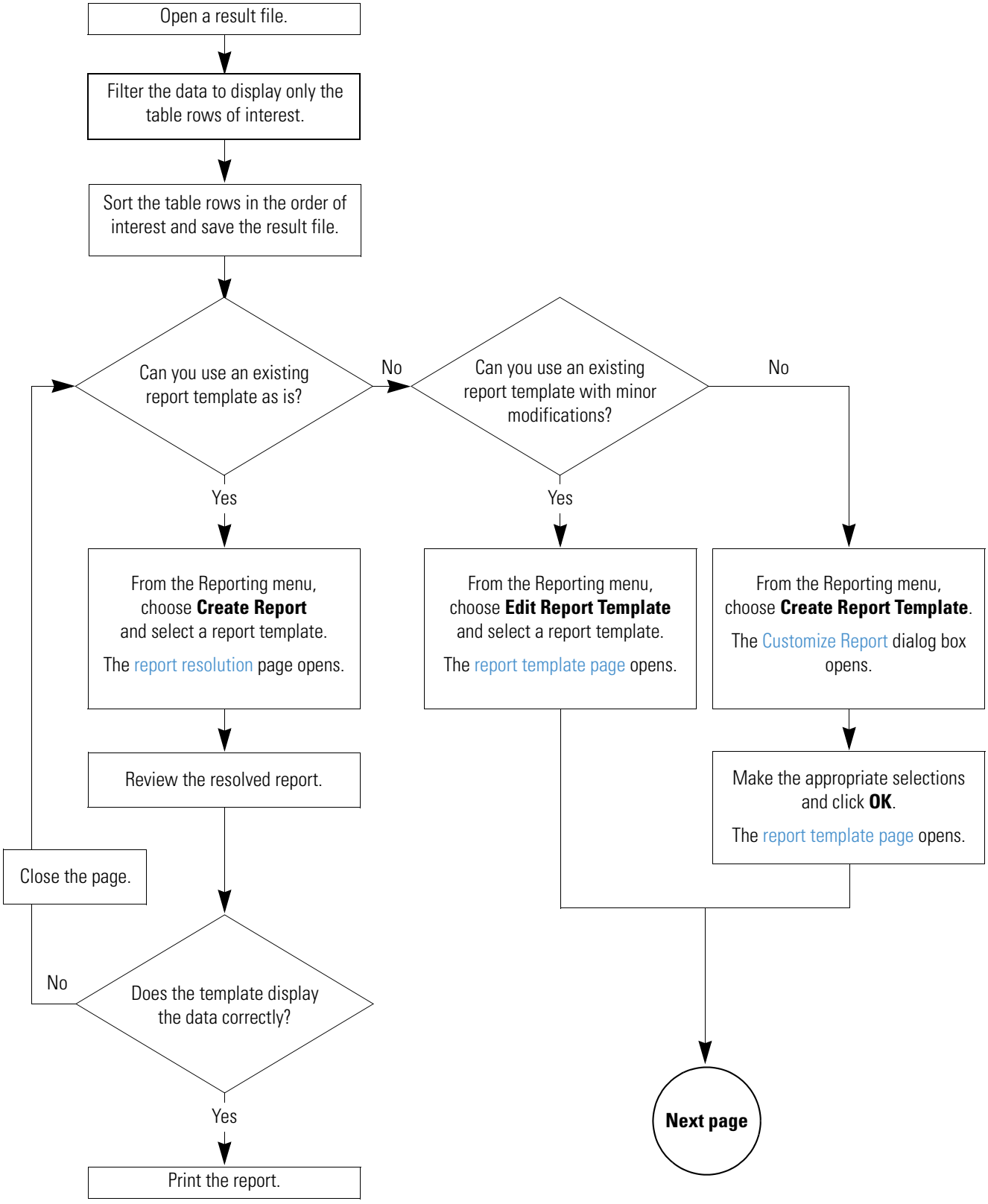
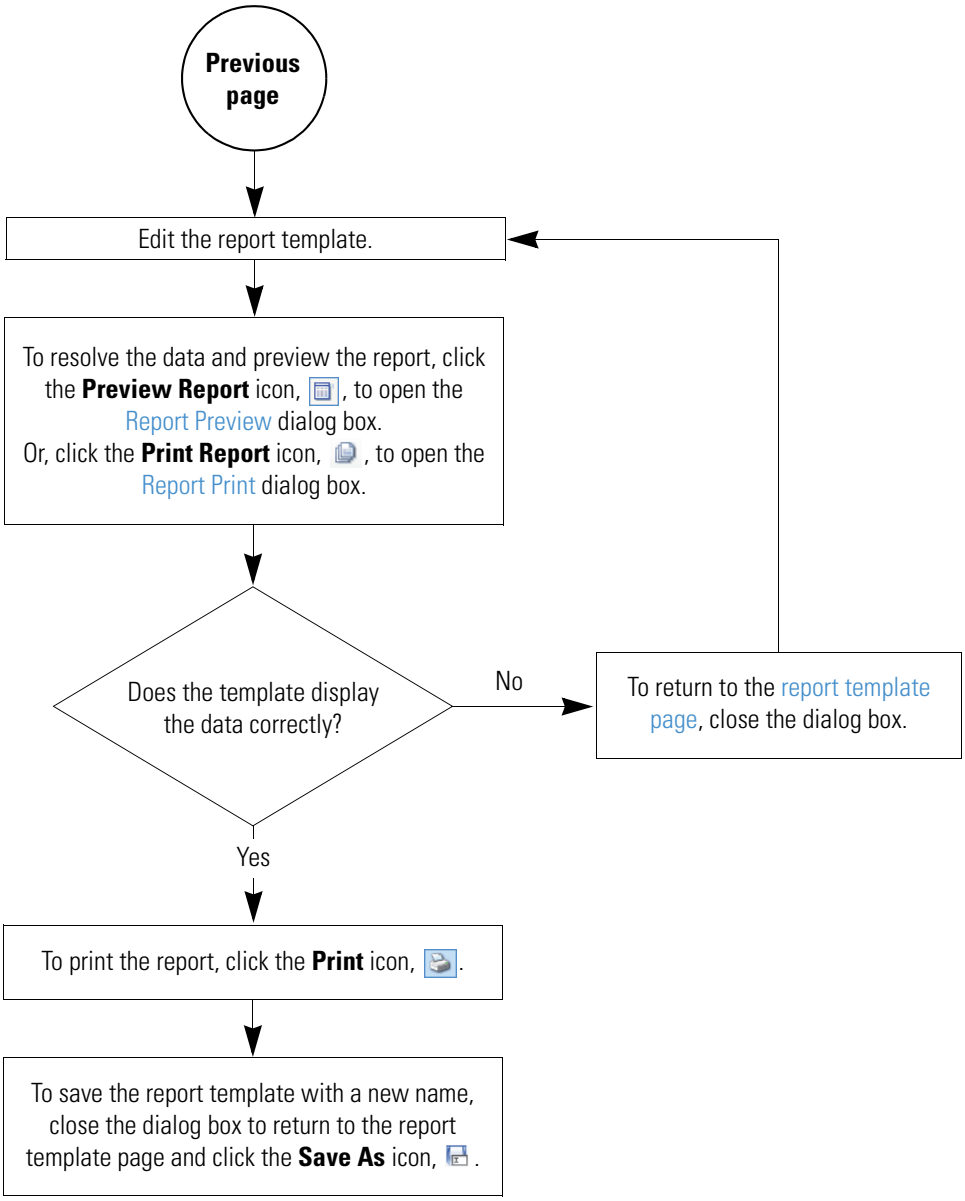


Figure 151. Reporting workflow (page 2)



Generate a report with an existing report template

You can use one of the report templates provided with the application or one of your own custom report templates to produce reports that display items of interest in a result file.

For details, see these topics:

- Report templates provided with the application
- Preview and print a report by using an existing report template

Report templates provided with the application

The Compound Discoverer application comes with several report templates. The report templates reside in the following folder:

drive:\ProgramData\Thermo\Compound Discoverer 3.3\Common Templates\ReportTemplates

For LC studies, the application comes with the nine defined report templates.

Table 167. LC report templates provided with the application (Sheet 1 of 2)

Report template name	Description
Compounds No Graphs A4	Generates single row for each visible compound in the Compounds table. Reports the structure, name, and formula when available. Reports the calculated molecular weight and group areas.
Compounds with Graphs A4	Generates a single page for each visible compound in the Compounds table. Reports the structure, name, and formula when available. Reports the calculated molecular weight and group areas. The report includes a chromatogram plot, an MS1mass spectrum plot, and an MS2 spectrum plot.
Expected Compounds No Graphs A4	Generates a single row for each visible compound in the Expected Compounds table. Reports the parent compound, formula, calculated molecular weight, retention time, dealkylations, transformations, composition change, FISh coverage, and group areas.
Expected Compounds per File No Graphs A4	Generates a single row for each visible compound in the Expected Compounds table. Reports the parent compound, formula, calculated molecular weight, retention time, ions and the *m/z* values of the ions, composition change, chromatographic peak area, and study file ID.
Expected Compounds per File with Graphs A4	Generates a separate page for each visible compound in the Expected Compounds per File table. Includes the following graphs: MS1 spectrum, chromatogram, and MS2 spectrum.
Expected Compounds with Structures No Graphs A4	Generates a single row for each visible compound in the Expected Compounds table. Reports the parent compound, formula, calculated molecular weight, composition change, retention time, FISh coverage, and group areas. Reports the structure and name when available.

Table 167. LC report templates provided with the application (Sheet 2 of 2)

Report template name	Description
Expected Compounds with Structures with Graphs A4	Generates a separate page for each visible compound in the Expected Compounds table. Reports the parent compound, formula, calculated molecular weight, composition change, retention time, FISh coverages, and group areas. Reports the name when available. Includes the following graphs: chromatogram, MS1 spectrum, and MS2 spectrum with fragment annotations.
Expected Compounds with Graphs A4	Generates a separate page for each visible compound in the Expected Compounds table. Reports the parent compound, formula, calculated molecular weight, retention time, dealkylations, transformations, composition change, FISh coverage, and group areas. Reports the name and structure when available. Includes the following graphs: chromatogram, MS1 spectrum, and MS2 spectrum with fragment annotations.
Compounds with Graphs and mzCloud Mirror Plot	Generates a single page (or more depending on the number of mzCloud matches the analysis found for the compound) for each visible compound in the Compounds table. Reports the structure, name, and formula when available. Reports the calculated molecular weight. The report includes a chromatogram plot, an MS1 mass spectrum plot, and mirror plots.

Preview and print a report by using an existing report template

❖ To preview and print a report by using an existing report template

1. Open a result file. See "Open, close, and update result files."

   In the application window, the reporting menu commands and the reporting toolbar icons ( ) become available.

2. Determine which main table you want to include in the report and filter the data in this table as appropriate. See "Filter the data for data reduction."

   For LC studies, you can use the report templates provided with the application with one of these tables as described in the template name: Compounds table, Expected Compounds table, or Expected Compounds per File table.

3. To select an existing report template, choose **Reporting > Create Report** from the menu bar or click the **Create Report** icon,  .

   The Open Report Design Template dialog box opens to the Report Templates folder.

To select an appropriate report template, you must know what data the report template is designed to resolve. Typically, a report template resolves the filtered data from one of the main tables and one or more of the graphs associated with the table. A report template can also resolve data from one or more related tables. The predefined report templates resolve the data in the Compounds table or the Expected Compounds table.

4. Select the appropriate report template and click **Open**.

   The report resolution page opens with the thumbnail pane on the right and a report preview on the left.

   The tab format for the report resolution page is as follows:

   Report Template Name

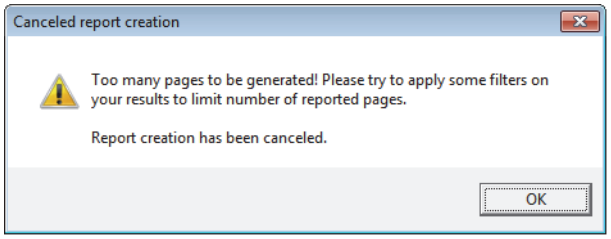
   As the application resolves the data with the report template, the following icon displays the progress.

   When the data is resolved, the progress icon disappears, and the application begins rendering the report pages. The current page/estimated pages box lists the progress.

   If the selected template does not contain ReportInfo items, the application displays the pages as it renders them. If the selected template contains a ReportInfo item, the application does not display the rendered pages until it has rendered all of the report pages. ReportInfo items include the time stamp in the upper left and the page number at the center bottom of the defined report templates.

   If the report contains too many pages, the application cancels the report generation and the following message box appears.

5. If the application cancels the report generation, repeat step 2 to step 4. This time, reduce the number of reported items by modifying the filters.

6. Review the contents of the report.

7. On the report resolution page, click the **Print** icon, , in the toolbar to print the report.

   The Print dialog box opens.

8. Select the appropriate printer and the page range that you want to print.

   The report templates that come with the application default to printing on A4 paper.

9. If you are not printing on A4 paper, change the printer setting.
10. Click **OK** to print the report.

Create new report templates

This topic describes how to create a new report template by using the Customize Report dialog box where you do the following:

- Select the data to be included in the report:
  - Columns of interest in the main table
  - Graphs associated with the main table
  - Columns of interest in any of the related tables
  - Graphs associated with any of the selected related tables
- Change the appearance of the tables:
  - Transpose the column orientation from left to right to top to bottom
  - Add Separator lines below the column headings
  - Indent the related tables below the main table
  - Select background colors for the table headers and table rows
- Select the paper type (PaperKind parameter), page orientation, and logo image

For details, see these topics:

- Create a new report template by using the Customize Report dialog box
- Add, remove, or modify the color schemes for a report template
- Customize Report dialog box parameters

Create a new report template by using the Customize Report dialog box

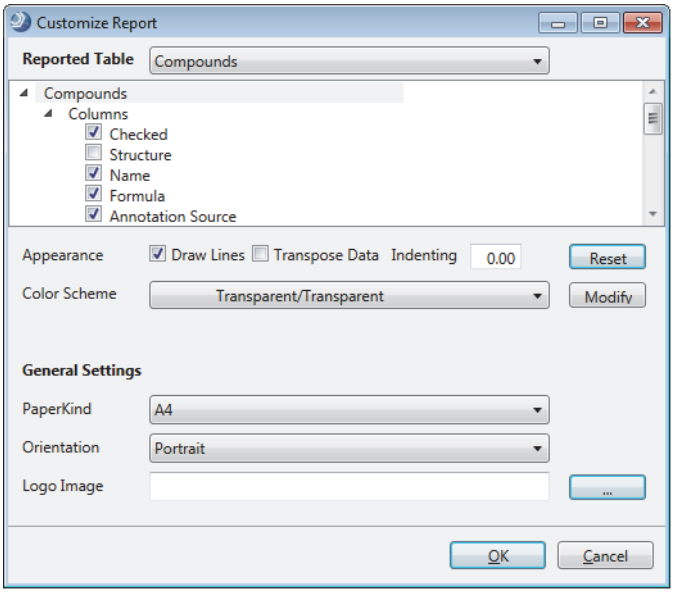
When you create a new report template by using the Customize Report dialog box, the application automatically adds a date-and-time stamp on the left side of the report header, the Compound Discoverer logo on the right side of the report header, and the page number in the report footer. By default, the application displays information from the currently selected main result table on A4 paper in the portrait orientation with the data columns listed left to right. You can select a different main table, add related tables and graphs (chromatogram, mass spectrum, mirror plot), and change the paper type, page orientation, and logo image.

❖ To create a report template by using the Customize Report dialog box

1. Open a result file. See "Open, close, and update result files."
2. Do one of the following:
   - From the menu bar, choose **Reporting > Create Report Template**.
   - In the toolbar, click the **Create a New Report Template** icon, .

   The Customize Report dialog box opens in front of the New Report Template page.

   Figure 152. Customize Report dialog box for the Compounds table



3. In the Reported Table list at the top of the dialog box, select the main table for the report template.

   A list of data items for the selected table appears. By default, the Columns list is expanded, and the Graphs and Related Tables lists are collapsed.

4. To select the columns for the main table, any of the associated graphs, and any of the main table's related tables, do the following:
   a. Under the selected table name, click each expand icon, , to open these sections:
      - Columns
      - Graphs
      - Related Tables
   b. In the expanded sections, select the check box for each column, graph, or related table (and associated columns) that you want to include in the generated reports.

5. To add a separator line above the column heading row for each result table, select the **Draw Lines** check box.

(Default layout for the main result table)				
Column 1 label	Column 2 label	Column 3 label	Column 4 label	Column 5 label
Data text box	Data text box	Data text box	Data text box	Data text box
(Related table)				
Column 1 label	Column 2 label	Column 3 label	Column 4 label	Column 5 label
Data text box	Data text box	Data text box	Data text box	Data text box

Tip For result tables with a large number of data columns, transpose the columns by selecting the Transpose Data check box. Otherwise, you might need to resize the data columns to fit the page.

6. To transpose the tabular data from columns to rows, do the following:
   a. Select the main result table and the related tables for the report.
   b. In the data item list, select the table that you want to transpose as follows:
      - To transpose the columns in the main table, select the main table name (the first data item) in the Customize Report dialog box.
      - To transpose the columns in a related table, select the check box to the left of the related table name and click the table name to make sure that it is highlighted in blue.
   c. Select the **Transpose Data** check box.

      Note Selecting another table clears the Transpose Data check box.

   Each selected data column appears as a two-column row in the report template. The first column displays the column heading and the second column displays the data from a table row.

(Default layout for the main table)		
Column 1 label	Column 2 label	Column 3 label
Data text box	Data text box	Data text box
(Transposed layout for the main table)		
Column 1 label	Data text box	
Column 2 label	Data text box	
Column 3 label	Data text box	

7. To indent a related table, do the following:
   a. Select the related table in the expanded list of data items.

b. In the Indenting box, type the indentation value from **0.00** to **1.00** inch.

(Default layout for the main result table)

Column 1 label	Column 2 label	Column 3 label	Column 4 label	Column 5 label
Data text box	Data text box	Data text box	Data text box	Data text box

(Related table indented by 1 inch)

	Column 1 label	Column 2 label	Column 3 label	Column 4 label
	Data text box	Data text box	Data text box	Data text box

8. To select a color scheme for a report table, do the following:
   a. In the report item list, select the table of interest, for example, the main table or one of the related tables.
   b. In the Color Scheme list, select one of the available color schemes.

      Each scheme consists of two colors: the first color for the background of the table headers and the second color for the background of the table rows. The default color scheme is Transparent/Transparent.
9. Under General Settings, do the following:
   - In the PaperKind list, select the default paper size for the report.
   - In the Orientation list, select the page orientation.
   - Next to the Logo Image box, click the browse icon, . Then, in the Open Image File dialog box, select the graphic file for the logo image and click **Open**.
10. To apply the settings and close the Customize Report dialog box, click **OK**.

    Your selections appear on the report template page. The tab format for the report template page is as follows:

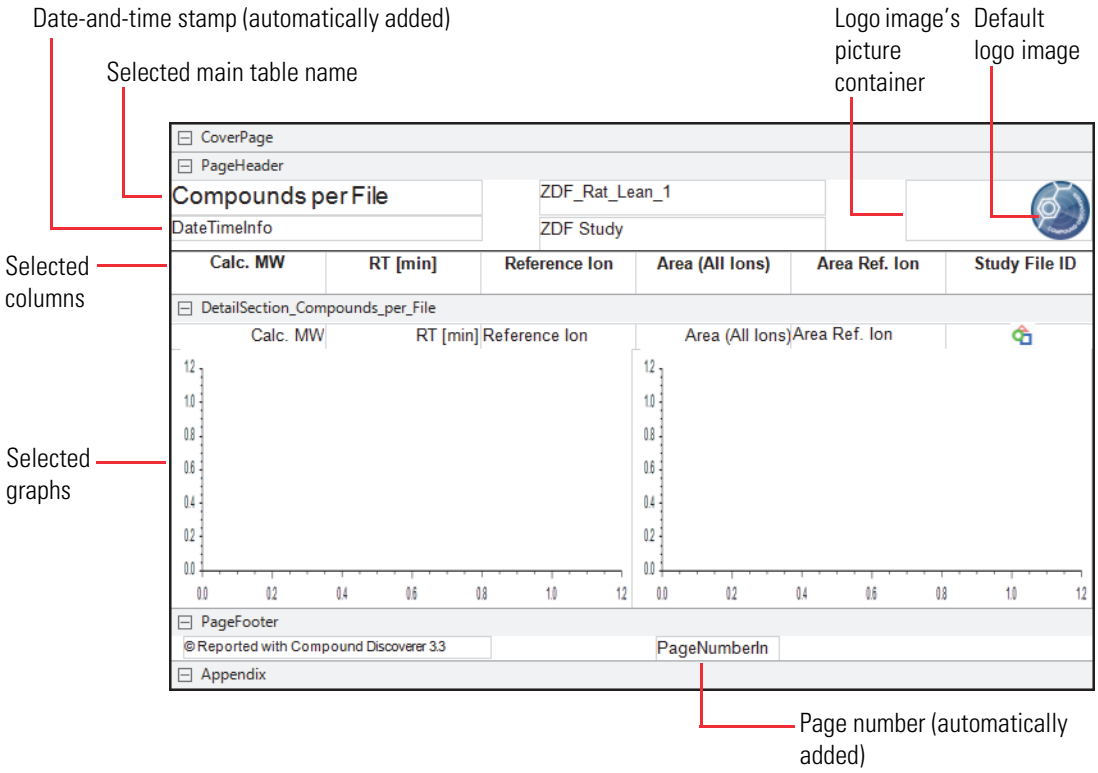
    Main Result Table
11. To save the template with a different name, click the Save As icon ( ) in the upper-left corner of the report template page.

    For information about editing the report template, see "Edit existing report templates."

Figure 153 shows a report template for selected columns in the Compounds per File table and two associated graphs. The default report template uses the Compound Discoverer application icon. You can select a different image and resize its picture container as appropriate.

Note The Customize Report dialog box automatically adds the file name and study name fields to the page header section of the report template.

Figure 153. Report template with data from the Compounds per File table



Note The Customize Report dialog box automatically adds the file name and study name fields to the page header section of the report template.

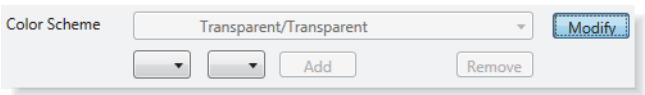
Add, remove, or modify the color schemes for a report template

In the Customize Report dialog box, follow this procedure to modify, add, or remove the color schemes for the report tables.

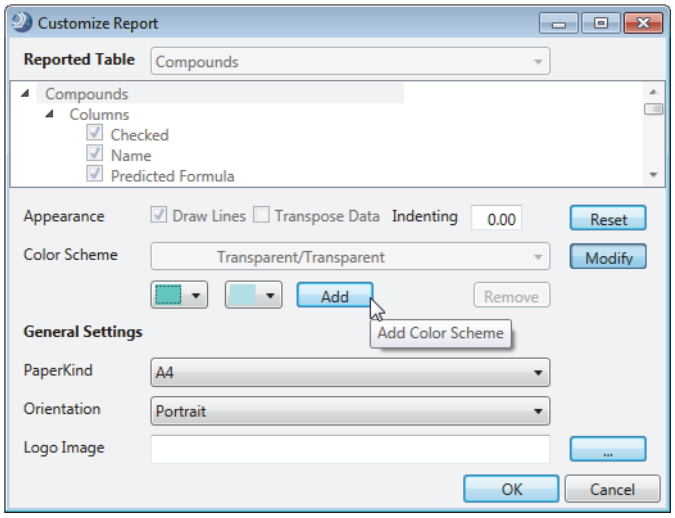
❖ **To modify the current color scheme or to add or remove color schemes from the list**

1. Open the Customize Report dialog box. See "Create new report templates."
2. Select the main result table and the related tables for the report.
3. Click **Modify**.

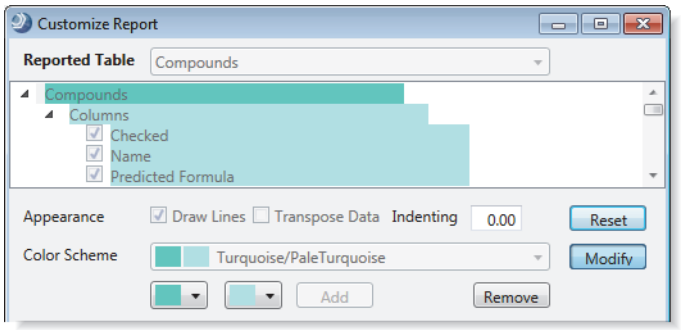
   Two color selection lists appear below the Color Scheme list. The list on the left changes the background color for the column headings. The list on the right changes the background color for the data columns.



4. From the color lists, select one or two background colors, and then click **Add**.



The application displays the effect of the color scheme in the data item list, adds the new color scheme to the Color Scheme list, and makes the Remove button available.



Note Accepting the settings in the Customize Report dialog box adds the new color scheme to the ColorScheme.xml file that is located in the following folder:

C:\Users\Public\Public Documents\Thermo\Compound Discoverer 3.3 \Common Templates\ReportTemplates

If you remove the new color scheme before you click OK at the bottom of the Customize Report dialog box to accept the settings, the application does not add the new color scheme to the ColorScheme.xml file.

5. To change the color selection, do one or both of the following:

   - If you do not want to apply the new color scheme to the currently selected table, click **Reset**.

     The application undoes the color selections, applies the default color scheme (Transparent/Transparent), and closes the color lists. When you click OK to accept the settings and close the Customize Reports dialog box, the application adds the new color scheme to the ColorScheme.xml file.

- If you do not want to keep the new color scheme, click **Remove**.

  The application undoes the color selections, leaves the color lists open, and removes the color scheme from the Color Scheme list.

Customize Report dialog box parameters

Table 168 describes the parameters in the Customize Report dialog box.

Table 168. Customize Report dialog box parameters (Sheet 1 of 3)

Parameter	Description
Reported Table	Lists the main tables in the result file.
Columns	Lists the columns for the selected main table.
Graphs	Lists the graphs for the selected main table.
Related Tables	Lists the tables related to the selected main table.
Columns	Lists the columns for the selected related table.
Graphs	Lists the graphs for the selected related table.
Related Tables	Lists the second-level related tables for the selected related table.
Appearance	
Draw Lines	Specifies whether the application draws a line above the table column headers. Default: Selected
Transpose Data	Specifies the layout of the data in the result table columns. The default layout (check box cleared) matches the result table layout, with columns displayed from left to right and rows displayed from top to bottom. Select this check box to transpose the columns to rows. Default: Cleared
	Tip When you select a table item in the data item list, the application automatically clears the Transpose Data check box. For each table that you want to transpose, select the table name and make sure that it is highlighted in blue. Then select the **Transpose Data** check box.
Indenting	Specifies the indentation of the selected related table data from the left edge of the page, from 0.00 to 1.00 inch. Default: 0.00 in.

Table 168. Customize Report dialog box parameters (Sheet 2 of 3)

Parameter	Description
Color Scheme	
Color Scheme	Specifies the color scheme for the selected table. Each color scheme consists of two colors. The first color is the background of the column headings. The second color is the background of the table rows. You can modify the Color Scheme list by adding or removing color schemes. Default: Transparent/Transparent **Note** Accepting the settings in the Customize Report dialog box adds the new color schemes to the ColorScheme.xml file that is stored in the same folder as the common report templates.
General Settings	
PaperKind	Specifies the size of the paper for printing the report. Select the appropriate paper size before sending the report to the printer. Default: A4
Orientation	Specifies the orientation of the report, either Portrait or Landscape. Default: Portrait
Logo Image	Specifies the logo image to appear by default in the upper-right corner of each report page. The default size of the picture container for the logo is 1.823 × 0.492 in. (width × height). When the selected image is larger than the picture container, the container clips the image. You can edit the properties of the picture container in the report template.
Buttons	
Reset	Resets the color scheme to the default scheme.
Modify	Opens two color selection lists.
Add	Selecting colors in one or both of the color selection lists (below the Color Scheme list) makes this button available. Applies the new color scheme to the selected table and adds the new color scheme to the Color Scheme list.
Remove	Removes the selected color scheme from the Color Scheme list.

Table 168. Customize Report dialog box parameters (Sheet 3 of 3)

Parameter	Description
OK	Applies the selected settings to the new report template.
Cancel	Cancels your selections and closes the dialog box.

Edit existing report templates

Use the report template page to modify a report template. The report template page shows the items that you selected using the Customize Report dialog box or the items in the existing report template that you selected. Some of the items appear as containers (a rectangular box) where you can add text, images, or data graphs.

Note You can open more than one report template page in the application window.

Tip For reference information about the toolbars, shortcut menus, and so on, see "Reference information for the report template page." For information about changing the paper type and page orientation, see "Select the paper type, print width, page orientation, and watermark for a report template."

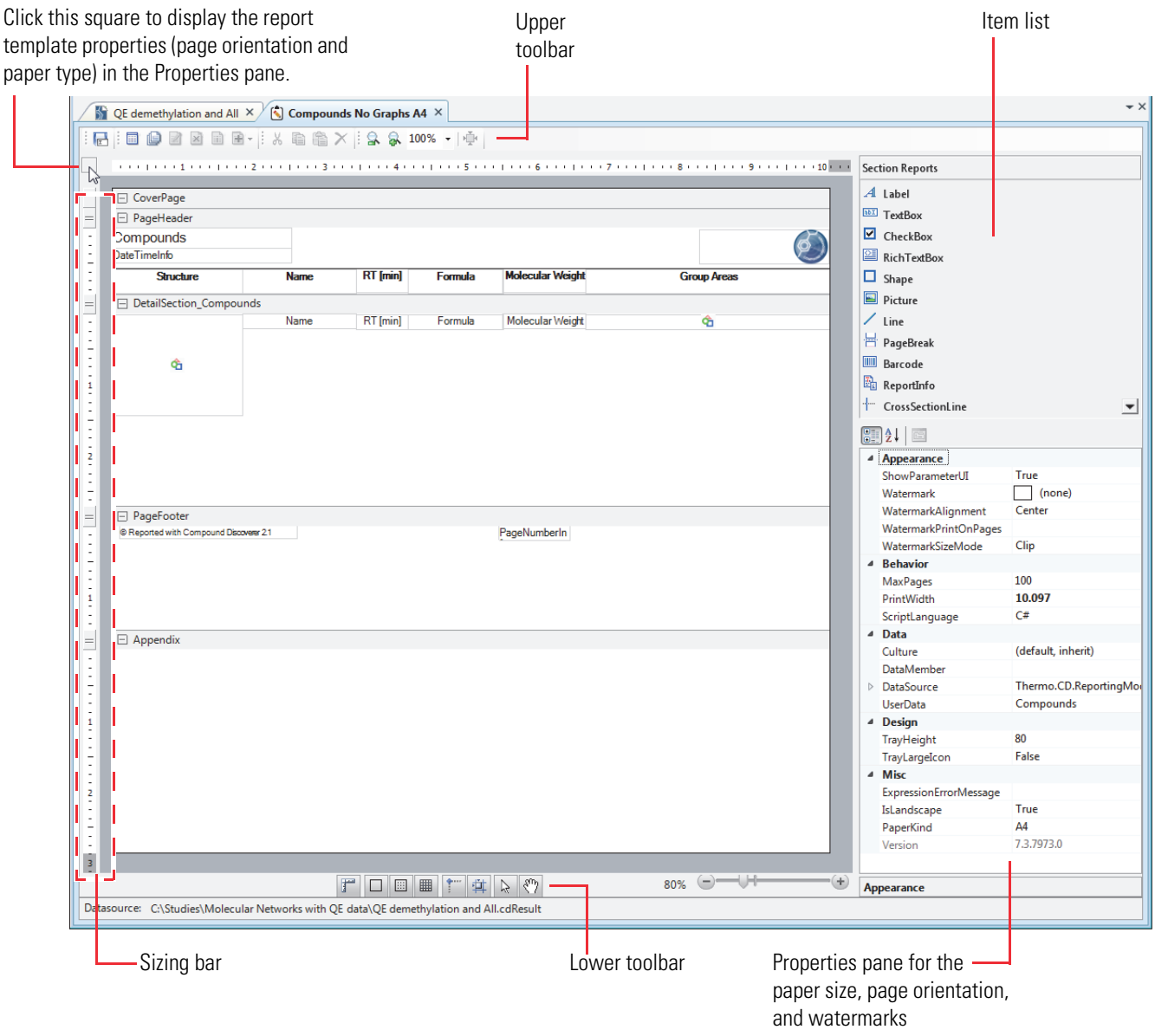
To modify a report template, follow these procedures as applicable:

- Open a report template for editing
- Add a cover page to a report template
- Change the logo image for a report template
- Change the format of the date and time field in a report template
- Add items in the Section Reports pane to a report template
- Add a rich text box to a report template
- Add main table columns to a report template
- Add data graphs to a report template
- Add mzCloud mirror plots to a report template
- Add related table columns to a report template
- Edit the properties of subreport columns in a report template
- Move a subreport column to the main table of a report table
- Modify the properties of a section report item
- Add page breaks to a report template
- Delete a pair of workspace sections on the report template page

- Resize the sections of a report template
- Add, align, and transpose columns in a report template by using the shortcut menu commands
- Add a border to an item by using the Format Border command

Figure 154 shows the Compounds No Graphs template on the report template page.

Figure 154. Report template page



Open a report template for editing

The Compound Discoverer application comes with several report templates.

❖ To open a report template

1. Open a result file. See "Open, close, and update result files."
2. From the application window, do one of the following:
   a. Choose **Reporting > Create Report Template** from the menu bar, or click the **Create a New Report Template** icon, , in the toolbar.

      The Customize Report dialog box opens.

   b. Make the appropriate selections and click **OK**.

      The report template page opens as a tabbed document. The tab format is as follows:

      Main Result Table Name

Add a cover page to a report template

By default, the cover page is not visible in the report templates that you create by using the Customize Report dialog box.

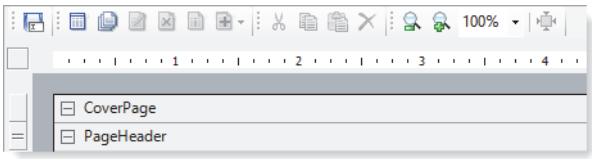
The default items on the cover page are as follows:

- Name of the main result table
- Date and time stamp
- Logo

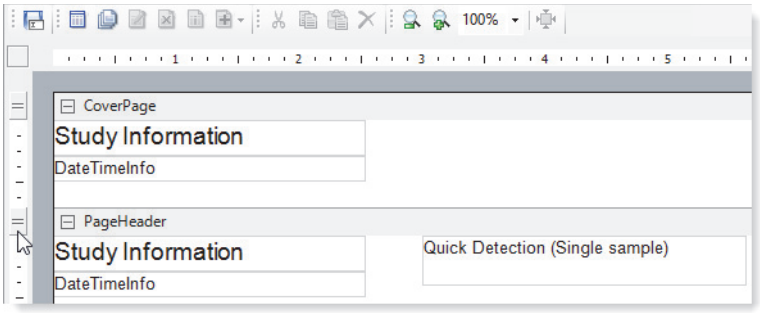
❖ To display and edit the cover page of a report template

1. Open the report template that you want to edit. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window. Typically, the cover page section is closed.



2. (Optional) To view the items in the cover page section that you might want to edit, drag down the sizing handle to the left of PageHeader. Then, edit the items as applicable.



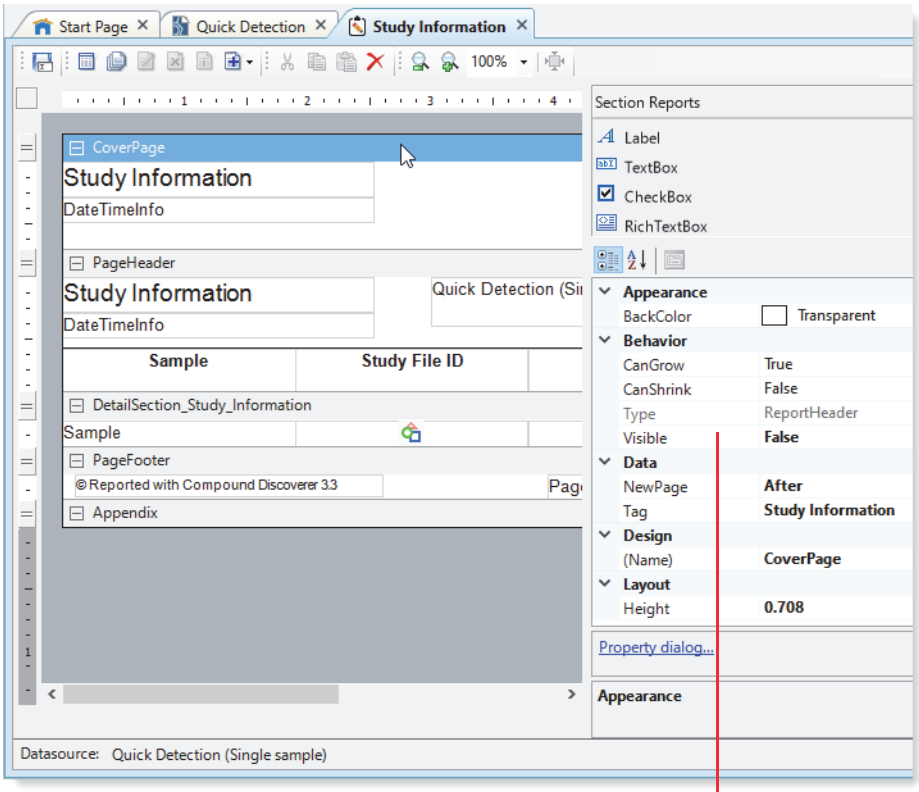
Sizing handle next to the beginning of the page header section

3. To add the cover page to the report, do the following:

   a. Click the cover page title bar to select it.

      The properties for the cover page appear in the Properties pane.

      Figure 155. Cover page properties



Cover page properties

   b. In the properties pane, select **True** for Visible in the Behavior section.

Change the logo image for a report template

❖ **To change the logo image in a report template**

1. Open the report template. See "Open a report template for editing."

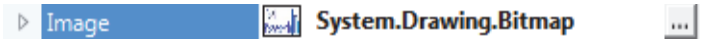
   The report template opens as a tabbed page in the application window.

2. Select the logo image container.

   The picture properties appear in the Properties pane.

   Note The Compound Discoverer icon is the default logo for the common templates and the templates that you create with the Customize Reports dialog box.

3. In the Data area, click the browse icon, ..., to the right of the Image property. You might have to click the row to make the browse icon appear.

   The Open dialog box opens with a setting of All image files for the file type.

4. Browse to the folder where you stored the logo of interest, select the logo, and click **Open**.

   The selected image appears in the container.

5. Modify the Layout properties as appropriate.

Change the format of the date and time field in a report template

The templates that come with the application include a DateTimeInfo field (date and time stamp) in the Cover Page section and the Page Header section.

❖ **To change the format of the date-and-time field**

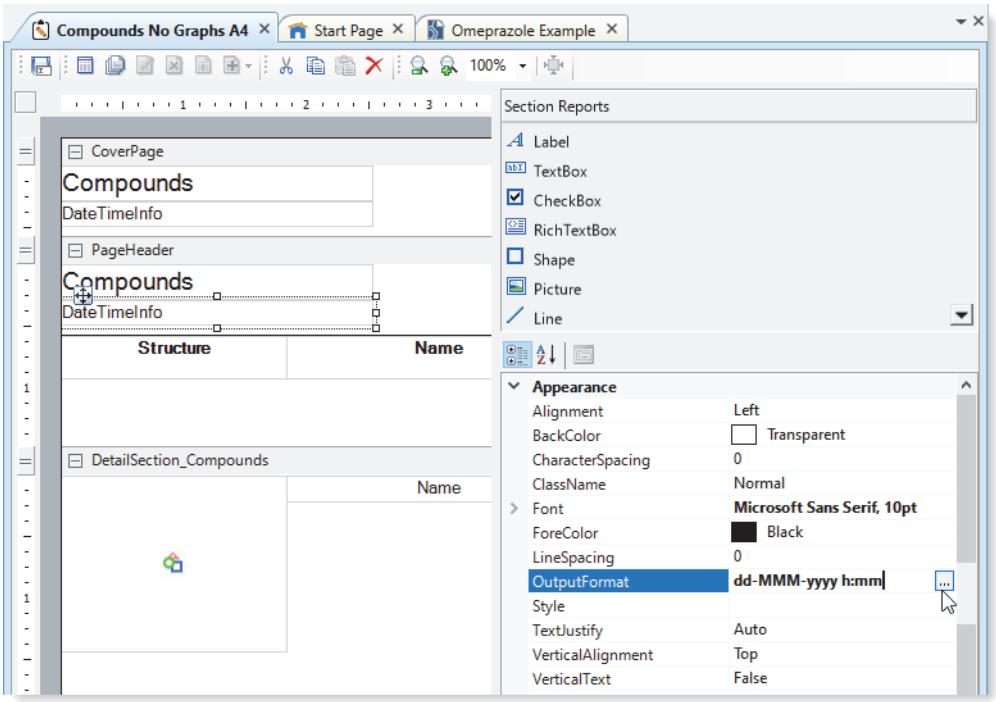
1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. Select the **DateTimeInfo** item.

   The properties for this item appear in the Properties pane.

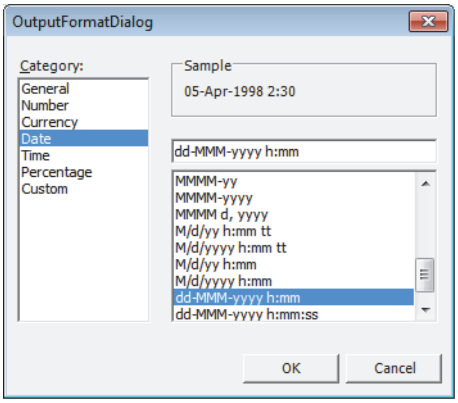
Figure 156. Output Format box for the Date Time Info field in the report templates



3. Under Appearance, click the **OutputFormat** box to make the browse icon appear. Then click the browse icon.

   The Output Format dialog box opens.

Figure 157. Output Format dialog box



4. Select the format of interest.
5. Click **OK** to accept the setting.

Add items in the Section Reports pane to a report template

You can add any of the items in the Section Reports pane to a report template. See "Section report items for a report template."

❖ To add an item to the template

1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. From the Section Reports pane to the right of the workspace area, drag an item to the appropriate location on a workspace section of the page.

   Some of the items appear as containers (boxes) where you can add text or images.

3. Select the item to open its properties below the Section Reports pane.

4. Edit the properties of the item as necessary.

Add a rich text box to a report template

A rich text box contains fixed text that is not dynamically populated from the contents of the result file.

❖ To add rich text box to a report template

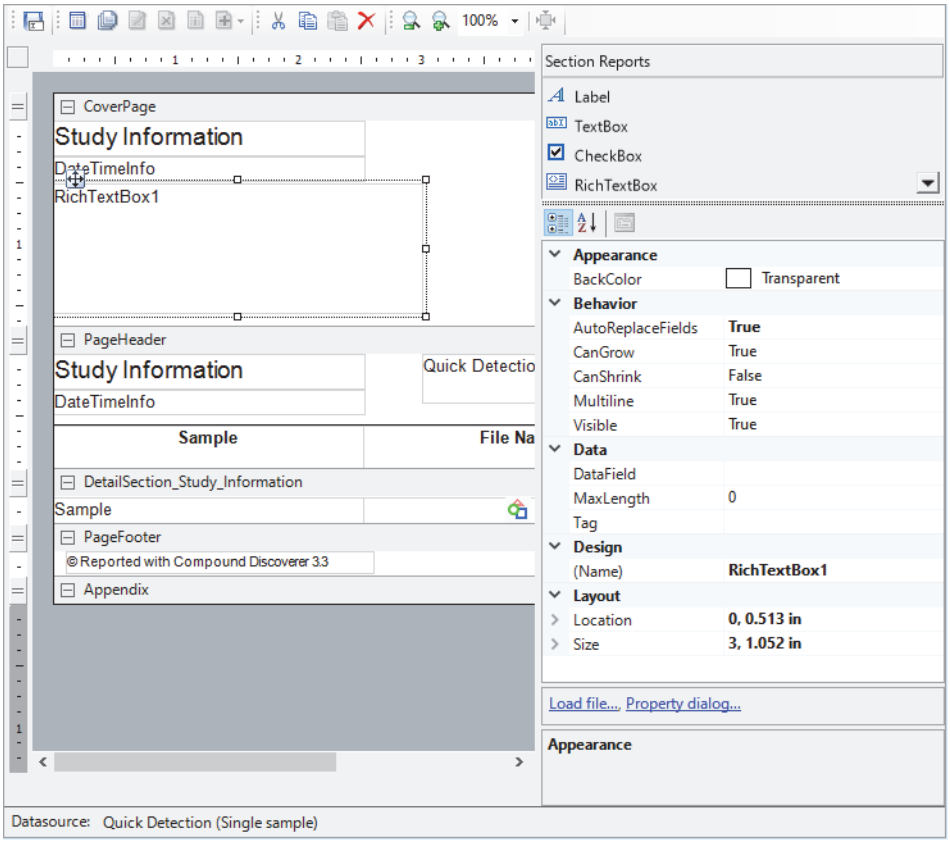
1. Open a report template for editing. See "Open a report template for editing."

2. From the Section Reports pane to the right of the workspace area, drag the RichTextBox item to the appropriate location on a workspace section of the page.

3. Do one of the following:

   - Type text in the rich text box.
   - Click the **Load File** link below the properties pane to open the Open dialog box. Then, select the file type (RTF, TXT, HTML, or HTM), browse to the file location, select the file, and click **Open**. Figure 158 shows the properties for the rich text box and the Load File link below the properties pane.

Figure 158. Properties for the rich text box



Add main table columns to a report template

Use the Add Field shortcut menu command or the Add Items icon in the upper toolbar to add data fields from a result table to the report template.

❖ To add a main table column to the report template

1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. Depending on the orientation of the table columns, do the following:

   - If the result table columns are arranged horizontally from left to right, go to step 3.
   - If the result table columns are arranged vertically from top to bottom, go to step 5.

3. To add a main table column to a column set that is arranged horizontally, do either of the following:

   - To place the new column to the right of the current column set, select the **PageHeader** bar.
   - To place the new column to the right of a specific column, select the column heading.

4. Do one of the following:

   - Right-click the **PageHeader** bar or a specific column heading, and then choose **Add Field** > ***Data Column*** from the shortcut menu.

   –or–

   a. Click the **PageHeader** bar or a specific column heading.

   b. In the toolbar, click the **Add Items** icon,  , to open a list of data column selections.

      The available items in the list include the unused data columns in the current main table. The data columns that are already in the template are unavailable and grayed out.

   c. Select an available data column from the list.

      The new data column appears to the right of the selected column or the current column set. If there is a gap to the right of the selected column or to the right of the column set, the new column fills the gap. If there is no space to the right of the selected column or to the right of the column set, the new column shares the space with the selected column or the last column in the column set.

5. To add a main table column to a column set that is arranged vertically, do the following:

   a. Use the sizing bar to display all of the data column rows.

   b. Right-click the Label column (heading) of the two-column row that is above where you want to add the new two-column data row, and choose **Add Field** > ***Data Column***.

      The new two-column data row appears below the selected two-column row.

Add data graphs to a report template

You can add the following data graphs to a report template from a compounds table—MS1 Spectrum, MS2 Spectrum, Chromatogram Trace.

❖ **To add a data graph that is associated with the main table to the report template**

1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. Do one of the following:

   - Right-click the **DetailSection_*Main_Table_Name*** bar and choose the **Add Field > *Data Graph*** of interest from the shortcut menu.

   –or–

   a. Click the **DetailSection_*Main_Table_Name*** bar.

   b. In the toolbar, click the **Add Items** icon,  , to open a list of data graphs and related table column and graph selections.

      The available items in the list include the data graphs associated with the current main table and the related tables and graphs for the current main table.

   c. Select an available data graph from the list.

The new data graph appears below the right of the last graph currently in the template.

Add mzCloud mirror plots to a report template

When the processing workflow includes the Search mzCloud node, you can add mirror plots to the report template.

- Add the mirror plots for each mzCloud hit for a compound to a report
- Create a report template for the mzCloud Results table that includes a mirror plot

Add the mirror plots for each mzCloud hit for a compound to a report

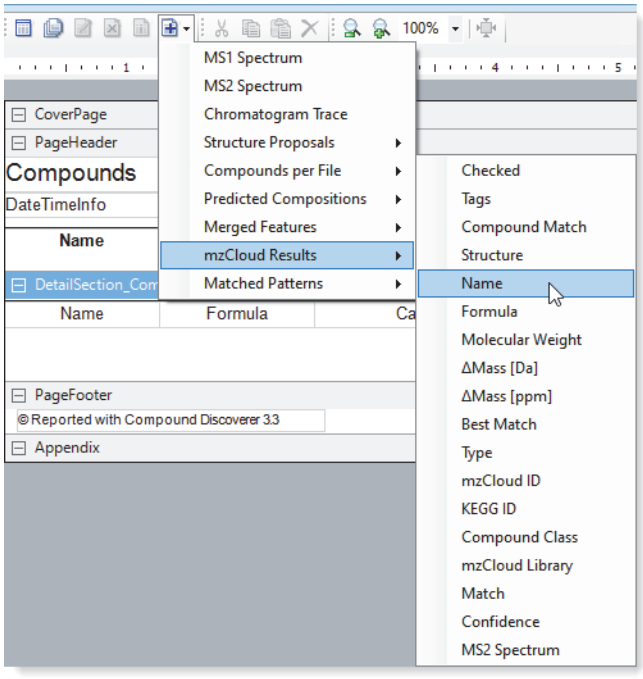
❖ **To add an mzCloud mirror plot for a to a report template**

1. Add a sub report for the mzCloud results table to the details section as follows:

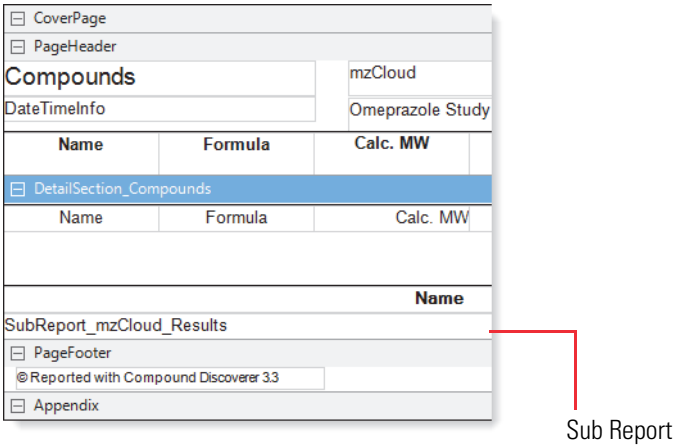
   a. Click the **DetailSection_Main_Table_Name** bar to select it.

   b. In the toolbar, click the **Add Items** icon,  , and choose **mzCloud Results > Name** (or any table columns that you want to report). See Figure 159.

Figure 159. Menu selections for the mzCloud Results table



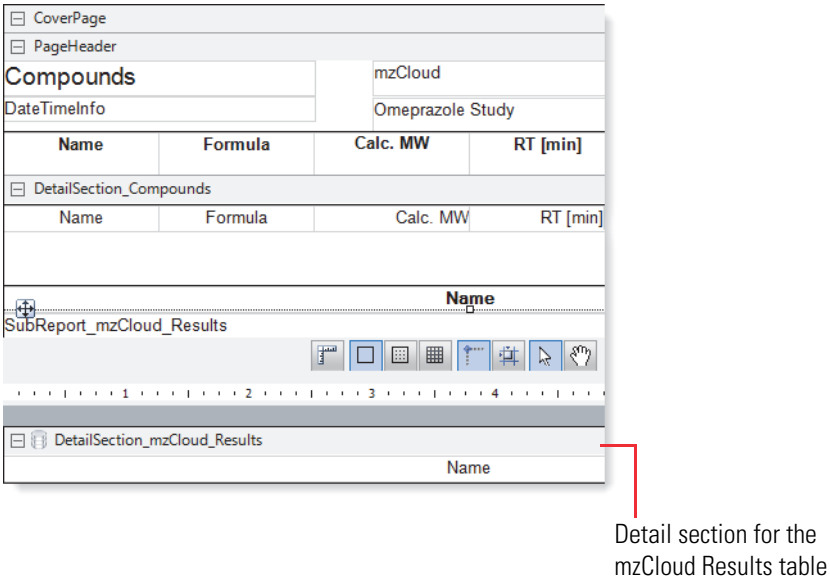
The SubReport_mzCloud_Results report appears in the DetailSection area.



2. Double-click **SubReport_mzCloud_Results**.

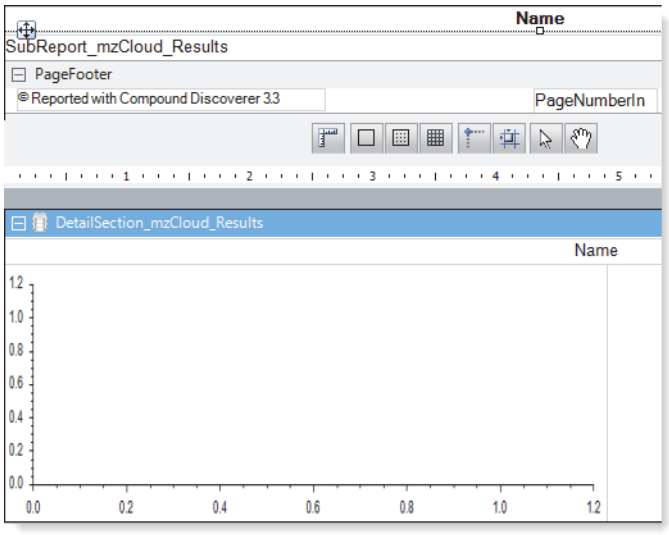
   The DetailSection mzCloud_Results area appears below the bottom toolbar. See Figure 160.

Figure 160. Detail section for the mzCloud Results table selections



3. Right-click DetailSection_mzCloud_Results and choose **Add Field > MS2 Spectrum**.

   The MS Spectrum data field appears in the detail section for the related mzCloud Results table.



Create a report template for the mzCloud Results table that includes a mirror plot

❖ **To create a report template for the mzCloud hits in the mzCloud Results table**

1. From the application menu bar, choose **Reporting > Create Report Template**.

   The Customize Report Dialog box opens.

2. In the Reported Table list, select **mzCloud Results**.

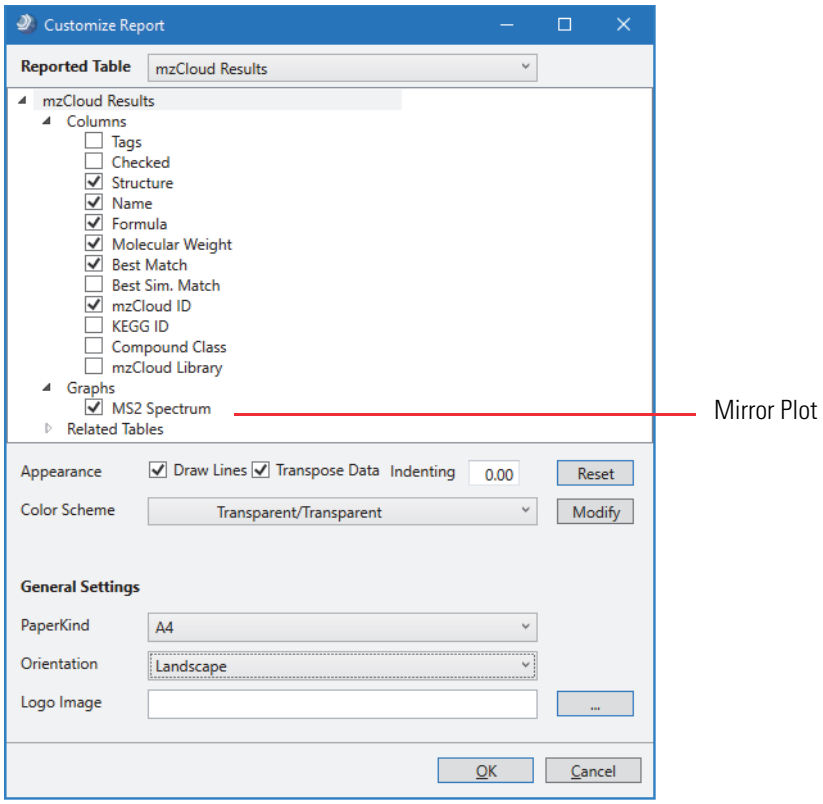
3. Under Columns select the check boxes for the table columns you want to include in the report.
4. Expand Graphs and select the **MS2 Spectrum** check box.

> **Note** The MS2 Spectrum under Graphs for the mzCloud Results table is a mirror plot of the best MS2 spectrum for the compound and its best match spectrum from the mzCloud mass spectral database.

5. Make the appropriate selections for the appearance, color scheme, paper kind, orientation, and logo image.

   For example, select the **Draw Lines** and **Transpose Data** check boxes. And, select **Landscape** for the paper orientation. See Figure 161.

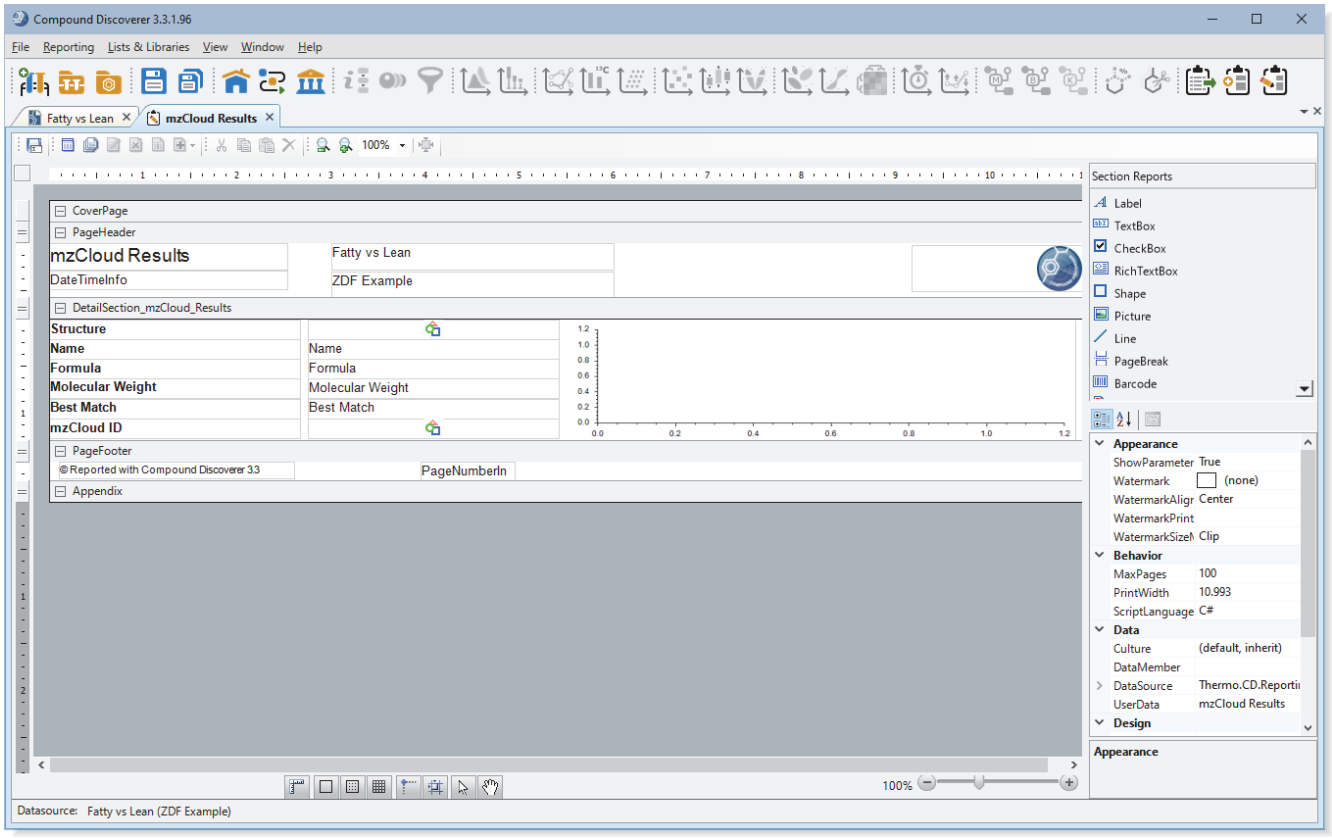
Figure 161. Customize Report box for the mzCloud Results table



6. Click **OK**.

   The template appears on the report designer page. The default print width for the landscape orientation on A4 paper is 10.993 inches. See Figure 162.

Figure 162. Report designer page with a report template for the mzCloud Results table

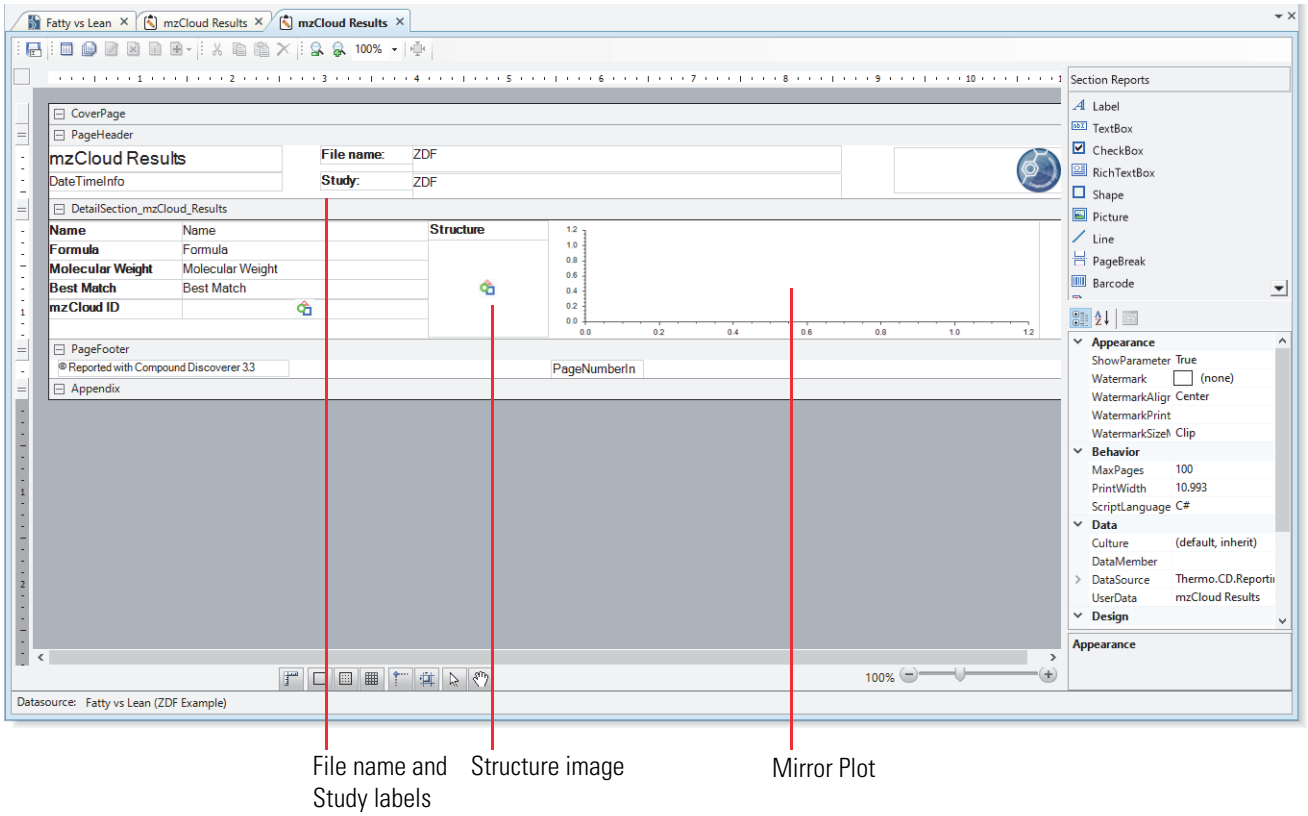


7. Modify the report template as appropriate.

   - In the Page Header section, add labels to the left of the Result File container and the Study File container by dragging the Label item from the Section Reports area at the right of the report designer page, aligning it to the left of the left of the data field container, and then typing the appropriate text in the Label container.
   - Expand the vertical size of the Detail Section for the mzCloud Results table. Then, do the following:
     - Move the Structure data field and the container for the structure image to the right of the other table columns. Then enlarge the size of the container for the structure image.
     - Adjust the widths of the Name, Formula, Molecular Weight, Best Match, and mzCloud columns on the left as appropriate.
   - In the Page Footer section, center the Page Number In container.

     By default, the x axis location of the page number is 3.948 inches and the print width for the page is 10.993 inches. To center the page number, change the location of the page number under the Layout property to 5.5 inches.

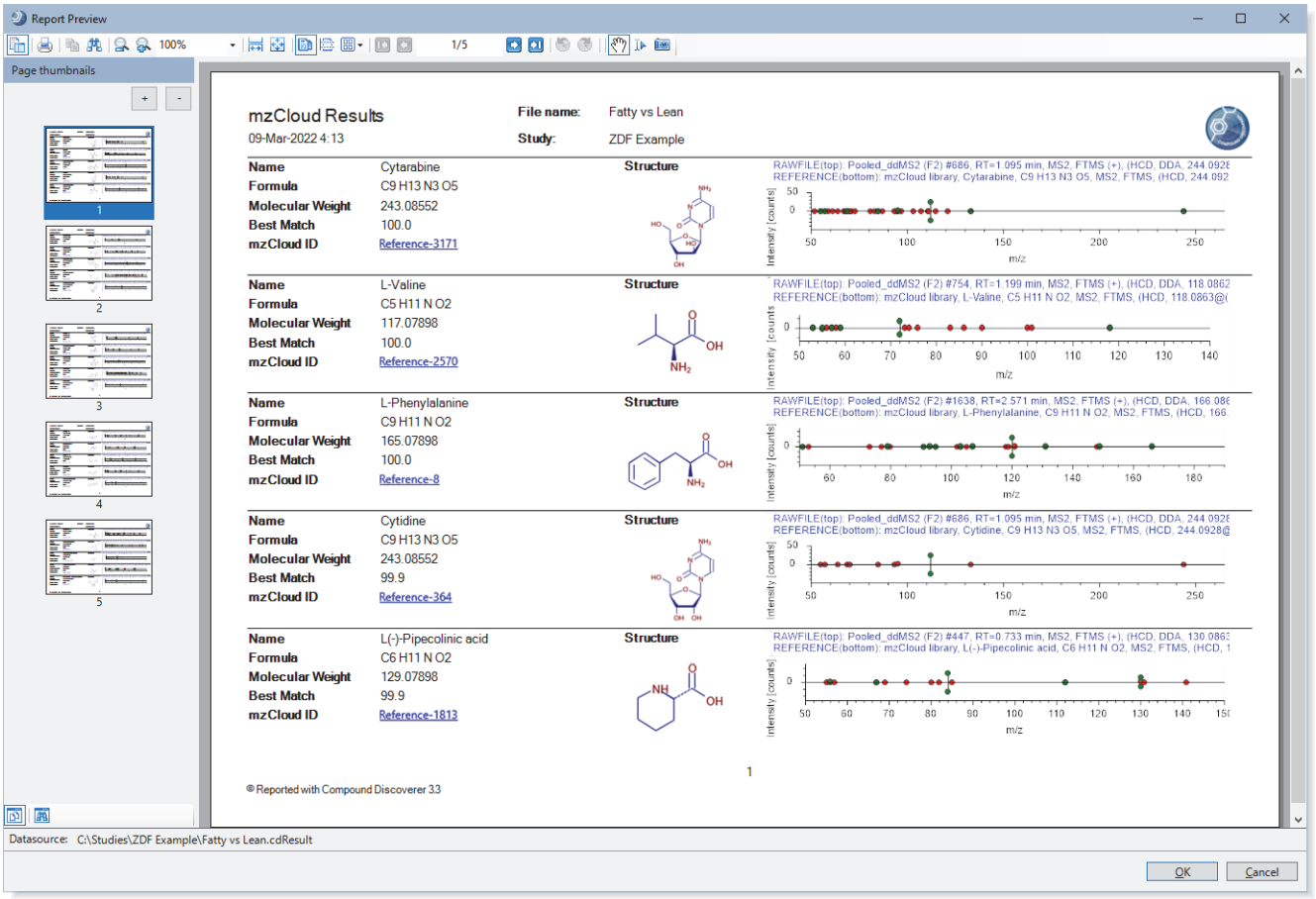
Figure 163. Modified report template for the mzCloud Results table



8. To preview the report, click the **Preview Report** icon,  .

   Figure 164 shows the report review.

Figure 164. Preview for the mzCloud Results table report



9. To save the report, do the following:
   a. In the toolbar at the top of the report designer page, click the **Save As** icon, .

      The Save Report Template As dialog box opens.

   b. Select the directory location, change the file name as appropriate, and click **Save**.

Add related table columns to a report template

When you add table columns from a related table to a report template, a subreport item appears in the report template.

❖ To add a column from a related table to a report template

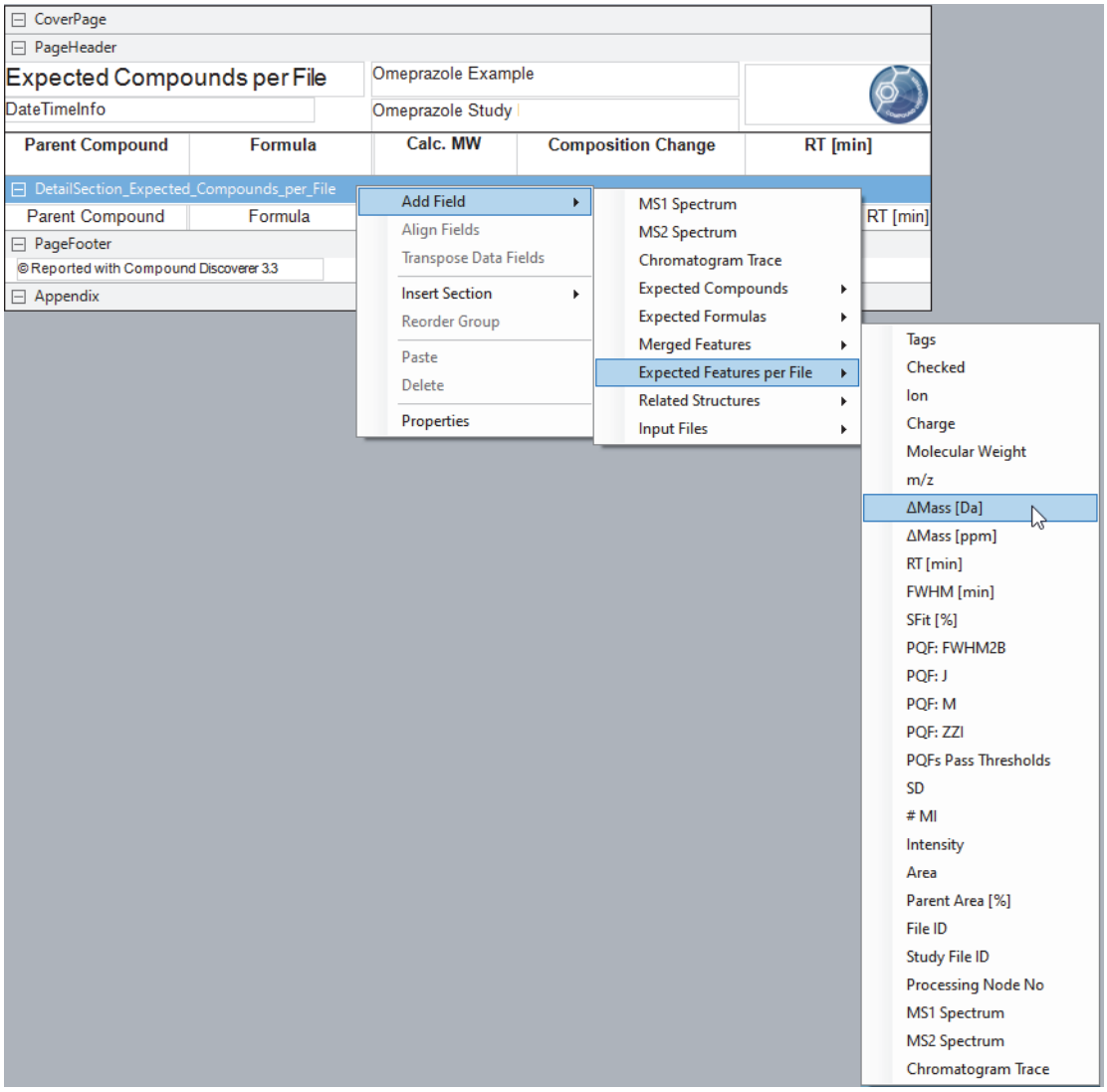
1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. Do one of the following:

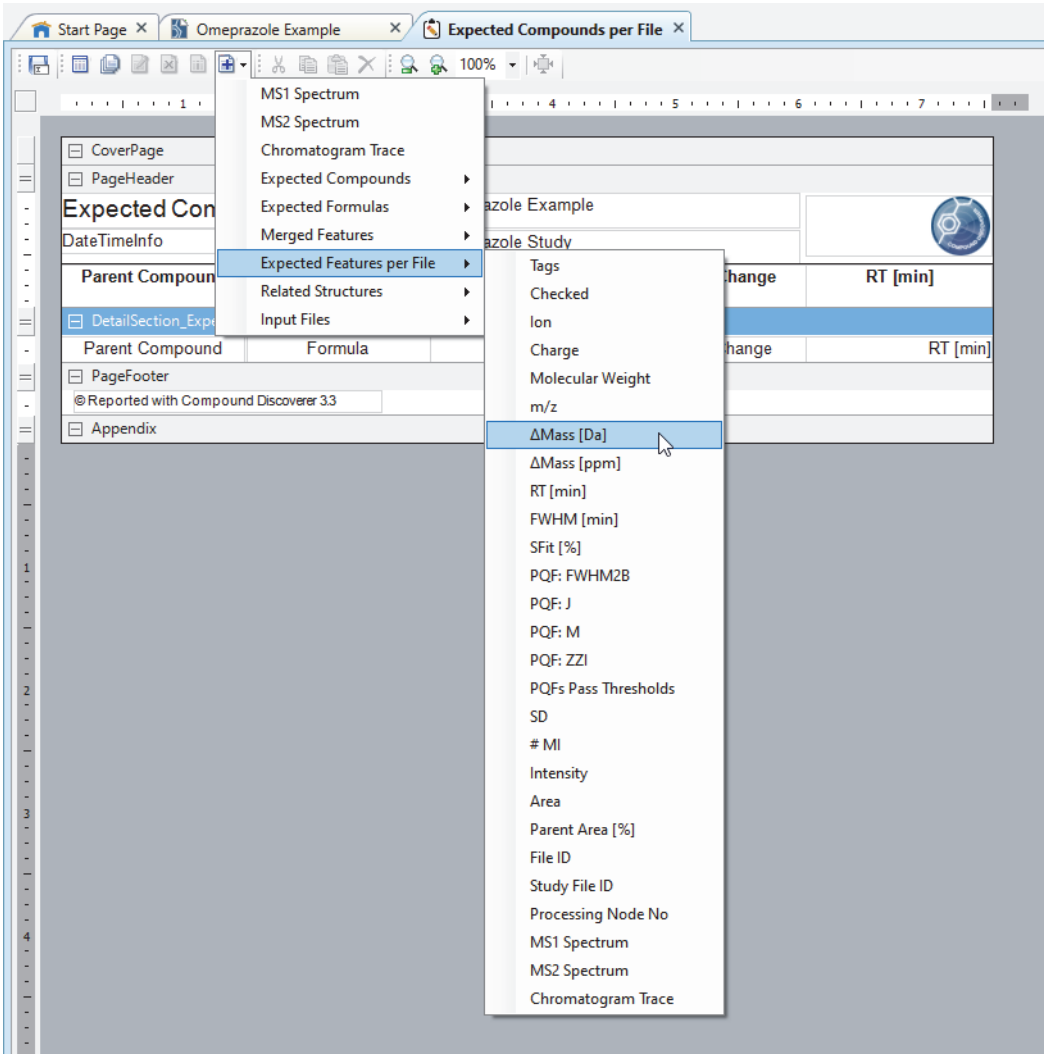
   - Right-click the **DetailSection_*Main_Table_Name*** bar and choose **Add Field > *Related Table Name* > *Column of Interest***.

     Figure 165. Using the shortcut menus to select a column from a related table



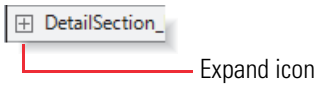
- Select the **DetailSection_*Main_Table_Name*** bar. Then, in the toolbar, click the **Add Items** icon, , select an available related table from the first list, and then select a table column from the second list.

Figure 166. Using the Add Items list to select a column from a related table



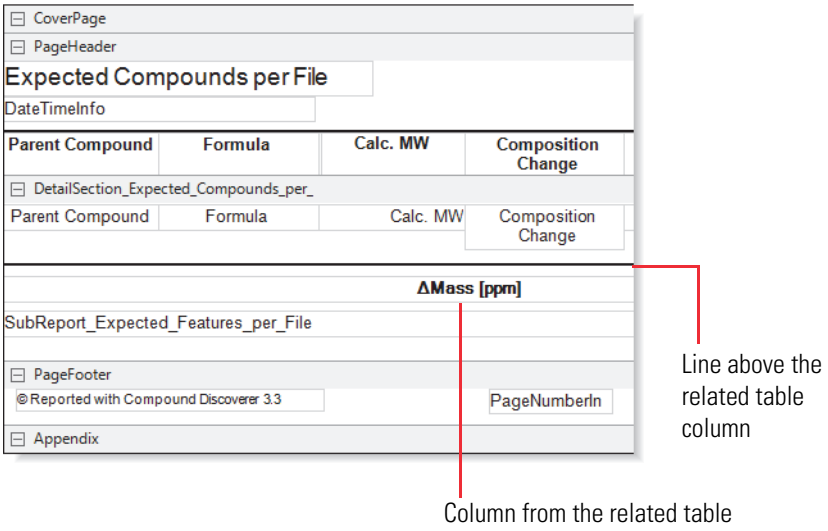
Note The available items in the first list include the data graphs associated with the current main table and the related tables for the current main table. When you select a related table from the first list, the second list includes the available columns for that table.

3. If the DetailSection is collapsed, click the expand icon to open the section.



The added table column appears at the bottom of the DetailSection (data area). The application automatically adds a line above the column heading.

Figure 167. Expected Compounds per File table with the ΔMass [ppm] column from the related Expected Features per File table



Edit the properties of subreport columns in a report template

❖ To edit the properties of subreport columns

1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. To open the subreport editor area, do one of the following:

   - Double-click the **Subreport_*Related_Table_Name*** box.

   –or–

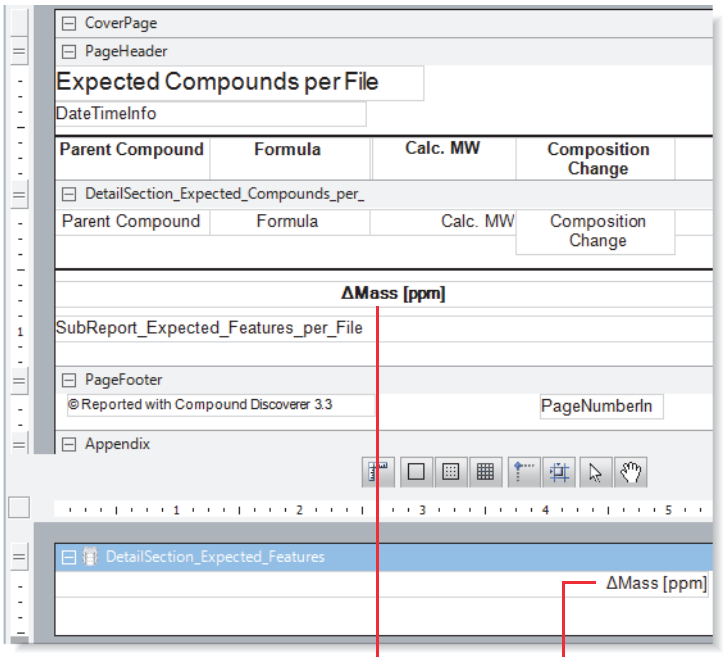
   a. Select the **Subreport_*Related_Table_Name*** box.

      The Edit Sub-Report icon, , becomes available.

   b. Click the **Edit Sub-Report** icon.

The TextBox item for the related table column appears in a separate section. The container for the item is sized to the full width of the page.

Figure 168. Report template page with the subreport section open

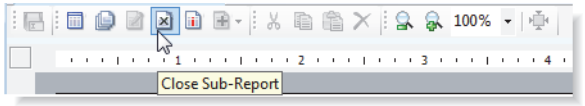


3. To change the properties of the TextBox item in the subreport section, select it.

   The properties for the selected item appear in the properties pane to the right of the workspace.

4. Make changes as necessary in the properties pane, or click the property dialog link below the properties pane to open the TextBox dialog box and make similar changes.

5. To close the subreport section, click the **Close Sub-Report** icon in the report designer toolbar.



Move a subreport column to the main table of a report table

❖ **To move a subreport column up to the set of main table columns**

1. Open the report template. See "Open a report template for editing."

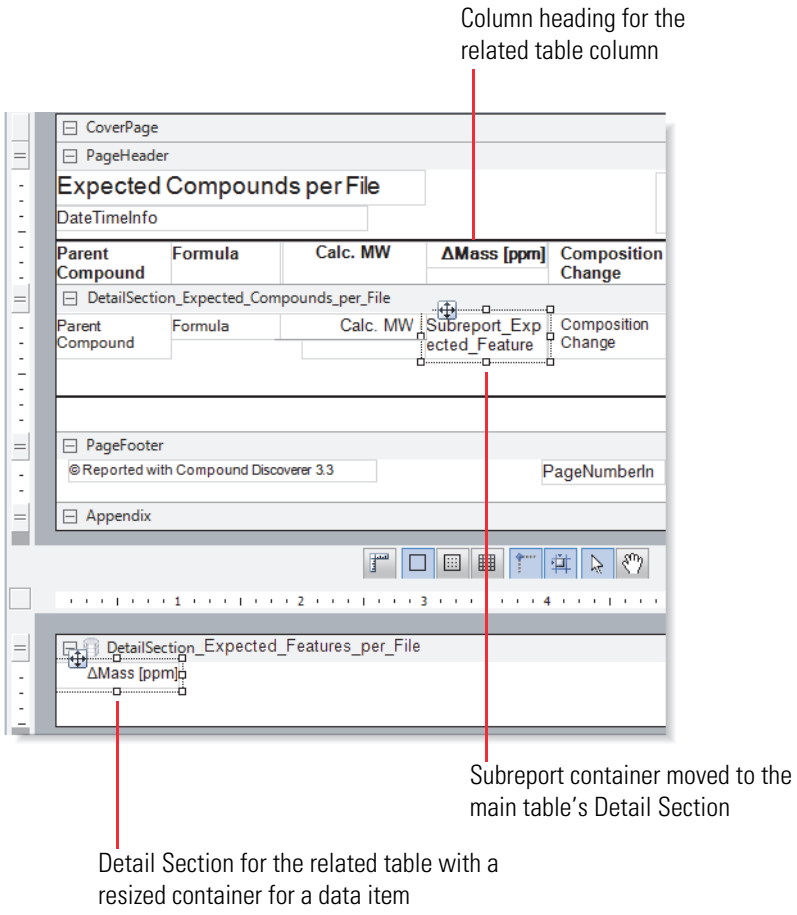
   The report template opens as a tabbed page in the application window.

2. Resize the column heading container for the subreport column. Then, move it to an appropriate location in the set of labels for the main table columns.
3. Resize the Subreport_*Related_Table_Name* container. Then, move it to the appropriate location in the Detail Section.
4. Double-click the Subreport_*Related_Table_Name* container that you moved to the Detail Section.

   The DetailSection_*Related_Table_Name* appears below the bottom toolbar.
5. In the related table's Detail Section, resize the containers for the data items from the related table.

   Figure 169 shows a report template for the Expected Compounds per File table with an additional column from the related Expected Features per File table.

Figure 169. Related table column moved up to the main table



Modify the properties of a section report item

On the report template page, you can edit the position and size of an item by using the mouse or the properties pane on the right. You can also edit other properties for an item from the properties pane or the specific dialog box for the item.

❖ To modify the properties of a section report item

1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. Select the item.

   The properties for the selected item appear in the properties pane, at the bottom right of the report template page. For information about the properties of each item, see "Property settings for the sections and items in a report template."

3. Do any of the following:

   - To move the item to another position, do either of the following:
     - Move the item by dragging it (or you can use the arrow keys on the keyboard).
     - In the Properties pane, under Layout, expand Location, and then change the X and Y values.
   - To resize the container for the item, do either of the following:
     - Resize the item by dragging the handle points of the container.
     - In the Properties pane, under Layout, expand Size, and then change the Width and Height values.
   - To change other properties for the item, do either of the following:
     - Modify the properties in the Properties pane.
     - Click the **Property Dialog** link at the bottom right of the report template page, and then modify the property in the item-specific dialog box.

     Note For the RichTextBox item, in addition to the Property Dialog link, you can click the Load File link to load text from a file. See "Add a rich text box to a report template."

Add page breaks to a report template

❖ **To add a page break between reported result table rows**

1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. On the report template page, drag the PageBreak item from the Section Reports pane to the bottom of the Detail Section of the report template.

Delete a pair of workspace sections on the report template page

Note The report template page pairs these sections together:

- Cover Page and Appendix
- Page Header and Page Footer

When you select one of the paired sections to delete, the application removes both sections. You cannot delete one section without deleting the other, and you cannot delete the Detail Section section.

❖ **To delete a pair of workspace sections**

1. Open the report template. See "Open a report template for editing."

   The report template opens as a tabbed page in the application window.

2. Select one of the workspace sections by clicking the section header or by clicking within the section area.

3. From the shortcut menu, choose **Delete**.

Resize the sections of a report template

Use the sizing bar to the left of the workspace to resize each workspace section vertically, except for the Appendix section. See "Workspace sections and sizing bar on the report template page."

Tip Make sure to enlarge the workspace section enough to hold all of the items that you want to add to that section of the template.

The size of a section on the report template page is not necessarily the same as its size in the generated report.

❖ To vertically resize a workspace section

1. Open the report template. See "Open a report template for editing."

   The report template page opens as a tabbed page in the application window.

2. Do any of the following:

   - For the CoverPage, PageHeader, DetailSection, and PageFooter sections, do the following
     - In the sizing bar, drag the sizing handle.
     - To vertically enlarge a workspace section, drag down the handle that is aligned with the header of the subsequent section. To reduce a workspace section, drag the handle up.
   - To enlarge the Appendix section, drag it down by the bottom edge of the report template page. To reduce this workspace section, drag the bottom edge up.

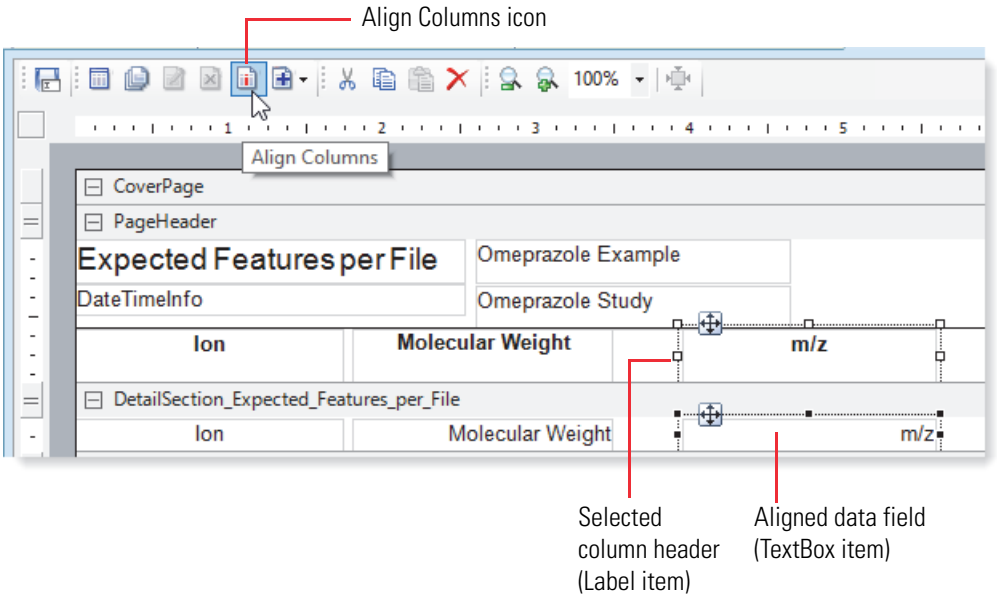
Add, align, and transpose columns in a report template by using the shortcut menu commands

See the following table for information about using the shortcut menu for the report template page to modify a report template.

Table 169. Using the shortcut menu commands on the report template page (Sheet 1 of 2)

Task	Do the following
Open the shortcut menu for the report template page.	Right-click the report template page.
Add an item to a section of the report template.	Right-click the section bar of a section area and choose **Add Field >** ***Item of Interest***.

Table 169. Using the shortcut menu commands on the report template page (Sheet 2 of 2)

Task	Do the following
Align a column heading to its associated data field.	1. In the PageHeader section, right-click the column heading (Label item) that you want to align with its associated data field (TextBox item). The Align Columns icon becomes available.  2. From the shortcut menu, choose **Align Fields**.
Transpose the data fields (columns to row or rows to columns)	1. Right-click a column heading (Label) or a column data field (TextBox) and choose **Transpose Data Fields**. 2. To undo the change, if necessary, right-click a column heading (Label) or a column data field (TextBox) and choose **Transpose Data Fields**.

Add a border to an item by using the Format Border command

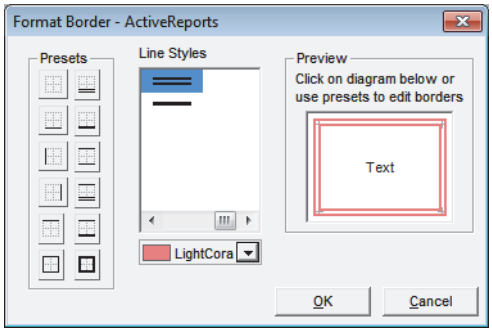
You can add a border or modify the current border of any item in the workspace area of a report template.

❖ To add a border to an item

1. Open the report template that you want to edit.
2. Right-click the item of interest in the workspace of the report template and choose **Format Border**.

   The Format Border dialog box opens.

Figure 170. Format Border dialog box with the selection of a coral, double-line border



3. To set up the border, click one of the icons in the Presets area or select the line style in the Line Styles area, and click the appropriate sides of the square in the Preview area.

Reference information for the report template page

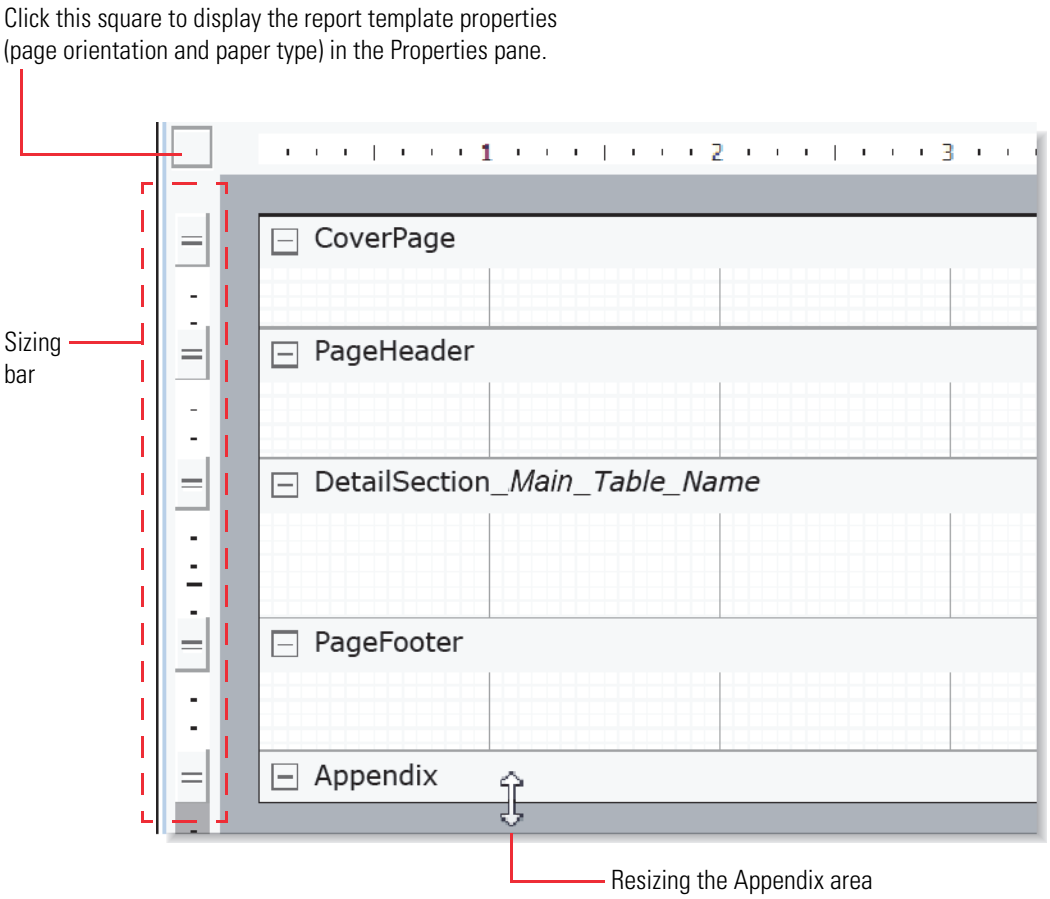
For information about the editing tools on the report template page, see these topics:

- Workspace sections and sizing bar on the report template page
- Report template page toolbars
- Shortcut menu commands for the report template page
- Section report items for a report template
- Property settings for the sections and items in a report template
- Open the property dialog box for a workspace section or a specific report item

Workspace sections and sizing bar on the report template page

Figure 171 shows the five workspace sections, the sizing bar on the left, and the icon that opens the page orientation and paper type options in the upper-left corner.

Figure 171. Workspace sections, sizing bar, and icon that opens the page size options



By default, the workspace on the report template page has five sections. Table 170 lists these sections, from top to bottom.

Table 170. Default workspace sections (Sheet 1 of 2)

Workspace section	Description
Cover Page	Appears as the first page of a report with the following property selections: • True—For the Visible parameter in the Behavior section of the properties pane. Default: False • After—For the NewPage parameter in the Data section of the properties pane. Default: After. See "NewPage." To display the Cover Page section without a page break between it and the next section, select **True** for the Visible parameter and **None** for the New Page parameter. Use this section to add nonrepeating information, such as the report title, date-and-time stamp, and company logo.
Page Header	Adds items to the top of each report page. The standard templates include a Label item with the main table name, a TextBox item with a time stamp, and a Picture item with a company logo. The column headings (Label items) appear here when you add table columns to the report.
Detail Section (concatenated with the selected *Main_Table* name)	Adds data from the result file, such as the repeating items (TextBox item) of a main table or the data graphs for each table row.
Page Footer	Adds information to the footer of each report page, for example, the page number. Report templates created with the Customize Reports dialog box automatically include a page number at the bottom of each page. The page number is a TextBox item.

Table 170. Default workspace sections (Sheet 2 of 2)

Workspace section	Description
Appendix	Adds information to an appendix section of the report. An Appendix section appears after the last page of a report, with the following property settings: • True—For the Visible parameter in the Behavior section of the properties pane Default: False • Before—For the NewPage parameter in the Data section of the properties pane Default: Before To display the Appendix section without a page break between it and the previous section, select **True** for the Visible parameter and **None** for the NewPage parameter.

Report template page toolbars

Table 171 describes the toolbars on the report template page.

For more information about the report template page, see "Edit existing report templates."

Table 171. Toolbars on the report template page (Sheet 1 of 4)

Icon	Description
Top toolbar	
	Save Active Item—Saves the report template using the same file name. By default, the template file name is the same name as the main table that you selected in the Customize Report dialog box. See "Create new report templates."
	Save As—Saves the report template using a different file name.
	Preview—Opens the Report Preview dialog box. See "Preview and print a report."
	Print—Opens the Report Print dialog box.

Table 171. Toolbars on the report template page (Sheet 2 of 4)

Icon	Description
	Edit Sub-Report—Enlarges a selected subreport so that you can edit it. Selecting a subreport item makes this icon available. When you click this icon, the report designer opens the subreport in a separate Detail Section workspace section. You can zoom in on this temporary section or zoom out of it. Increasing the size of this temporary section does not affect the report template page. **Note** Related tables that you select in the Customize Report dialog box appear as subreports on the report template page.
	Close Sub-Report—Closes the separate subreport workspace section. Clicking anywhere in the separate subreport workspace makes this icon available.
	Align Columns—Aligns the Label (column heading) and Textbox (data) containers for the selected column or columns. Selecting a report column makes this icon available.
	Add Items—Opens a list of items that you can add to the currently selected section of the report template. Clicking within a workspace section or the section header makes this icon available. The list of items varies depending on the selected section: • CoverPage and DetailSection sections: You can add related table columns or graphs that are not currently in the template. • PageHeader section: You can add main table columns that are not currently in the template. The column heading appears in the PageHeader section as a Label item, and the container for the column data appears in the DetailSection as a TextBox item.
	Cut—Deletes the selected item without confirmation.
	Copy—Copies the selected item.
	Paste—Pastes the selected item.
	Delete—Deletes the selected item after you click OK in the confirmation dialog box.

Table 171. Toolbars on the report template page (Sheet 3 of 4)

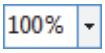
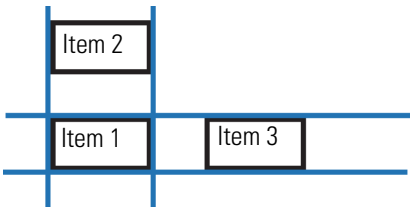
Icon	Description
	Zoom Out—Reduces the magnification of the page.
	Zoom In—Increases the magnification of the page.
	Magnification box—Displays the magnification percentage.
	Actual Size—Displays the page at 100% magnification. Changing the magnification by using the Zoom In and Zoom Out icons or by typing a value in the magnification box makes this icon available.
Bottom toolbars	
	Dimension Lines—Displays dimension lines () as you resize an item by using the mouse.
	Hide Grid—Clears the grid on the page.
	Show Dots—Shows the main grid lines and the small dots within the grid.
	Show Lines—Shows the main grid and the smaller lines within the grid.
	Snap Lines—When you move an item on the page, blue alignment lines appear. When the selected item (Item 1 below) is horizontally aligned with another item, two vertical lines bracket the aligned items. When the selected item is vertically aligned with another item, two horizontal lines bracket the aligned items. 
	Snap to Grid—When you move an item on the page, this mode automatically snaps it to the smaller grid lines.
	Select Mode—Use this mode to select items on the page. To select multiple items, press the SHIFT key while you select the items.

Table 171. Toolbars on the report template page (Sheet 4 of 4)

Icon	Description
	Pan Mode—When the page is zoomed in, use this mode to move to a different part of the page.
	Magnification bar—Move the slider to the left to zoom out and to the right to zoom in. The magnification percentage appears to the left of the slider.

Shortcut menu commands for the report template page

Table 172 describes the shortcut menu commands for the report template page.

Table 172. Report template page shortcut menu (Sheet 1 of 2)

Command	Description
Add Field	Adds the item that you choose to the selected workspace section.
Align Fields	Aligns a column header or subreport with the associated data. This command becomes available when you select a column header or a subreport.
Transpose Data Fields	Transposes the data from columns to rows or from rows to columns. This command becomes available when you select a column header.
Note The Insert Section command is available if the template does not already include a Report Header/Footer section or a Page Header/Footer section.	
Insert Section > Report Header/Footer	Inserts the ReportHeader and ReportFooter sections.
Insert Section > Page Header/Footer	Inserts the PageHeader and PageFooter sections.
Copy	Copies the selected item.
Paste	Pastes the selected item.
Cut	Removes the selected item without confirmation.
Delete	Deletes the selected item after you click OK in the confirmation dialog box.
Bring to Front	Moves the selected item to the front, on top of other surrounding items.
Send to Back	Moves the selected item to the back, beneath all other surrounding items.

Table 172. Report template page shortcut menu (Sheet 2 of 2)

Command	Description
Format Border	Opens the Format Border dialog box where you can change an item's border layout, line style, and color.
Properties	Highlights the (Name) property in the properties pane of the report template page.

Section report items for a report template

The Section Reports pane to the right of the workspace on the report template page contains all of the different items that you can add to the report template.

Figure 172. Section Reports pane of the report template page

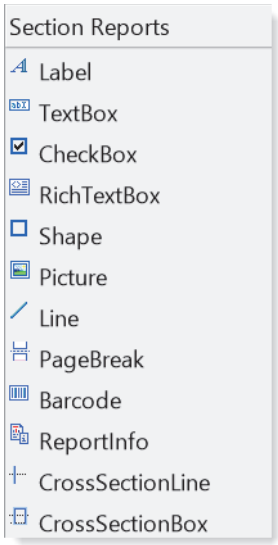


Table 173 describes the items in the Section Reports pane.

Table 173. Items in the Section Reports pane (Sheet 1 of 3)

Item	Description
Label	A text label that you can add to the report. For example, the File Name and Study Name labels in the Page Header section of the report templates provided with the application are labels.
TextBox	A text box that is usually used to group multiple items together. The application uses the TextBox item to display the repeating tabular data in the result file.
	IMPORTANT Use the Rich Text Box item rather than the TextBox item to add fixed (non-dynamic) text to the report's cover page.
CheckBox	A check box that you can select or clear.

Table 173. Items in the Section Reports pane (Sheet 2 of 3)

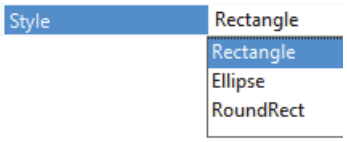
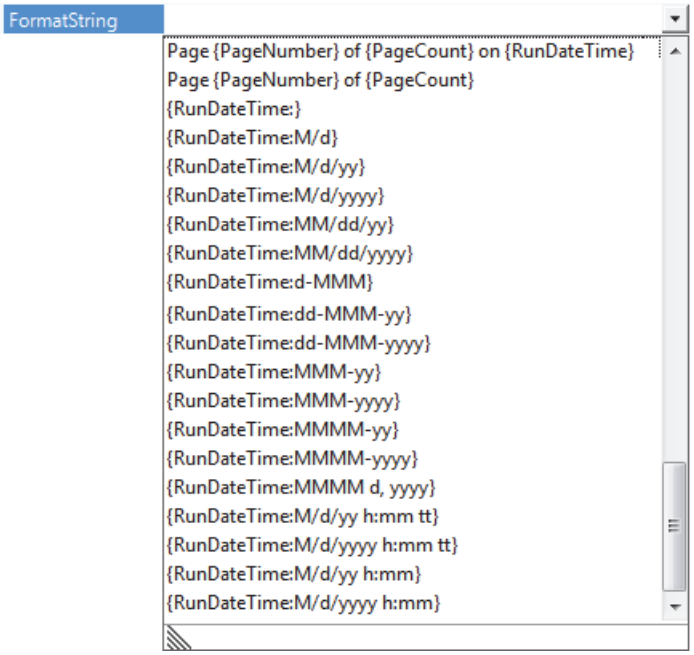
Item	Description
RichTextBox	A text box that you can populate by typing text in the box or by loading text from a file. Use the Load File link below the properties pane on the right to select and open a text file.
Shape	A geometric shape such as a rectangular or square box (with either square or rounded corners), an ellipse, or a circle.  **Tip** When you add this item, by default, it appears as a rectangular box with square corners. To change to a different shape, modify the Style property under Appearance in the properties pane.
Picture	A container for a graphic.
Line	A straight line.
PageBreak	A break to push the subsequent content to the next page. To place reported table rows on separate pages, add a page break at the bottom of the DetailSection.
Barcode	A bar code. For information about setting up the Barcode properties, refer to the *ActiveReports User Guide* on the company website for Grape City.

Table 173. Items in the Section Reports pane (Sheet 3 of 3)

Item	Description
ReportInfo	A variable that the application automatically replaces with real-time data in the generated report. Use the ReportInfo item to show the current page number or to add a date-and-time stamp. Select the page number or date-and-time stamp from the FormatString list under Appearance in the Properties pane. 
CrossSectionLine	A line that can span across multiple workspace sections on the report template page. **Note** You cannot add this item to the Detail Section workspace section. However, you can add it to another section (for example, the Page Header section) and have it span across the Detail Section section.
CrossSectionBox	A box that can span across multiple workspace sections on the report template page. **Note** You cannot add this item to the Detail Section workspace section. However, you can add it to another section (for example, the Page Header section) and have it span across the Detail Section section.

Property settings for the sections and items in a report template

On the report template page, the properties pane to the bottom right of the workspace includes all of the property settings that you can use to format a workspace section or an item in the report template. The settings vary depending on the selected workspace section or item.

If it is available, click the expand icon, ▷, to open the settings for a particular property or the collapse icon, ◢, to close the settings.

The properties pane contains these property groups, from top to bottom:

- Appearance properties
- Behavior properties
- Data properties
- Design properties
- Layout properties
- Miscellaneous properties

IMPORTANT The Summary properties are not functional.

Tip To open a report template for editing, see "Open a report template for editing."

For information about opening the properties dialog box for a report item, see "Open the property dialog box for a workspace section or a specific report item."

Appearance properties

Table 174 describes the Appearance properties for report template items.

Table 174. Appearance properties in the Properties pane (Sheet 1 of 3)

Property	Description
AnchorBottom	(For the Line item only) Specifies whether the line is anchored to the bottom of the workspace section. Selections: • False—Does not anchor the line to the bottom of the workspace section. • True—Anchors the line to the bottom of the workspace section.
Alignment	(For the Label, TextBox, ReportInfo, and Barcode items) Specifies the horizontal alignment of the text within the container. (For the Barcode item) Specifies the horizontal alignment of the caption text that is associated with the bar code. You enable the caption text by setting the CaptionGrouping and CaptionPosition properties.
BackColor	Specifies the background or fill color.
BarHeight	(For the Barcode item only) Specifies the height of the bar code.
CaptionGrouping	(For the Barcode item only) Selections: • False—Does not enable a text caption to be associated with the bar code. • True—Enables a text caption.
CaptionPosition	(For the Barcode item only) Sets the position of the caption container relative to the bar code symbol.  Selections: • None—Hides the caption. • Above—Sets the position above the symbol. • Below—Sets the position below the symbol, as in the figure above.
CharacterSpacing	(For the Label and TextBox items) Specifies the spacing between the characters in the text, in points. Default: 0

Table 174. Appearance properties in the Properties pane (Sheet 2 of 3)

Property	Description
ClassName	Specifies the name of the class for a particular format. Default: Normal
Font	(For the Label, TextBox, and CheckBox items) Specifies the name of the font and other font characteristics such as the style, size, effects, and script. Clicking the browse icon, ..., opens the Font dialog box where you can specify the font characteristics. Clicking the expand icon, ▷, expands the settings.
Font > GdiCharSet	Specifies the GDI character set to use. For a list of valid values, refer to the GdiCharSet Property in the Microsoft Developer Network (MSDN) Library.
Font > GdiVerticalFont	Specifies that the font is derived from a GDI vertical font.
ForeColor	(For the Label, TextBox, and CheckBox items) Specifies the font color.
FormatString	(For the ReportInfo item only) Specifies the format of the generated content as a page number or a date-and-time string.
LineColor	Specifies the color of a line or border.
LineSpacing	Specifies the spacing between multiple lines of content, in points.
LineStyle	Specifies the style of a line or border.
LineWeight	Specifies the thickness of a line or border, in pixels.
NarrowBarWidth	(For the Barcode item only) Specifies the width of the narrow bars in the bar code (a value of 1.0 equals 0.864 points). **Tip** At a thicker width for the narrow bars, the entire bar code might be too large for the container. In this case, enlarge the size of the container to see the entire bar code.
NWRatio	(For the Barcode item only) Specifies the ratio of the width of the wide bars relative to the width of the narrow bars in the bar code. The larger the ratio, the thicker the wide bars appear. **Tip** At a thicker width for the wide bars, the entire bar code might be too large for the container. In this case, enlarge the size of the container to see the entire bar code.

Table 174. Appearance properties in the Properties pane (Sheet 3 of 3)

Property	Description
OutputFormat	(For the TextBox item only) Specifies the format settings for custom content, or for a number, currency, date, time, or percentage. Clicking the browse icon, ..., for this property opens the OutputFormatDialog box (see Figure 157 on page 583) where you can change the settings. Do not change the OutputFormat settings for data fields from a result table column.
PictureAlignment	(For the Picture item only) Specifies the alignment of the selected image with respect to the container. For proper alignment, the container must be larger than the image. Selections: TopLeft, TopRight, Center, BottomLeft, and BottomRight
QuietZone	(For the Barcode item only) Specifies the left, right, top, and bottom margins of the quiet zone for the bar code, in inches.
Rotation	(For the Barcode item only) Specifies the rotation of the bar code within the container. **Tip** At a rotation of 90 or 270 degrees, the entire bar code might be too large for the container. In this case, enlarge the size of the container to see the entire bar code.
Style	Specifies the format settings such as color, alignment, font, geometric shape, or bar code properties.
SupplementOptions	(For the Barcode item only) Specifies the supplement options (2- or 5-digit add-ons for EAN/UPC bar codes).
TextJustify	(For the Label and TextBox items) Specifies how to distribute the text when you set the Alignment property to Justify.
VerticalAlignment	(For the Label and TextBox items) Specifies the vertical alignment of the text within the container. Selections: Top, Middle, and Bottom
VerticalText	Specifies the vertical alignment for the text. • False—Does not render the text according to the vertical layout settings. • True—Renders the text according to the vertical layout settings.
WrapMode	Specifies that a long line of text wraps to the beginning of the next line to fit in the container.

Behavior properties

Table 175 describes the Behavior properties for report template items.

Table 175. Behavior properties in the Properties pane (Sheet 1 of 3)

Behavior property	Description
Angle	Specifies the slope of the text within the container, in degrees.
AutoReplaceFields	(For the RichTextBox item only) Specifies whether the data in the container is automatically replaced with the data from the data source as specified by the Data Field property selection. • False—Does not automatically replace the fields of the object with the fields in the data source that are assigned to the current workspace section. • True—Automatically replaces the fields of the object with the fields in the data source that are assigned to the current workspace section.
AutoSize	(For the Barcode item only) Specifies whether the barcode item stretches to fill its container. Selections: True or False
CanGrow	Specifies whether the container or section can increase in height to fit its contents. Selections: True or False
CanShrink	Specifies whether the container or section can decrease in height to fit its contents. Selections: True or False
CheckAlignment	(For the CheckBox item only) Specifies the alignment of the check box in the container.
Checked	(For the CheckBox item only) Specifies whether the CheckBox item appears with or without a check mark in the report. Selections: • False—Shows the check box selected. • True—Shows the check box cleared.
CheckSumEnabled	(For the Barcode item only) Specifies whether the application computes and includes a checksum in the bar code. Selections: True or False

Table 175. Behavior properties in the Properties pane (Sheet 2 of 3)

Behavior property	Description
ColumnDirection	(For the Detail Section workspace section only) Specifies whether to display the data columns in the down-and-across direction or the across-and-down direction, for a multi-column (newspaper-style) report. Selections: DownAcross or AcrossDown
Enabled	(For the PageBreak item only) Specifies whether the PageBreak item is enabled. Selections: True or False
KeepTogether	(For the Detail Section and Appendix workspace sections only) Specifies whether the contents of the current section prints on a single page. This property does not shrink items to fit; rather, it acts like a page break between reported table rows. Selections: True or False
MultiLine	(For the Label, TextBox, ReportInfo, and RichTextBox items only) Specifies whether the report template displays only the content that fits on one line or displays all the lines that fit in the container. Selections: True or False
PrintAtBottom	(For the Appendix workspace section only) Specifies where the design items in the Appendix section are printed. Selections: • False—Places the Appendix design items immediately after the DetailSection and before the page footer information. • True—Places the Appendix design items at the bottom of the current page just above the page footer information.
RepeatToFill	(For the Detail Section workspace section only) False—Does not repeat content to fill the report page. True—Repeats content to fill the report page.
RightToLeft	(For the Label, TextBox, and ReportInfo items) Specifies whether the text is aligned with the right side of the container. Also supports locales that use right-to-left fonts. Selections: True or False

Table 175. Behavior properties in the Properties pane (Sheet 3 of 3)

Behavior property	Description
ShrinkToFit	Specifies whether the font size of the text within the selected container shrinks to fit the container. If the WrapMode property under Appearance is set to WordWrap, the application first wraps the text to fit the container and then shrinks the text to fit the container. Selections: True or False
Visible	Specifies whether the selected item appears in the report. By default, the Cover Page and Appendix sections are set to False, and therefore, do not appear in the report. Selections: True or False

Data properties

Table 176 describes the Data properties.

Table 176. Data properties in the Properties pane (Sheet 1 of 3)

Data property	Description
ColumnCount	(For the Detail Section workspace section only) Specifies the number of columns in the report, similar to a newspaper layout. Default: 1 When the template contains data columns that match the layout of the main table (data columns displayed from left to right), use the default value of 1 (ColumnCount = 1) for the number of columns. **Tip** Increasing the number of columns per page works with transposed data columns (transposed from rows to columns).
CountNullValues	(For the Textbox item only) False—Does not include null values as zeros in the summary fields. True—Includes null values as zeros in the summary fields.
ColumnSpacing	(For the Detail Section workspace section only) Specifies the space between columns (newspaper style) in a multi-column report.
Culture	(For the Textbox item only) Formats the report data based on the selected culture from a particular country or region. Default: Inherit

Table 176. Data properties in the Properties pane (Sheet 2 of 3)

Data property	Description
DataField	Specifies the data source (main table column, related table column, or data graph) for the content. **IMPORTANT** For best results, do not manually modify the content of this box; that is, do not select from the associated dropdown list or type text in the box. To change an item to another item, delete the current item. Then, add a new item as described in these topics: • Add main table columns to a report template • Add data graphs to a report template.
Description	(For the Picture item only) Not implemented.
Hyperlink	Sets to a URL address for a specific location. The application automatically converts this URL to a hyperlink in the HTML or PDF exported reports.
Image	(For the Picture item only) Opens the Open dialog box where you can find and select the image file. The default file types for the search are image files.
MaxLength	(For the Rich Textbox item only) Specifies the maximum number of characters to be displayed.
NewColumn	(For the Detail Section workspace section only) Specifies where a new column is printed. The default number of report columns is 1. The standard report templates contain only one column and the Customize Reports dialog box creates reports with one column. In this context, a column is a formatting option, not a table column from a result table.

Table 176. Data properties in the Properties pane (Sheet 3 of 3)

Data property	Description
NewPage	Specifies whether a page break is inserted before, after, or both before and after the section. Default settings: • CoverPage—After • DetailSection—None • Appendix—Before CoverPage section: • None—No page break between the cover page and the next section. • Before—No effect. • After—Adds a page break between the cover page and the next section. • BeforeAfter—Adds a page break between the cover page and the next section. DetailSection: • None—No page break between the table rows. • Before—Adds a page break between each table row. • After—Adds a page break between each table row. • BeforeAfter—Adds a page break between each table row. Appendix section: • None—No page break. • Before—Adds a page break before the Appendix section. • After—No effect. • BeforeAfter—Adds a page break before the Appendix section.
Tag	Displays information associated with an object on the page. **IMPORTANT** Do not modify or delete the Tag property.
Text	For a Label item, you can type text here. For the column headings, this box displays the column heading text. For the TextBox item, this box displays the name of the data source (table column in the result file).
Title	(For the Picture item only) Not implemented.

Design properties

Table 177 describes the Design property.

Table 177. Design properties in the Properties pane

Design property	Description
(Name)	Displays the internal name of an object on the report template page, used by the application to uniquely identify each individual object.

Layout properties

Table 178 describes the Layout properties.

Table 178. Layout properties in the Properties pane (Sheet 1 of 2)

Layout property	Description
End	(For the CrossSectionLine and CrossSectionBox items only) Specifies the X and Y coordinates of the end of the line or the bottom-right corner of the box, based on the rulers at the top and left side of the report template page.
Height	(For a workspace section only) Specifies the height of the section, based on the ruler to the left of the template workspace.
Location	Specifies the X and Y coordinates of the upper-left corner of an object, based on the rulers at the top and to the left of the template workspace.
Padding	Specifies the values in points for the space to the left, top, right, and bottom of the textual content within the container.
Radius	(For the CrossSectionBox item only) Specifies the percentage value for the roundness of the corners of the box. The default value of 0 creates corners with no rounding. A value of 100 creates top and bottom sides that look like half circles.
RoundingRadius	(For the Shape item only) Specifies the percentage value for the roundness of the corners when you select RoundRect (rectangle with rounded corners) for the Style property.
Size	Specifies the width and height of an object on the page, in inches.
SizeMode	(For the Picture item only) Specifies how the report designer sizes the image to fit in the container. Selections: • Clip—Clips images that are larger than the container. • Stretch—Stretches images to fit the container. • Zoom—Decreases the image size to fit the container.

Table 178. Layout properties in the Properties pane (Sheet 2 of 2)

Layout property	Description
Start	(For the CrossSectionLine and CrossSectionBox design items only) Specifies the X and Y coordinates of the start of the line or the top-left corner of the box, based on the rulers at the top and to the left of the template workspace.
X1	(For the Line item only) Specifies the coordinate of the left end of a line, based on the horizontal ruler at the top of the report template page.
X2	(For the Line item only) Specifies the coordinate of the right end of a line, based on the horizontal ruler at the top of the report template page.
Y1	(For the Line item only) Specifies the coordinate of the left end of a line, based on the vertical ruler to the left of the template workspace.
Y2	(For the Line item only) Specifies the coordinate of the right end of a line, based on the vertical ruler to the left of the template workspace.

Miscellaneous properties

Table 179 describes the Miscellaneous properties.

Table 179. Miscellaneous properties in the Properties pane (Sheet 1 of 2)

Miscellaneous property	Description
Code128	(For the Barcode item only) When you select Code_128_x for the Style property in the Appearance area, use this property to define the code.
Code49	(For the Barcode item only) When you select Code49 for the Style property in the Appearance area, use this property to define the code.
DataMatrix	(For the Barcode item only) When you select the DataMatrix option for the Style property in the Appearance area, use this property to define the code.
PDF417	(For the Barcode item only) When you select Pdf417 for the Style property in the Appearance area, use this property to define the code.

Table 179. Miscellaneous properties in the Properties pane (Sheet 2 of 2)

Miscellaneous property	Description
QRCode	(For the Barcode item only) When you select QRCode for the Style property in the Appearance area, use this property to define the code. A QR code (quick response code) is a matrix (2D) barcode. Because smartphones can convert QR codes to URLs, QR codes can provide quick access to websites.
RssExpandedStacked	(For the Barcode item only) When you select RssExpandedStacked for the Style property in the Appearance area, use this property to define the code.

Open the property dialog box for a workspace section or a specific report item

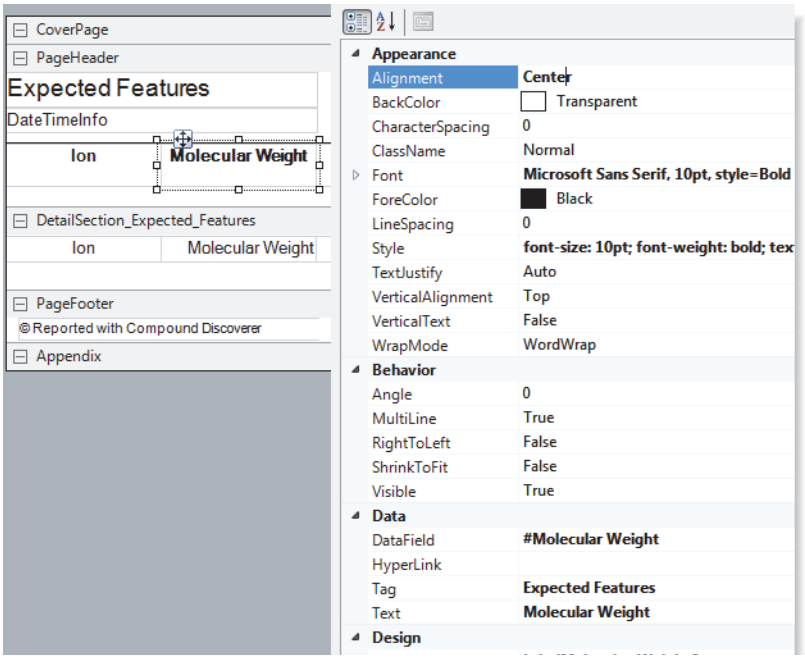
The reporting feature for the application includes a property dialog box for each item in the Section Reports pane. Using this dialog box, you can modify the formatting parameters for a selected item on the report template page. The available properties vary depending on the selected workspace section or item. Most of these parameters are similar to the properties listed in the properties pane, although some have slightly different names.

❖ To open the property dialog box for an item

1. Select the item of interest in the workspace.

   The properties pane for the selected item appears.

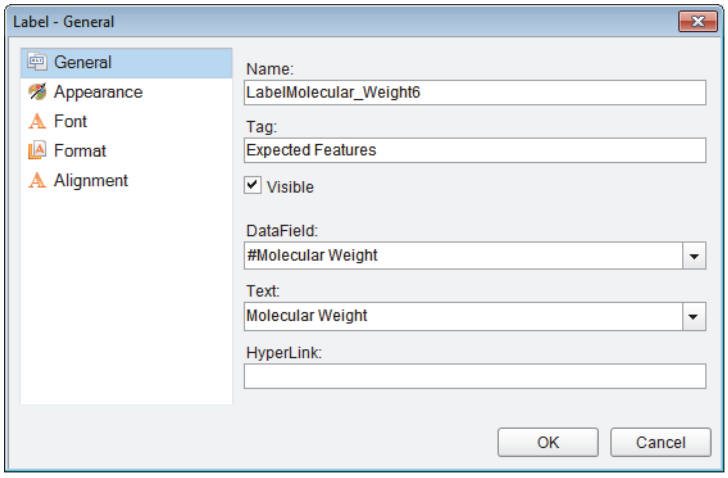
   Figure 173. Properties pane for a label item



2. At the bottom-right corner of the report template page, click the **Property Dialog** link.

   The property dialog box for the selected object opens (Figure 174).

   Figure 174. Property dialog box for the Label item



Note For the RichTextBox item, in addition to the Property Dialog link, you can click the Load File link to load text from a file into the box. See "Add a rich text box to a report template."

The parameters in the property dialog boxes have equivalent parameters in the properties pane.

Select the paper type, print width, page orientation, and watermark for a report template

On the report template page, you can add a watermark, change the print width and the orientation of the report template (portrait or landscape), and select the type of paper that you want the printer to use.

See the following topics:

- Open the property settings for a report template
- Add a watermark to a report template
- Change the print width of a report template
- Change the page orientation of a report template
- Change the page orientation of a report template
- Change the paper size for the printer

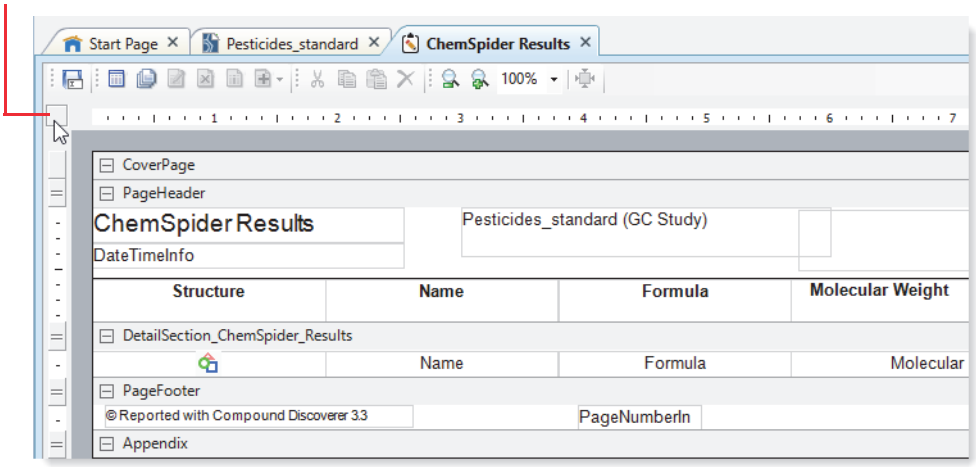
Open the property settings for a report template

❖ To open the property settings for the report template

1. Open a report template for editing. See "Open a report template for editing."
2. Click the unfilled square in the upper-left corner (above the vertical sizing bar) of the report template page.

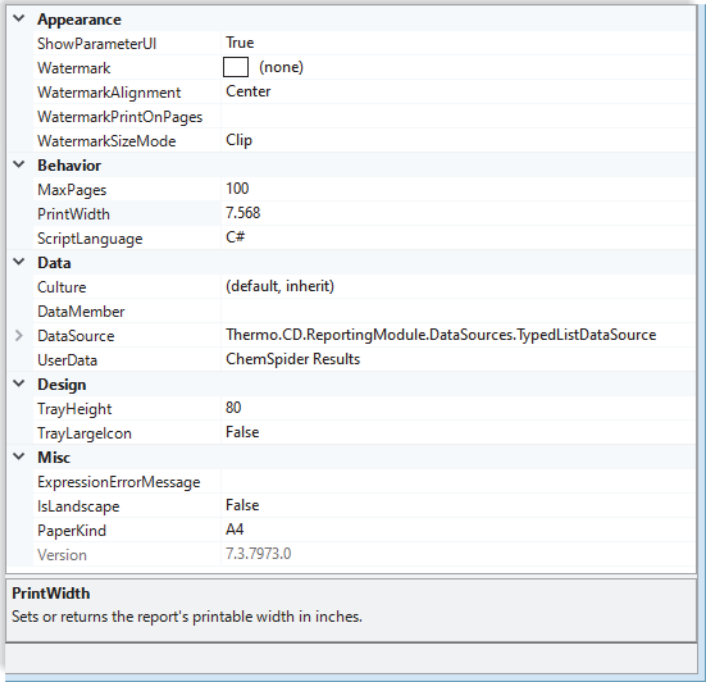
Figure 175. Square in upper-left corner of the report template grid

Opens the report template properties in the Properties pane



The watermark properties appear in the Appearance group, and the orientation and paper size properties appear in the Miscellaneous group.

Figure 176. Report template properties (in the Properties pane)



Add a watermark to a report template

By default, the Watermark property for a report template is set to None.

❖ To add a watermark to a report template

1. Open the property settings for the report template. See "Open the property settings for a report template."
2. Under Appearance, click the browse icon,  , to the far right of the Watermark property.

   The Open dialog box opens with the file type setting for all image files.
3. Find and select the image file of interest and click **Open**.
4. In the WatermarkAlignment list, select the appropriate alignment.
5. In the WatermarkPrintOnPages box, type the page number of the page where you want the watermark to appear.
6. In the WatermarkSizeMode list, select whether you want to clip the image if it is larger than the container, stretch the image to fit the container, or reduce the image size to fit the container.

Change the print width of a report template

❖ To change the print width of a report template

1. Open the property settings for the report template. See "Open the property settings for a report template."
2. Under Behavior, type a numeric value in the PrintWidth box.

Tip When you change the page layout from portrait (IsLandscape = False) to landscape (IsLandscape = True) or landscape to portrait, the numeric value in the PrintWidth box automatically updates, but the grid ruler does not update.

To update the grid ruler, type the print width in the PrintWidth box.

Change the page orientation of a report template

❖ To change the page orientation of the report template

1. Open the property settings for the report template. See "Open the property settings for a report template."
2. Under Misc, select **True** for Landscape or **False** for Portrait in the IsLandscape list.

Change the paper size for the printer

❖ **To change the paper size used by the printer**

1. Open the property settings for the report template. See "Open the property settings for a report template."
2. Under Misc, select the appropriate paper size from the PaperKind list.

   To open the list to the paper size of interest, type the first letter of the paper-size name. For example, if you want to change the size from A4 to Letter, type an L in the box. If the paper size does not appear in the box, continue typing the next letter of its name. The application cycles through the paper sizes that begin with this letter or letters.

Preview and print a report

This topic describes how to work with the Report Preview and Report Print dialog boxes and the report resolution page.

You can print all of the report pages from the report resolution page or the Report Print dialog box. You can print up to five pages from the Report Preview dialog box.

Perform these tasks as applicable:

- Preview a report for up to five rows in the main result table
- Preview a report for all the visible rows in the main result table
- Open the Report Resolution page
- Find a text item in a resolved report
- Copy a portion of a report to the Clipboard
- Export the contents of a report to an external document
- Print a report
- Report preview toolbar
- Page thumbnails pane

Preview a report for up to five rows in the main result table

To preview a report, use the Report Preview dialog box to preview up to five rows.

❖ **To open the Report Preview dialog box**

1. Open a report template for editing. See "Open a report template for editing."
2. In the toolbar on the report template page, click the **Preview Report** icon,  .

The application opens the Report Preview dialog box and resolves the current result file with the current template on the report template page. The Page Thumbnails pane displays up to five resolved pages.

A red line in the right page margin indicates that the print width does not fit on the selected page size, and the printer will print an empty page with every report page it prints, unless you resize the template. See "Change the print width of a report template."

Preview a report for all the visible rows in the main result table

To preview a report for all the visible rows in the selected main result table, use the Report Preview dialog box.

❖ **To open the Report Print dialog box**

1. Open a report template. See "Open a report template for editing."
2. In the toolbar on the report template page, click the **Print Report** icon, .

   The application opens the Report Print dialog box and resolves the current result file with the current template on the report template page. The Page Thumbnails pane displays all of the report pages.

Open the Report Resolution page

❖ **To open the report resolution page**

1. Open a result file.
2. Select an existing report template as follows:
   a. Choose **Reporting > Create Report** from the menu bar or, click the **Create Report** icon, .

      The Open Report Design Template dialog box opens to the Report Templates folder.

   b. Select the appropriate report template and click **Open**.

      The application resolves the current result file with the selected template. The Page Thumbnails pane displays all of the report pages.

Find a text item in a resolved report

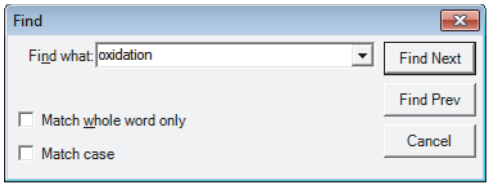
❖ **To find a text item in a resolved report**

1. On the report template page, resolve the report by clicking the **Print Report** icon, , or the **Preview Report** icon, .
2. In the toolbar of the Report Print dialog box or the Report Preview dialog box, click the **Find** icon, .

The Find dialog box opens.

3. In the Find What box, type the text that you want to find.

Figure 177. Find dialog box with a text entry



4. Select the appropriate check boxes.
   - To match whole words only, select the **Match Whole Word Only** check box.
   - To match the case—uppercase or lowercase, select the **Match Case** check box.
5. Click **Find Next** or **Find Prev**.

Copy a portion of a report to the Clipboard

❖ To copy a portion of a report to the Clipboard

Do one of the following:

a. To copy a specific item to the Clipboard, click the **Selection Mode** icon, , in the Report Preview toolbar.

b. Click the item that you want to copy, and then click the **Copy** icon, .

–or–

a. To copy a rectangular portion of the report to the Clipboard, click the **Snapshot Mode** icon, .

b. Drag the cursor across the area of interest.

Export the contents of a report to an external document

❖ To export the contents of a report to an external document

1. Open the report resolution page or the Report Print dialog box.
2. In the toolbar, choose **Export > *File Type***, where the *File Type* is one of the following:
   - Text—text file
   - PDF—portable document format file
   - RTF—rich text format file
   - Excel—Microsoft spreadsheet

- HTML—web page that opens in a browser
- Printing a report

Print a report

After you review the items in your Compound Discoverer result file and reduce the number of table rows to report to a reasonable number, open an existing report template or create a new report template, resolve the template, and then print a report.

❖ **To print a report for the visible table rows in a result file**

1. Open the result file of interest. See "Open, close, and update result files."
2. Review and filter the data. See "Filter the data for data reduction."
3. Do one of the following:
   a. From the menu bar, choose **Reporting > Create Report**.

      The Open Report Design Template dialog box opens.

   b. Select an appropriate template and click **Open**.

      The report resolution page opens.

   –or–

   - From the report template page, open the Report Print dialog box by clicking the **Print Report** icon, .
4. In the toolbar, click the **Print** icon,  .

   The Print dialog box opens.
5. Select the appropriate printer and the page range that you want to print.
6. Click **OK** to print the report.

Report preview toolbar

The Report Preview and Report Print dialog boxes and the report resolution page share a common toolbar. Table 180 describes the icons in the toolbar, from left to right.

Table 180. Report preview icons (Sheet 1 of 3)

Icon	Description
	Toggle Sidebar—Opens and closes the Page Thumbnails pane. See "Page thumbnails pane."
	Print—Opens the Print dialog box where you select the appropriate print options and send the report to the selected printer.

Table 180. Report preview icons (Sheet 2 of 3)

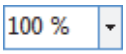
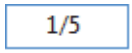
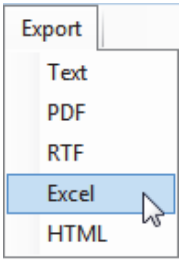
Icon	Description
	Copy—Copies the selected item to the Clipboard. Clicking the Selection Mode icon makes the Copy available.
	Find—Opens the Find dialog box where you can search for a particular word or phrase in the report.
	Zoom Out—Reduces the magnification of the report view. The current zoom box displays the magnification.
	Zoom In—Increases the magnification. The current zoom box displays the magnification.
	Current zoom—Use to change the on-screen magnification of the report by selecting or typing a percentage from 10 to 800 in this box, and then pressing ENTER.
	Fit Width—Sizes the width of the report to the screen width. The current zoom box displays the magnification.
	Fit Page—Sizes the current report page to the screen width and height, while maintaining the aspect ratio. The current zoom box displays the magnification.
	Single Page View—Fits the current report page to the full-screen view and removes the scroll bar. To view the report pages, you must use the First Page, Previous Page, Next Page, and Last Page icons or the Page Thumbnails pane.
	Continuous View—Changes the magnification to 100% and makes the scroll bar available so that you can scroll through the document.
	Multipage view—Changes the display to the selected multi-page view.
	First Page—Displays the first page of the report.
	Previous Page—Displays the previous page of the report.
	Current Page—Indicates the current page and the estimated number of pages in the report.
	Next Page—Displays the next page of the report.
	Last Page—Displays the last page of the report.
	Backward—Displays the previously selected page in the report. Selecting pages as you browse makes the Backward icon available.
	Forward—Displays the next selected page in the report. Clicking the Backward icon makes the Forward icon available.

Table 180. Report preview icons (Sheet 3 of 3)

Icon	Description
	Pan Mode—Use the hand cursor to drag the page on the screen.
	Selection Mode—Use to copy a report item to the Clipboard.
	Snapshot Mode—Use to copy a rectangular area to the Clipboard.
	Export—Use to export the contents of the report to an external document of one of these types: Text, PDF, RTF, Excel, or HTML.

Page thumbnails pane

The Page Thumbnails pane appears to the left of the page preview in the Report Preview and Report Print dialog boxes and the report resolution page. Each thumbnail represents a page in the report. The Report Preview dialog box resolves up to five pages of data. The Report Print dialog box resolves all of the data. In the Report Print dialog box, click a page thumbnail to jump to that page.

Table 181 describes the icons in the Page Thumbnails pane, from top left to bottom right.

Table 181. Page Thumbnails pane icons

Icon	Description
	Enlarge—Enlarges the size of the thumbnails.
	Reduce—Reduces the size of the thumbnails.
	Thumbnails Pane—Displays the Page Thumbnails pane.
	Search Results—Displays the Search Results pane where you can search for a particular word or phrase in the report. The found instances appear in the list of results.

Manage the lists and libraries

To modify the lists and libraries that you use to process mass spectral data and identify compounds in the Compound Discoverer application, see the following topics:

- Lists & Libraries manager
- Expected Compounds view
- Generate an Xcalibur inclusion list
- Adducts view
- Ion Definitions view
- Transformations view
- Neutral Losses view
- Mass Lists view
- Spectral Libraries view
- Metabolika Pathways view
- Edit new and existing Metabolika pathways
- Compound Classes view
- Load a structure from a structure file
- Find a structure in the ChemSpider database
- Structure drawing tools and commands
- Copy and paste InChi strings and MOL strings

Lists & Libraries manager

Clicking the Lists & Libraries Manager icon, , in the application toolbar opens the Lists & Libraries manager as a tabbed page. The buttons in the left pane open the individual views, and the buttons across the top of the page perform various tasks.

Not all the task buttons are available for every view. The Edit button is unavailable for the Spectral Libraries view, and the Replace button is visible only for the Mass Lists, Spectral Libraries, and Metabolika Pathways views.

Each view in the Lists & Libraries Manager page includes a table. For information about freezing panes, hiding and showing columns, freezing rows, sorting, and filtering the application tables, see "Common operations for manipulating data tables."

Expected Compounds view

The Expected Compounds view of the Lists & Libraries page contains a list of the expected (parent) compounds for targeted analyses in LC studies. See Figure 178.

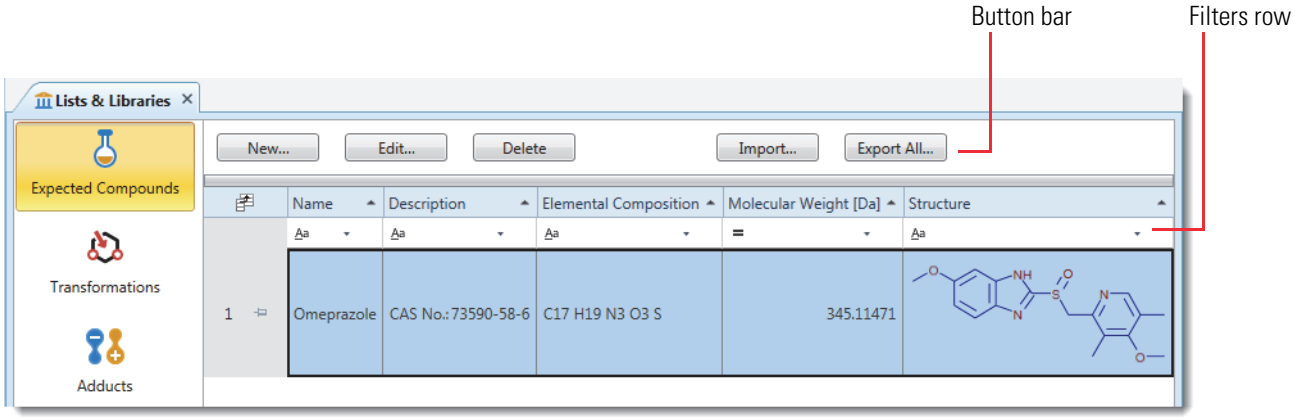
Tip To open the Expected Compounds view, choose **Lists & Libraries > Expected Compounds** from the application menu bar.

In a targeted analysis, the Generate Expected Compounds node generates a list of expected compounds by using the parent compounds and transformations that you specify. The Find Expected Compounds node then searches for these compounds in the raw data files that you submit for analysis.

The initial expected compounds list contains omeprazole, the targeted compound used in the *Compound Discoverer Metabolism Tutorial*.

Note To run a targeted processing workflow that includes the Generate Expected Compounds node, the Create FISh Trace node, or both of these nodes, you must first add the compounds of interest to the Expected Compounds list.

Figure 178. Expected Compounds view on the Lists & Libraries page



To modify the expected compounds list, see these topics:

- Expected Compounds view parameter descriptions
- Delete, import, or export expected compounds
- Add and edit expected compounds with the Compound Editor

For information about generating an Xcalibur inclusion list, see "Generate an Xcalibur inclusion list."

Expected Compounds view parameter descriptions

This table describes the buttons and columns in the Expected Compounds view of the Libraries & Lists page.

Table 182. Expected Compounds view parameters (Sheet 1 of 2)

Feature	Description
Buttons	
New	Opens the Compound Editor for adding new compounds to the Expected Compounds list.
Edit	Opens the Compound Editor for editing the selected compound. Selecting a compound makes this button available.
Delete	Deletes the selected compound. Selecting a compound makes this button available.
Import	Opens the Open dialog box for selecting an XML or SDF file.
Export All	Opens the Save As dialog box for exporting the entire Expected Compounds list as an XML file.

Table 182. Expected Compounds view parameters (Sheet 2 of 2)

Feature	Description
Generate Inclusion List	Opens the Generate Xcalibur Inclusion List dialog box for creating and exporting a list of compounds to include in an inclusion list for data acquisition. The application creates the inclusion list by generating a list of expected compounds by using the dealkylation and dearylation reactions, the transformation reactions, and the adduct ions that you specify. The application saves the list as a text file with the name and path that you specify.
Filters row	
Use this row to filter the table as appropriate. See "Filter the tables on a study page or a list or library view."	
Columns	
Name	Displays the user-specified compound name.
Description	Displays the user-specified description.
Elemental Composition	Displays the elemental composition that the application determines from the compound's structure.
Molecular Weight	Displays the molecular weight that the application calculates from the compound's elemental composition.
Structure	Displays the structure created by using the drawing tools or by importing a structure file.

Delete, import, or export expected compounds

You can perform the following tasks directly from the Expected Compounds view of the Lists & Libraries page.

Table 183. Expected Compounds view tasks (Sheet 1 of 2)

Task	Procedure
Delete a compound.	Select the compound in the expected compounds list and click **Delete**. Then, click **Yes** at the prompt.
Import compounds from an XML file or and SDF file.	Click **Import**, select the XML or SDF file of interest, and click **Open**. Then, click **OK** at the prompt. The application only imports new entries; it does not import entries that are already in the expected compounds list. After the application imports the new compound entries, it provides a tally of the number of imported compounds versus the number of skipped compounds.

Table 183. Expected Compounds view tasks (Sheet 2 of 2)

Task	Procedure
Export compounds to an XML file or an SDF file.	1. Click **Export All**. 2. Select a folder, name the file, and click **Save**. The application exports the list to the selected file type: XML or SDF. 3. At the prompt, click **OK**.

Add and edit expected compounds with the Compound Editor

Use the Compound Editor dialog box to create new compound entries or edit existing entries in the Expected Compounds view.

Note Similar Compound Editor dialog boxes open from the Mass List and Metabolika Pathways editors. For information about using the structure drawing tools, see "Structure drawing tools and commands."

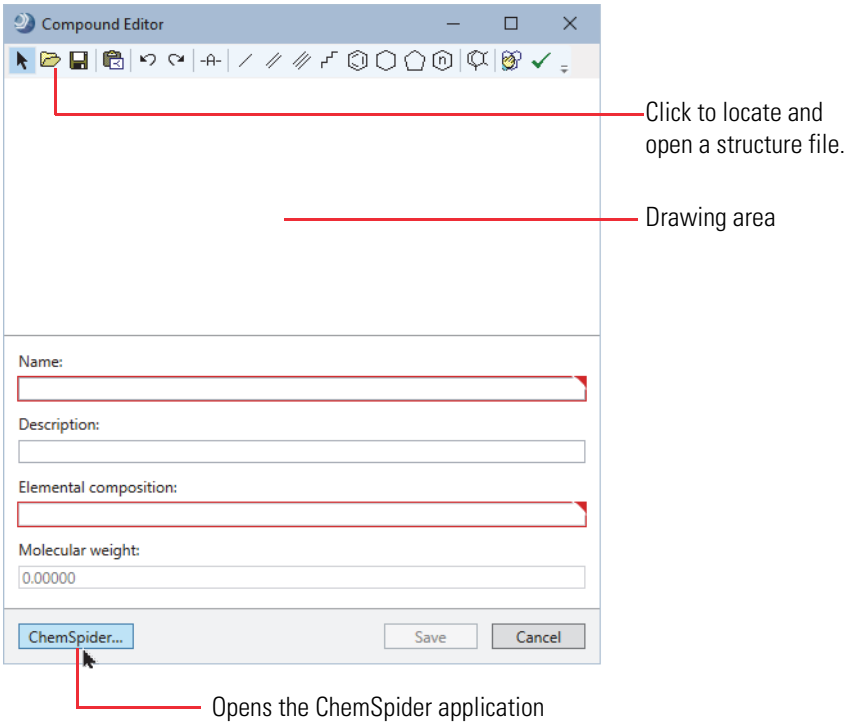
❖ To add a new compound or edit an existing compound

1. Open the Expected Compounds view on the Library & Lists page.
2. Do one of the following:
   - To edit the definition of a compound, double-click the entry or select the entry and click **Edit**.

     The Compound Editor dialog box opens with information for the selected entry.
   - To add a compound to the Expected Compounds list, click **New**.

     The Compound Editor dialog box opens. As indicated by the red borders you must name the compound and enter its elemental composition to save it.

Figure 179. Compound Editor dialog box for a new compound



3. To enter or edit the elemental composition of the compound, do any of the following:
   - Draw or edit the structure in the drawing area. See "Structure drawing tools and commands."
   - Paste an InChi or MOL string from the Clipboard.
   - Open a structure file. See "Load a structure from a structure file."
   - Click **ChemSpider** to find the structure. See "Find a structure in the ChemSpider database."

   The application automatically populates the Elemental Composition and Molecular Weight boxes with read-only values. To change the elemental composition and the molecular weight, you must modify the chemical structure in the drawing area.
4. In the Name box, type the name of the compound.
5. (Optional) In the Description box, type a description for the compound.
6. Click **Save**.

   The dialog box closes and the new compound or the edited information for the existing compound appears in the expected compounds list.

Generate an Xcalibur inclusion list

An Xcalibur inclusion list is a text file that contains the formulas and *m/z* values of the adduct ions (found in the survey scan) that you want the mass spectrometer to fragment and acquire data-dependent scans for during data acquisition.

Note The application creates the inclusion list from the parent compounds (compounds in the Expected Compounds list), transformations, and adduct ions that you select. A parent compound is the beginning compound in a set of metabolic reactions.

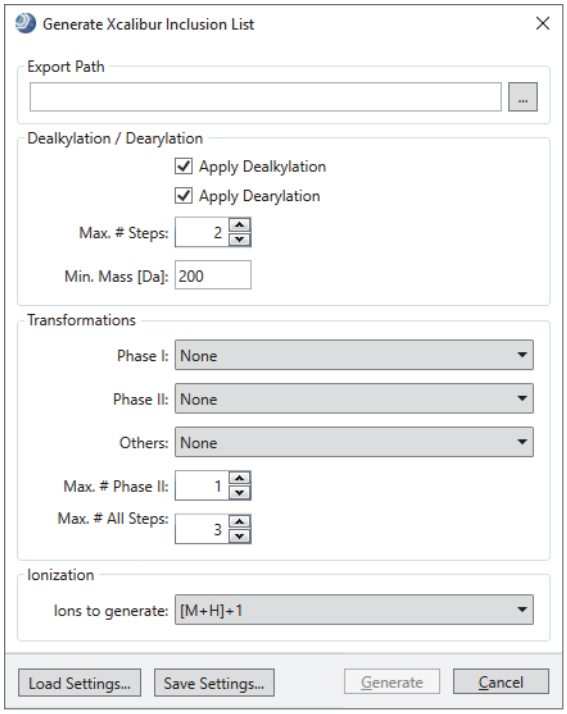
Tip For instructions on how to export inclusion and exclusion lists from the result tables of a result file, see "Export an Xcalibur inclusion or exclusion list from a compounds table."

❖ To generate an Xcalibur inclusion list from the Expected Compounds view

1. From the application menu bar, choose **Lists & Libraries > Expected Compounds**.
2. If the parent compounds of interest are not in the list, add them. See "Add and edit expected compounds with the Compound Editor."
3. Select the parent compounds that you want to add to the Xcalibur inclusion list.
4. In the command bar of the Expected Compounds view, click **Generate Inclusion List**.

   The Generate Xcalibur Inclusion List dialog box opens.

   Figure 180. Generate Xcalibur Inclusion List dialog box



5. Browse to the folder where you want to store the TXT file that this dialog box generates, and name the file.
6. Do one of the following:
   - Click **Load Settings**, select the inclusion settings file that includes all the parameter settings for generating the inclusion list, and then click **Open**.
   - Specify all the reactions that you want to use to generate the inclusion list, and select the adduct ions to generate.

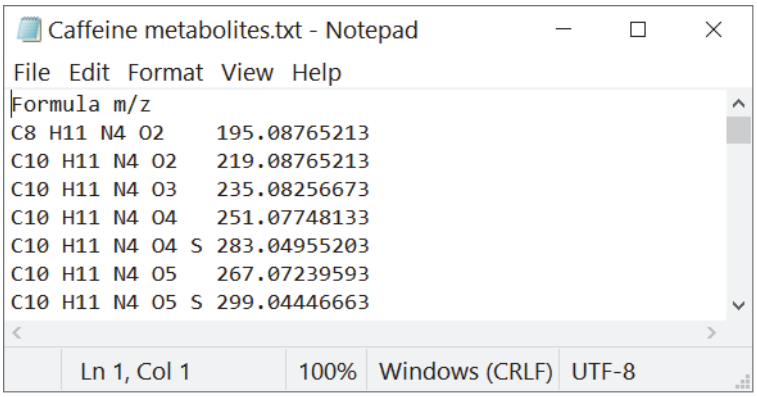
   Note For information about the parameters in the Dealkylation/Dearylation, Transformations, and Ionization areas of the dialog box, see "Generate Expected Compounds node."

   Tip If you expect to use these parameter settings for generating other inclusion lists, click **Save Settings** and save the settings to an inclusion settings file (.inclSet).
7. Click **Generate**.
8. At the prompt, verify the directory and file name for the inclusion list file, and then click **OK**.

   The application generates a list of adduct ions by using the user-specified parent compounds, and transformations, and ions. It exports the generated TXT file to the user-specified folder.

   The TXT file includes two columns. The first columns lists the formulas and the second column lists the *m/z* values of the ions that you want the mass spectrometer to include in a targeted DDA experiment. You can import the information in this file into the instrument method for your LC/MS system.

Figure 181. Xcalibur inclusion list for caffeine and its metabolites



Note The Generate Xcalibur Inclusion List dialog box retains the new parameter settings until you change them.

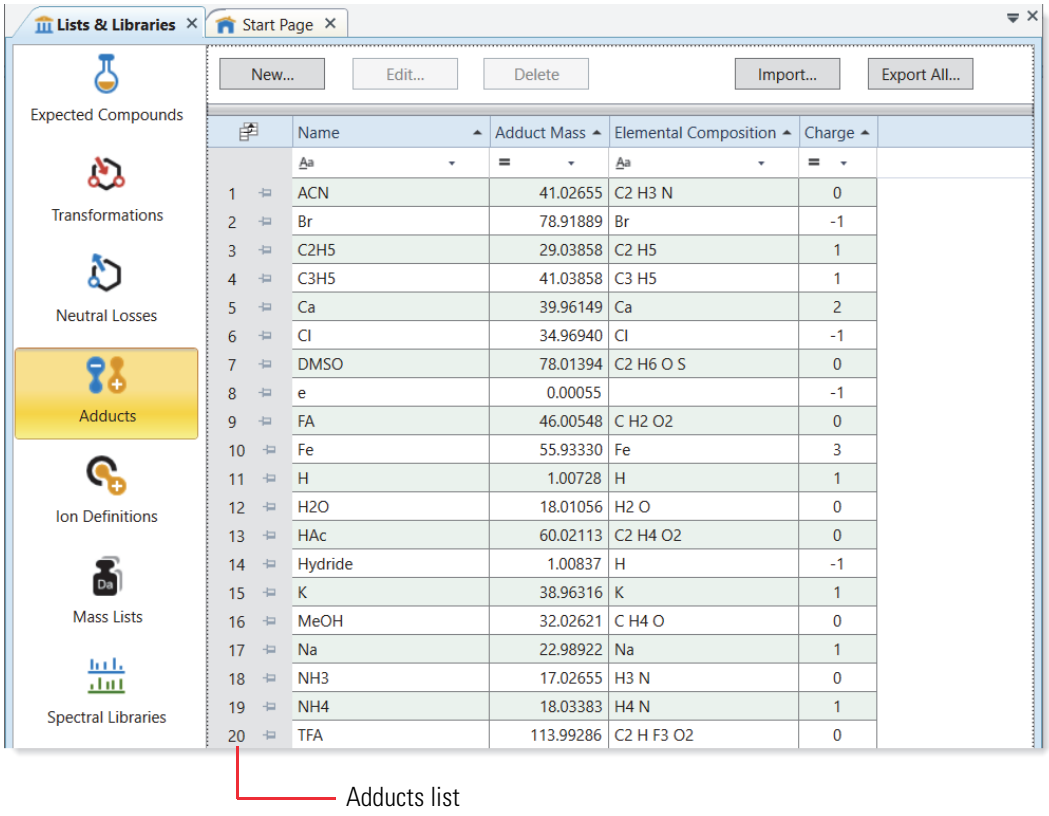
Adducts view

Use the Adducts view of the Lists & Libraries page to define the expected adducts in your samples. Adducts are part of the ion definition–that is, to create a new ion definition that uses an adduct that is not currently in the adducts list, you must first add the adduct to the adducts list.

Tip To open the Adducts view, choose **Lists & Libraries > Adducts** from the application menu bar.

The adducts list provided with the application contains 20 adducts. You can modify this list.

Figure 182. Adducts view



To modify the adducts list, see these topics:

- Adducts view parameter descriptions
- Delete, import, and export adducts
- Add and edit adducts with the Adduct Editor

Adducts view parameter descriptions

This table describes the buttons and table columns in the Adducts view of the Lists & Libraries page.

Table 184. Adducts view parameters

Feature	Description
Buttons	
New	Opens the Adduct Editor for defining an adduct.
Edit	Opens the Adduct Editor for editing the selected adduct. Selecting an adduct makes this button available.
Delete	Deletes the selected adduct. Selecting an adduct makes this button available. You cannot delete the following adducts: H, Na, K.
Import	Opens the Open dialog box for selecting an XML file.
Export All	Opens the Save As dialog box for exporting the entire adducts list to an XML file.
Filters row	
Use this row to filter the table as appropriate. See "Filter the tables on a study page or a list or library view."	
Table columns	
Name	Displays the specified name of the adduct.
Adduct Mass	Displays the mass that the application calculates from the specified elemental composition.
Elemental Composition	Displays the specified elemental composition of the adduct.
Charge	Displays the specified charge of the adduct.

Delete, import, and export adducts

You can perform the following tasks directly from the Adducts view of the Lists & Libraries page.

Table 185. Adducts view tasks (Sheet 1 of 2)

Task	Procedure
Delete an adduct	Select the adduct in the adducts list and click **Delete**. Then, click **Yes** at the prompt. You cannot delete the H, Na, or K adducts.

Table 185. Adducts view tasks (Sheet 2 of 2)

Task	Procedure
Import adducts from an XML file	1. Click **Import**. 2. In the Open dialog box, locate the file, and click **Open**. A message opens with a tally of the number of imported adducts versus the number of skipped adducts. The application only imports new entries; it does not import entries that are already in the list. 3. At the prompt, click **OK**.
Export a list of adducts to an XML file	1. Click **Export All**. 2. Select a folder, name the file, and click **Save**. The application exports the list to an XML file. 3. At the prompt, click **OK**.

Add and edit adducts with the Adduct Editor

Use the Adduct Editor dialog box to define additional adducts, which are part of the ion definition.

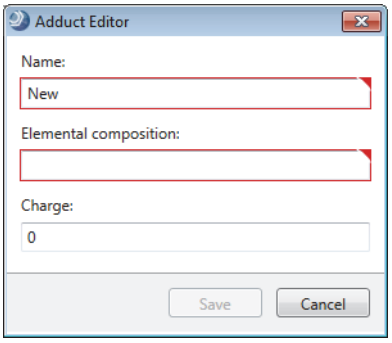
❖ To add or edit adducts

1. From the application menu, choose **Lists & Libraries > Adducts**.
2. In the Adducts view, do one of the following:
   - To edit the definition of an adduct, double-click the entry or select the entry and click **Edit**.

     The Compound Editor dialog box opens with information for the selected entry.
   - To add an adduct to the list, click **New**.

     The Adduct Editor dialog box opens. As indicated by the red borders, you must name the adduct and enter its elemental composition to save it.

Figure 183. Adduct Editor dialog box for a new entry



3. Define the new adduct or modify the existing adduct as follows:
   - In the Name box, select **New** and type a name for the adduct or keep or modify the name of the existing adduct.
   - In the Elemental Composition box, enter the elemental composition of the new adduct or keep or modify the elemental composition of the existing adduct.

     The editor validates the entry.
   - In the Charge box, enter the charge that the new adduct adds to the ion definition or keep or modify the charge of the existing adduct.

     Range: –10 to +10
4. Click **Save**.

   The new or modified adduct appears in the list.

Ion Definitions view

The Ion Definitions view of the Lists & Libraries page contains a list of adduct ions.

The application uses the entries in the Ion Definitions list in the following workflow nodes: Detect Compounds and Generate Expected Compounds.

Tip To open the Ion Definitions view, choose **Lists & Libraries > Ion Definitions** from the application menu bar.

To modify the ion definitions list, see these topics:

- Default list of ion definitions
- Delete an ion definition
- Import ion definitions from an XML file
- Export the ion definitions list to an XML File
- Add or edit ion definitions with the Ion Definition Editor

Ion Definition view parameters

Table 186 describes the parameters in the Ion Definitions view.

Table 186. Ion Definitions view parameters

Parameter	Description
Filter row	Use this row to filter the table as appropriate. See "Filter the tables on a study page or a list or library view."
Buttons	
New	Opens the Ion Definition Editor for editing the new ion definition.
Edit	Opens the Ion Definition Editor for editing the selected ion definition. Selecting an ion definition makes this button available.
Delete	Deletes the selected ion definition. Selecting an ion definition makes this button available.
Import	Opens the Open dialog box for selecting an XML file.
Export All	Opens the Save As dialog box for exporting the entire ion definitions list to an XML file.
Table columns	
Ion Definitions	Displays the user-specified ion definition.
Adducts Total Mass	Displays the difference between the exact mass of the neutral molecule and the molecular ion adduct or the exact mass of the neutral dimer and the ionized dimer.
Charge	Displays the charge of the ion.
Weight	Specifies the weighting factor for the ion definition when the ion definition is added to the list of possible ions in the Ions list for the Detect Compounds node.

Default list of ion definitions

The default list of ion definitions contains the most common adducts and dimers formed when using the electrospray-mass spectrometry (ESI-MS) technique in either the positive or negative ionization mode.

Table 187 lists the common adducts and dimers for the positive ionization mode.

Table 187. Common adducts and dimers in the positive ionization mode

Ion definition	Adducts total mass	Charge	Ion definition	Adducts total mass	Charge
M+H–H2O	–17.00329	1	M+H+Na	23.9965	2
M+H–NH3	–16.01927	1	M+H+MeOH	33.03349	1
M+H	1.00728	1	M+K	38.96316	1
2M+H	1.00728	1	2M+K	38.96316	1
M+2H	2.01455	2	M+H+K	39.97044	2
M+3H	3.02183	3	M+H+ACN	42.03383	1
M+NH4	18.03383	1	2M+H+ACN	42.03383	1
2M+NH4	18.03383	1	M+2H+ACN	43.0411	2
M+H+NH4	19.0411	2	M+Na+ACN	64.01577	1
M+Na	22.98922	1	2M+Na+ACN	64.01577	1
2M+Na	22.98922	1	M+H+DMSO	79.02121	1

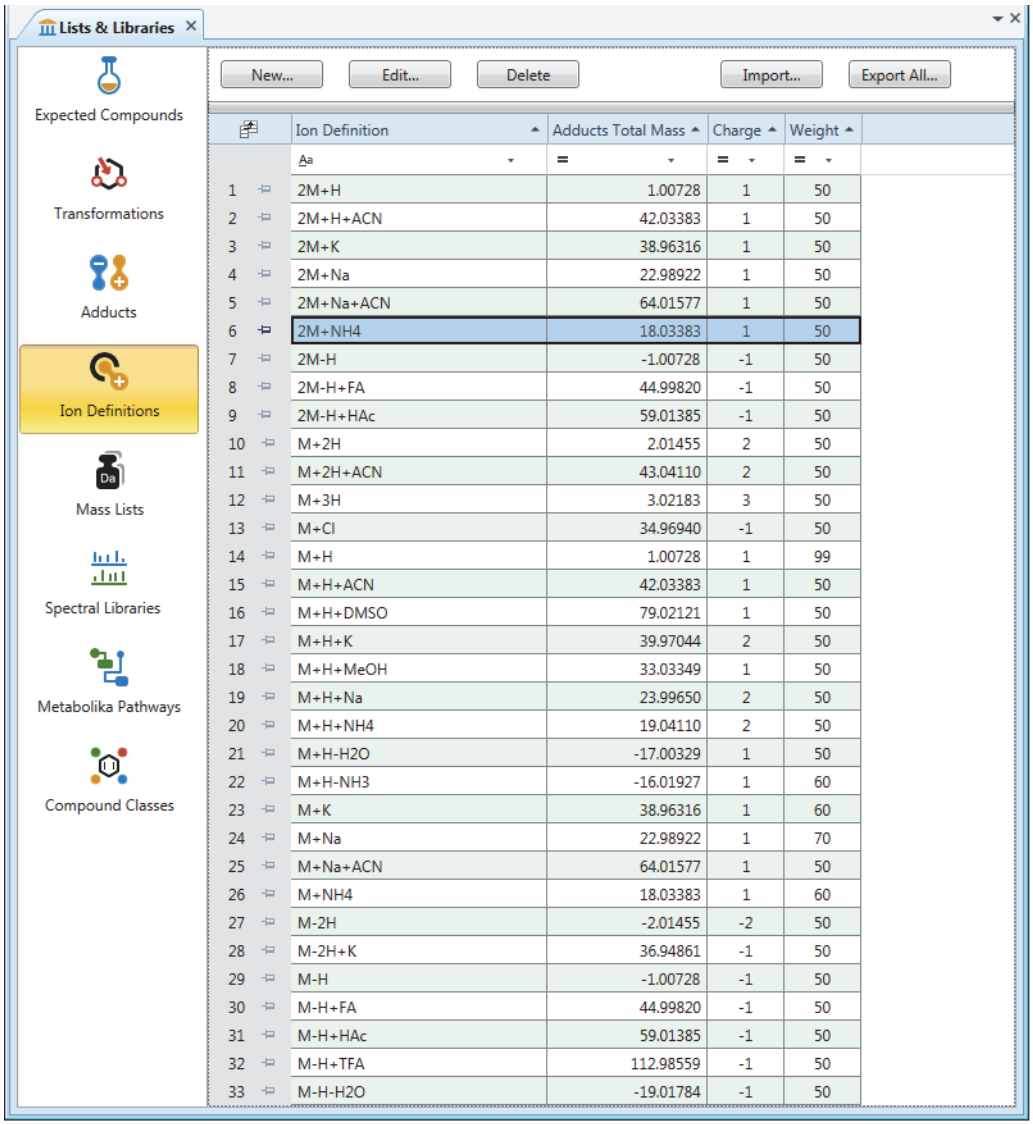
Table 188 lists the common adducts and dimers for the negative polarity mode.

Table 188. Common adducts and dimers in the negative ion mode

Ion definition	Adducts total mass	Charge	Ion definition	Adducts total mass	Charge
M–H	–1.00728	–1	M–H+FA	44.9982	–1
2M–H	–1.00728	–1	2M–H+FA	44.9982	–1
M–2H	–2.01455	–2	2M–H+HAc	59.01385	–1
M–H–H2O	–19.01784	–1	M–H+HAc	59.01385	–1
M+Cl	34.9694	–1	M–H+TFA	112.98559	–1
M–2H+K	36.94861	–1			

Figure 184 shows the Ion Definitions view.

Figure 184. Ion Definitions view



Delete an ion definition

All the ion definitions are deletable.

❖ To delete an ion definition

1. From the application menu bar, choose **Lists & Libraries > Ion Definitions**.
2. Select the ion definition and click **Delete**.
3. At the prompt, click **Yes**.

Import ion definitions from an XML file

❖ **To import a list of ion definitions from an XML file**

1. From the application menu bar, choose **Lists & Libraries > Ion Definitions**.
2. Click **Import**.
3. Locate the file and click **Open**.

   A message opens with a tally of the number of imported ion definitions versus the number of skipped ion definitions. The application only imports new entries; it skips entries that are already in the list.
4. At the prompt, click **OK**.

Export the ion definitions list to an XML File

❖ **To export the entire list of ion definitions to an XML file**

1. From the application menu bar, choose **Lists & Libraries > Ion Definitions**.
2. Click **Export All**.
3. Select a folder, name the file, and click **Save**.

   The application automatically adds the file name extension (.xml).
4. At the prompt, click **OK**.

Add or edit ion definitions with the Ion Definition Editor

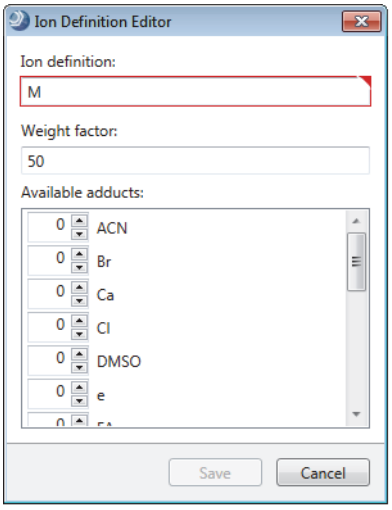
Use the Ion Definition Editor dialog box to create new or edit existing ion definitions.

❖ **To add new ion definitions or edit existing ion definitions**

1. From the application menu bar, choose **Lists & Libraries > Ion Definitions**.
2. Do one of the following:
   - To add a new ion definition, click **New**.

     The Ion Definition Editor dialog box opens. The Ion Definition box contains only an M for the uncharged molecule. Because the ion definition must include at least one additional component, a charge, or both, the box has a red border, and the Save button is unavailable.

Figure 185. Ion Definition Editor dialog box



- To edit an existing ion definition, double-click it or select it and click **Edit**.

3. To edit the ion definition, do any of the following:
   - Type the ion definition in the Ion Definition box.
   - Under Available Adducts, use the arrows to add or subtract components. Or, type a nonzero integer value for each component that you want to add or subtract.
4. In the Weight Factor box, type the weighting factor for the ion definition.

   Range: 0 to 99

   Note The Detect Compounds node uses the weight factor value for the ion definitions. With the exception of the protonated molecule $[M+H]^+$ in the positive polarity mode and the deprotonated molecule $[M–H]^–$ in the negative polarity mode, if you set the weight factor to 0, the Detect Compounds node does not look for the specified adduct in the mass spectrum.
5. To save the changes, click **Save**.

   The application calculates the ion's charge and the mass difference between the uncharged molecule and its adduct ion. The new ion definition appears in the list.

Table 189 describes the parameters in the Ion Definition Editor dialog box.

Table 189. Ion Definition Editor parameters

Parameter	Description
Ion Definition	Displays the current ion definition. Valid ion definitions include the neutral molecule, which is represented by M, and components from the component list. A red border indicates an invalid ion definition. As you edit the ion definition by using the component list, the application automatically updates the ion definition.
Weight Factor	Specifies the weighting factor for the ion definition.
Available Adducts list	Use this list to create custom ion definitions.

Transformations view

The Transformations view contains a table of possible transformations. The Generate Expected Compounds node uses a selection of entries from this table and the information in the expected compounds list to generate a table of expected transformations for a known (parent) compound.

With the addition of the PFAS Chain Shortening transformation in the Compound Discoverer SP2 release, the default Transformations list now contains 35 transformations.

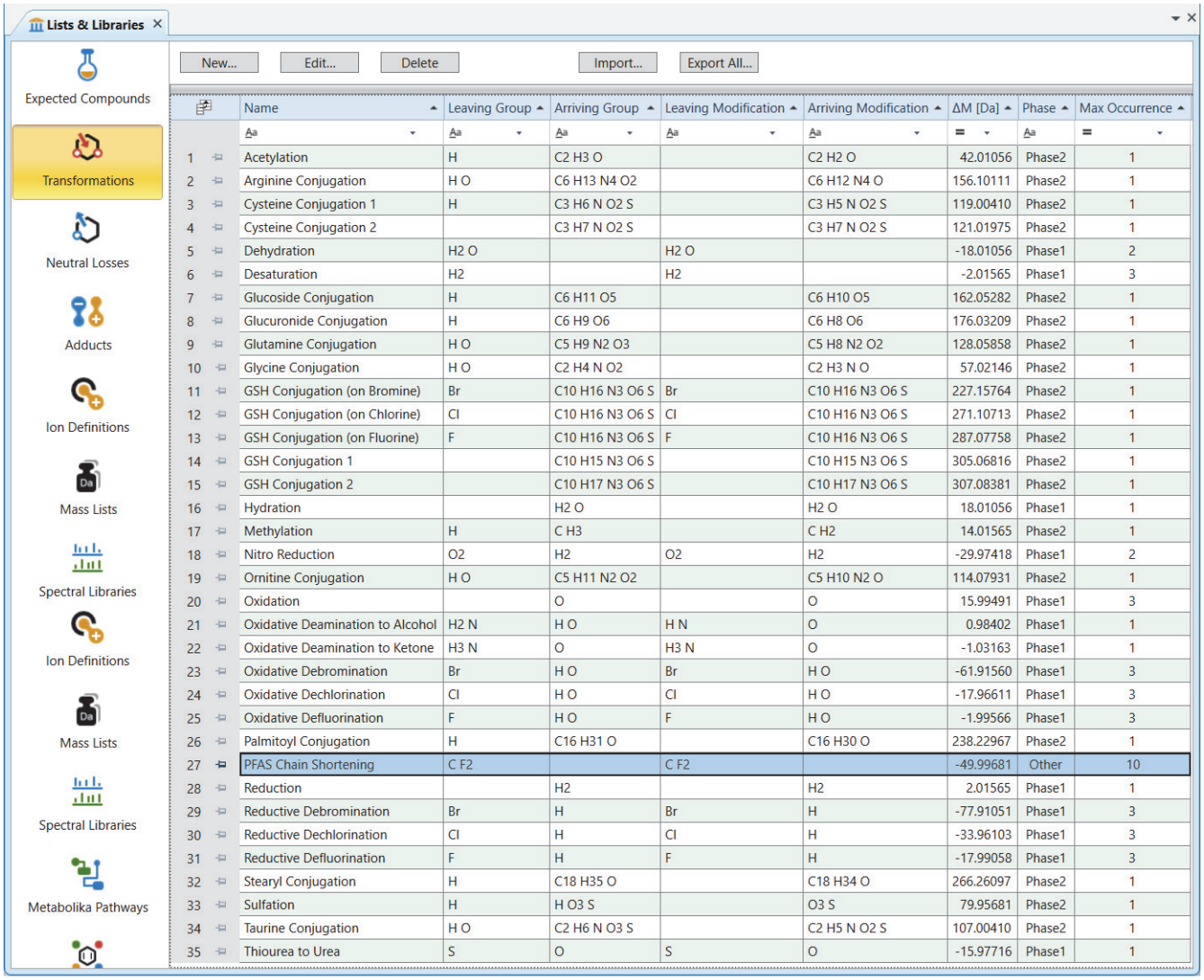
Tip To open the Transformations view, from the application menu bar, choose **Lists & Libraries > Transformations**.

To modify the transformations list, see these topics:

- Transformations view parameters
- Delete a transformation
- Import a list of transformations from an XML File
- Export the transformations list to an XML file

For details using the Transformation Editor to add or edit transformations, see "Add or edit transformations with the Transformation Editor."

Figure 186. Transformations view with the default transformations list



	Name	Leaving Group	Arriving Group	Leaving Modification	Arriving Modification	ΔM [Da]	Phase	Max Occurrence
1	Acetylation	H	C2 H3 O		C2 H2 O	42.01056	Phase2	1
2	Arginine Conjugation	H O	C6 H13 N4 O2		C6 H12 N4 O	156.10111	Phase2	1
3	Cysteine Conjugation 1	H	C3 H6 N O2 S		C3 H5 N O2 S	119.00410	Phase2	1
4	Cysteine Conjugation 2		C3 H7 N O2 S		C3 H7 N O2 S	121.01975	Phase2	1
5	Dehydration	H2 O		H2 O		-18.01056	Phase1	2
6	Desaturation	H2		H2		-2.01565	Phase1	3
7	Glucoside Conjugation	H	C6 H11 O5		C6 H10 O5	162.05282	Phase2	1
8	Glucuronide Conjugation	H	C6 H9 O6		C6 H8 O6	176.03209	Phase2	1
9	Glutamine Conjugation	H O	C5 H9 N2 O3		C5 H8 N2 O2	128.05858	Phase2	1
10	Glycine Conjugation	H O	C2 H4 N O2		C2 H3 N O	57.02146	Phase2	1
11	GSH Conjugation (on Bromine)	Br	C10 H16 N3 O6 S	Br	C10 H16 N3 O6 S	227.15764	Phase2	1
12	GSH Conjugation (on Chlorine)	Cl	C10 H16 N3 O6 S	Cl	C10 H16 N3 O6 S	271.10713	Phase2	1
13	GSH Conjugation (on Fluorine)	F	C10 H16 N3 O6 S	F	C10 H16 N3 O6 S	287.07758	Phase2	1
14	GSH Conjugation 1		C10 H15 N3 O6 S		C10 H15 N3 O6 S	305.06816	Phase2	1
15	GSH Conjugation 2		C10 H17 N3 O6 S		C10 H17 N3 O6 S	307.08381	Phase2	1
16	Hydration		H2 O		H2 O	18.01056	Phase1	1
17	Methylation	H	C H3		C H2	14.01565	Phase2	1
18	Nitro Reduction	O2	H2	O2	H2	-29.97418	Phase1	2
19	Ornitine Conjugation	H O	C5 H11 N2 O2		C5 H10 N2 O	114.07931	Phase2	1
20	Oxidation		O		O	15.99491	Phase1	3
21	Oxidative Deamination to Alcohol	H2 N	H O	H N	O	0.98402	Phase1	1
22	Oxidative Deamination to Ketone	H3 N	O	H3 N	O	-1.03163	Phase1	1
23	Oxidative Debromination	Br	H O	Br	H O	-61.91560	Phase1	3
24	Oxidative Dechlorination	Cl	H O	Cl	H O	-17.96611	Phase1	3
25	Oxidative Defluorination	F	H O	F	H O	-1.99566	Phase1	3
26	Palmitoyl Conjugation	H	C16 H31 O		C16 H30 O	238.22967	Phase2	1
27	PFAS Chain Shortening	C F2		C F2		-49.99681	Other	10
28	Reduction		H2		H2	2.01565	Phase1	1
29	Reductive Debromination	Br	H	Br	H	-77.91051	Phase1	3
30	Reductive Dechlorination	Cl	H	Cl	H	-33.96103	Phase1	3
31	Reductive Defluorination	F	H	F	H	-17.99058	Phase1	3
32	Stearyl Conjugation	H	C18 H35 O		C18 H34 O	266.26097	Phase2	1
33	Sulfation	H	H O3 S		O3 S	79.95681	Phase2	1
34	Taurine Conjugation	H O	C2 H6 N O3 S		C2 H5 N O2 S	107.00410	Phase2	1
35	Thiourea to Urea	S	O	S	O	-15.97716	Phase1	1

Transformations view parameters

Table 190. Transformations view parameters (Sheet 1 of 2)

Parameter	Description
Buttons	
New	Opens the Transformation Editor dialog box for creating new transformations.
Edit	Selecting an entry makes this button available. Opens the Transformation Editor dialog box for editing the selected transformation.

Table 190. Transformations view parameters (Sheet 2 of 2)

Parameter	Description
Delete	Selecting an entry makes this button available. Deletes the selected transformation from the library.
Import	Opens a dialog box for selecting an XML file to import.
Export All	Opens the Save As dialog box for saving the list as an XML file.
Filter row	Use this row to filter the table as appropriate. See "Filter the tables on a study page or a list or library view."
Columns	
Name	Displays the user-specified name for the entry.
Leaving Group	Displays the user-specified elemental composition of the leaving group for the transformation, if specified.
Arriving Group	Displays the user-specified elemental composition of the arriving group for the transformation, if specified.
Leaving Modification	Displays the elemental composition difference between the arriving group and the leaving group, if the transformed compound contains fewer atoms than the original compound.
Arriving Modification	Displays the elemental composition difference between the arriving group and the leaving group, if the transformed compound contains more atoms than the original compound.
ΔM [Da]	Displays the difference in mass between the original compound and the transformed compound in daltons.
Phase	Displays the user-specified category for the transformation.
Max Occurrence	Displays the user-specified value for the maximum number of times that this transformation can occur in a sequence of combinatorial transformations.

Delete a transformation

❖ **To delete an entry from the transformations list**

1. Open the Transformations view.
2. Select the entry and click **Delete**.
3. At the prompt, click **Yes**.

Import a list of transformations from an XML File

❖ **To import a list of transformations from an XML file**

1. Open the Lists & Libraries > Transformations view.
2. Click **Import**.
3. Locate the file and click **Open**.

   A message opens with a tally of the number of imported transformations versus the number of skipped transformations. The application only imports new entries; it does not import entries that are already in the library.
4. At the prompt, click **OK**.

Export the transformations list to an XML file

❖ **To export the entire transformations list to an XML file**

1. Open the Lists & Libraries > Transformations view.
2. Click **Export All**.
3. Select a folder, name the file, and click **Save**.
4. At the prompt, click **OK**.

Table 190 describes the parameters in the Transformations view.

Add or edit transformations with the Transformation Editor

Use the Transformation Editor to add entries to or to edit entries in the transformations list.

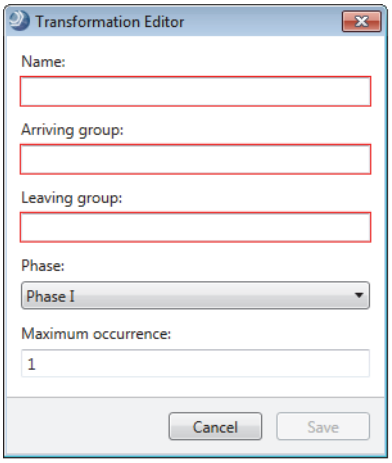
❖ **To add a new transformation or edit an existing transformation**

1. From the menu bar, choose **Lists & Libraries > Transformations**.
2. Do one of the following:
   - To add a new transformation, go to step 3.
   - To edit an existing transformation, go to step 4.
3. To add a transformation to the transformations list, do the following:
   a. Click **New**.

      The Transformation Editor dialog box opens. For details about the editor, see "Transformation Editor dialog box."

      The empty Name, Arriving Group, and Leaving Group boxes have a red outline. You must enter information in the Name box and in at least one of the group boxes.

Figure 187. Transformation Editor dialog box



b. In the Name box, type alphanumeric text to identify the transformation.

   The red outline disappears.

c. Define the transformation as follows:

   - In the Arriving Group box, type alphanumeric text for the arriving group of the transformation, if applicable.

     Valid alphabetic characters include all of the naturally occurring elements in the periodic table. The valid range of integers is from 1 to 100 000.

     After you define the arriving group, the red outline remains until you place the cursor in the Leaving Group box. If you leave the Arriving Group box empty, the red outline remains until you define the leaving group.

   - In the Leaving Group box, type alphanumeric text for the transformation's leaving group.

     The red outline disappears when you select a phase from the Phase list or place the cursor in the Maximum Occurrence box.

   - In the Phase list, select **Phase 1** or **Phase 2** for a biotransformation, or select **Other** for other transformation types.

   - In the Maximum Occurrence box, type an integer from **1** to **10**.

     The Transformation Editor validates the entries from top to bottom.

   After you make valid entries, the Save button becomes available.

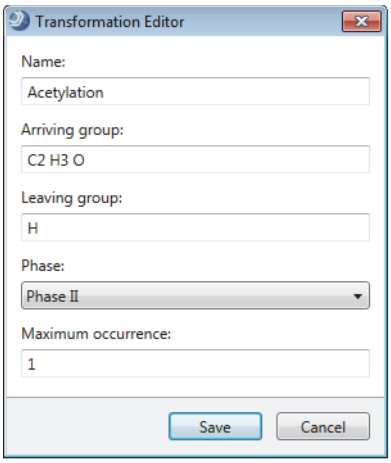
d. Click **Save**.

   The Transformation Editor dialog box closes and the new entry appears in the transformations library.

4. To edit an entry in the transformations list, do the following:
   a. Select the entry and click **Edit**.

      The Transformation Editor dialog box opens. The entry boxes are populated with the information for the transformation that you selected in the transformations list.

      Figure 188. Transformation Editor with information for an acetylation chemical reaction



   b. Make the appropriate changes.

      If the changes are invalid, the Save button becomes unavailable, the application outlines the invalid entries in red, and the invalid entries temporarily appear in the transformations library.

   c. Click **Save** and, at the prompt, click **Yes**.

Transformation Editor dialog box

Table 191 describes the parameters in the Transformation Editor dialog box.

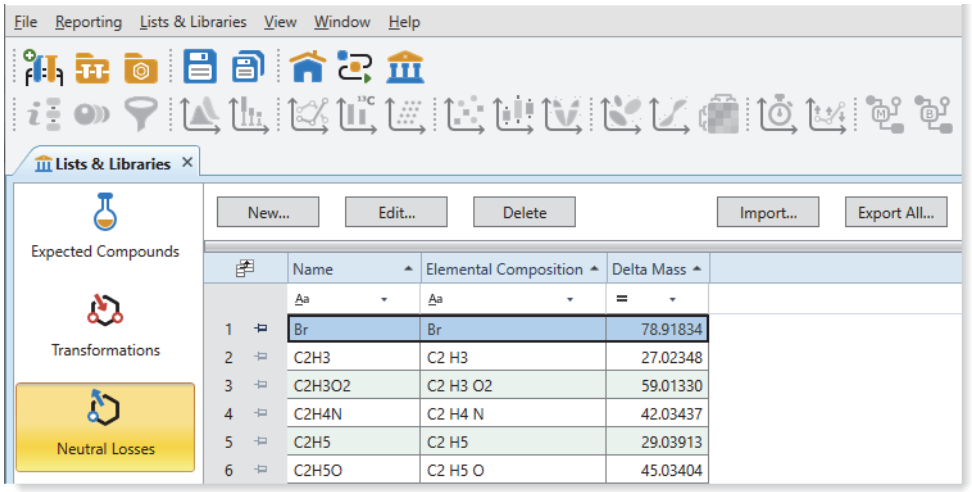
Table 191. Transformation Editor parameters

Parameter	Description
Name	Type alphanumeric text in this box.
Arriving Group	Type the elemental composition of the arriving group in this box.
Leaving Group	Type the elemental composition of the leaving group in this box.
Phase	Select a phase from this list. Selections: Phase I, Phase II, and Other
Maximum Occurrence	Type the maximum number of times that this reaction can occur in a set of combinatorial reactions. Default: 1; range: 1 to 10

Neutral Losses view

Use the Lists & Libraries > Neutral Losses view to modify the list of neutral losses that you can specify in an analysis that includes the Neutral Losses workflow node (for LC studies). See "Search Neutral Losses node."

Figure 189. Neutral Losses view



For more information, see these topics:

- Add, edit, delete, import, or export neutral loss entries
- Neutral Loss Editor
- Default neutral loss entries

Add, edit, delete, import, or export neutral loss entries

Table 192 describes the tasks that you can perform in the Neutral Losses view.

Table 192. Neutral Loss view tasks

Task	Procedure
Add a neutral loss entry to the list.	1. Click **New**. The Neutral Losses Editor opens. See "Neutral Loss Editor." 2. Do the following: • Type a name in the Name box. • Enter the elemental composition of the loss in the Elemental Composition box. 3. Click **Save**. By default, the new entry appears in the neutral loss list in alphabetical order.
Edit an existing neutral loss.	1. Select an entry and click **Edit**. 2. In the Neutral Loss Editor, edit the name, the elemental composition, or both. 3. Click **Save**.
Delete neutral losses.	1. Select the entries that you want to delete. Use the SHIFT key to select contiguous entries or the CTRL key to select noncontiguous entries. 2. Click **Delete**.
Import defined neutral losses.	1. Click **Import**. 2. Select the XML file that you want to import and click **Open**.
Export the neutral loss list to an XML file.	1. Click **Export All**. 2. Browse to the folder where you want to store the file. 3. Name the file. 4. Click **Save**.

Neutral Loss Editor

From the Lists & Libraries > Neutral Losses view, use the Neutral Loss Editor to add and edit neutral losses.

Tip To open the Neutral Loss Editor, click **New** in the Neutral Loss view or select an item in the neutral loss list and click **Edit**.

Figure 190. Neutral Loss Editor

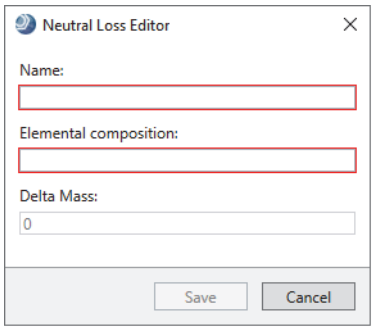


Table 193. Neutral Loss Editor

Parameter	Description
Name	Specifies the name of the elemental composition. The Name box accepts alphanumeric and special characters.
Elemental Composition	Specifies the elemental composition of the entry. The Elemental Composition box accepts any of the chemical symbols in the periodic table, D for deuterium, and T for tritium. For each chemical element, enter the element and the number of atoms for the element. Separate each element with a space.
Delta Mass	Displays the mass difference between the precursor ion and the product ion as the result of the neutral loss of the specified elemental composition. The application calculates the delta mass as you enter the elemental composition.
Save	Saves the new entry or the edited entry to the neutral losses table in the Neutral Losses view.

Default neutral loss entries

Table 194. Default neutral loss list (Sheet 1 of 2)

No.	Name	Elemental Comp.	Delta Mass	No.	Name	Elemental Comp.	Delta Mass
1	Br	Br	78.91384	36	Fatty_Acid_18.3	C18 H30 O2	278.22458
2	C2H3	C2 H3	27.02348	37	Fatty_Acid_20.4	C20 H32 O2	304.24023
3	C2H3O2	C2 H3 O2	59.01330	38	Fatty_Acid_22.5	C22 H34 O2	330.25588
4	C2H4N	C2 H4 N	42.03437	39	Fatty_Acid_22.6	C22 H32 O2	328.24023
5	C2H5	C2 H5	29.03913	40	Gluconuric Acid	C6 H10 O7	194.04265
6	C2H5O	C2 H5 O	45.03404	41	Glucuronide	C6 H8 O6	176.03209
7	C2H5OH	C2 H6 O	46.04186	42	H	H	1.00783
8	C2H6	C2 H6	30.04695	43	H2	H2	2.01565
9	C3H7	C3 H7	43.05478	44	H2C=CH2	C2H4	28.03130
10	C4H10	C4 H10	58.07825	45	H2C=O	C H2 O	30.01056
11	C4H7	C4 H7	55.05478	46	H2O	H2 O	18.01056
12	C4H8	C4 H8	56.06260	47	H2S	H2 S	33.98772
13	C4H9	C4 H9	57.07043	48	HBr	H Br	79.92616
14	CH2	C H2	14.01565	49	HCCH	C2 H2	26.01565
15	H2C=O	C H2 O	42.04695	50	HCl	H Cl	35.97668
16	CH3	C H3	15.02348	51	HCN	H Cl	27.01090
17	CH3CH=CH2	C3 H6	42.04695	52	Hexose	C6 H10 O5	162.05282
18	CH3CO	C2 H3 O	43.01839	53	Hexose-Hexose	C12 H20 O10	324.10565
19	CH3COOH	C2 H4 O2	60.02113	54	HF	H F	20.00623
20	CH3O	C H3 O	31.01839	55	HI	H I	127.91229
21	CH3OH	C H4 O	32.02621	56	HS	H S	32.97990
22	CH4	C H4	16.03130	57	I	I	126.90447
23	CH5O	C H5 O	33.03404	58	NH3	H3 N	17.02655
24	Cl	Cl	34.96885	59	NO	N O	29.99799
25	CO	C O	27.99491	60	NO2	N O2	45.99290
26	CO2	C O2	43.98983	61	OH	H O	17.00274
27	CO3	C O3	59.98474	62	Pentose	C5 H8 O4	132.04226
28	CONH2	C H2 N O	44.01364	63	Pentose-Hexose	C11 H18 O9	294.09508
29	Deoxyhexose	C6 H10 O4	146.05791	64	Pentose-Pentose	C10 H16 O8	264.08452

Table 194. Default neutral loss list (Sheet 2 of 2)

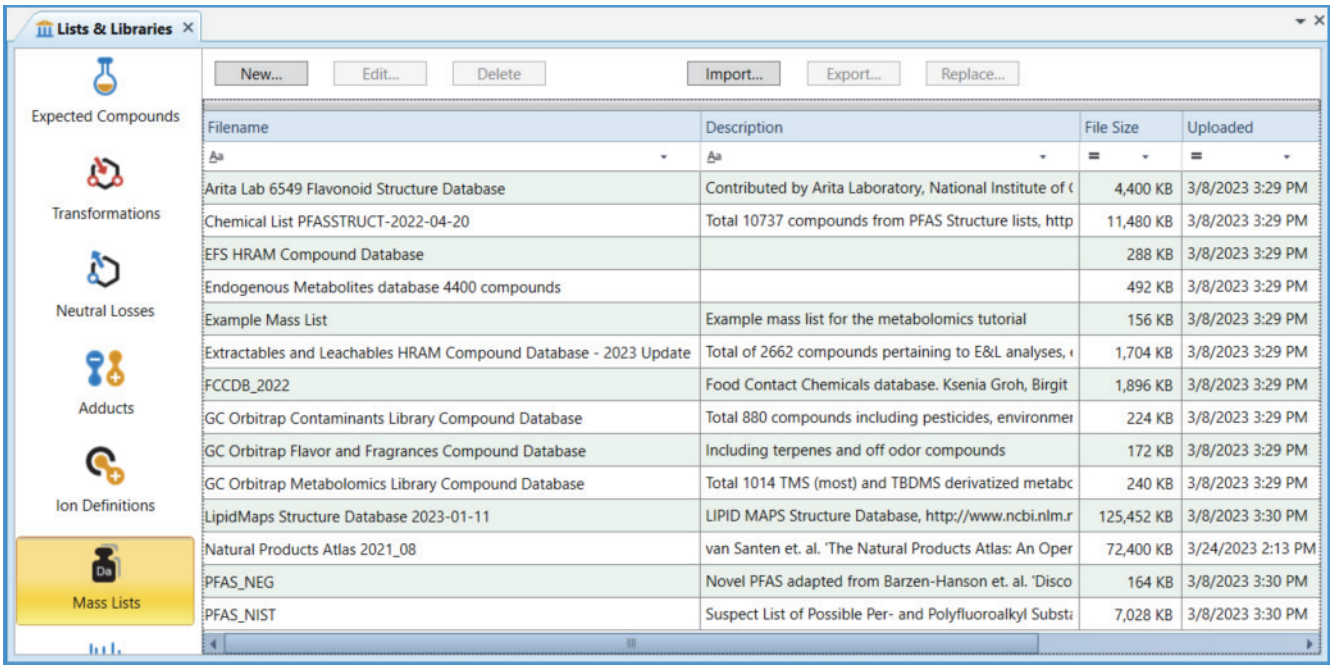
No.	Name	Elemental Comp.	Delta Mass	No.	Name	Elemental Comp.	Delta Mass
30	F	F	18.99840	64	Pyroglutamic Acid	C5 H7 N O3	129.04259
31	Fatty_Acid_16:0	C16 H32 0	256.24023	66	S	S	31.97207
32	Fatty_Acid_16:1	C16 H 30 02	254.22458	67	SO	O S	47.96699
33	Fatty_Acid_18:0	C18 H36 02	284.27153	68	SO2	O2 S	63.96190
34	Fatty_Acid_18:1	C18 H34 02	282.25588	69	y-GluAlaGly-2H	C10 H15 N3 O6	273.09609
35	Fatty_Acid_18:2	C18 H32 02	280.24023				

Mass Lists view

Use the Mass Lists view to create a library of available mass lists to use with the Search Mass Lists node—a processing workflow node that searches selected mass lists for matching compounds.

Tip To open the Mass Lists view, choose **Lists & Libraries > Mass Lists** from the application menu bar.

Figure 191. Mass Lists view



The application comes with 14 mass lists:

- Anita Lab 6549 Flavonoid Structure Database (with structures)
- Chemical List PFASSTRUCT-2022-04-20

- EFS HRAM Compound Database
- Endogenous Metabolites database 4400 compounds
- Example Mass List
- Extractables and Leachables HRAM Compound Database (with structures) 2023 Update

  Tip If you uninstall a previous version of Compound Discoverer 3.3 from your data processing computer before you install the latest service pack, your mass list will include the obsolete version of the Extractables and Leachables HRAM Compound Database and the current 2023 update of this mass list. To delete the obsolete mass list, select it and click **Delete**.

- FCCDB_2022

  For more information, go to https://doi.org/10.5281/zenodo.3240108.

- GC Orbitrap Contaminants Library Compound Database
- GC Orbitrap Flavor and Fragrances Compound Database
- GC Orbitrap Metabolomics Library Compound Database
- LipidMaps Structure Database 2021-09-13

  For more information, go to http://ncbi.nlm.nih.gov/pubmed/17098933.

- Natural Products Atlas 2021_08
- PFAS_NEG
- PFAS_NIST

  For more information, go to https://data.nist.gov/od/id/mds2-2387.

Note The Example Mass List file, which contains four amino acids, is specifically designed for the metabolomics tutorial for LC studies that you can access from the Help menu.

The application can read the following file types:

- The following types of CSV files:
  - CSV files with a molecular weight column that specifies the molecular weight to five decimal places, an elemental composition column, or both of these columns
  - CSV files created by exporting a ChemSpider Results table or a Compounds table as plain text

    Note The Export > As Plain Text shortcut menu command saves the data in the result table to a CSV file (ChemSpider Results.csv or Compounds.csv).

  - CSV files created by exporting data from the Thermo Scientific ToxID application

  - CSV files (MaConDa_*version#*_.csv) downloaded from the Mass Spectrometry Contaminant Database

- Mass lists files (.massList) created by the Compound Discoverer application
- XML files created by exporting all the compounds in the Expected Compounds library
- SDF files

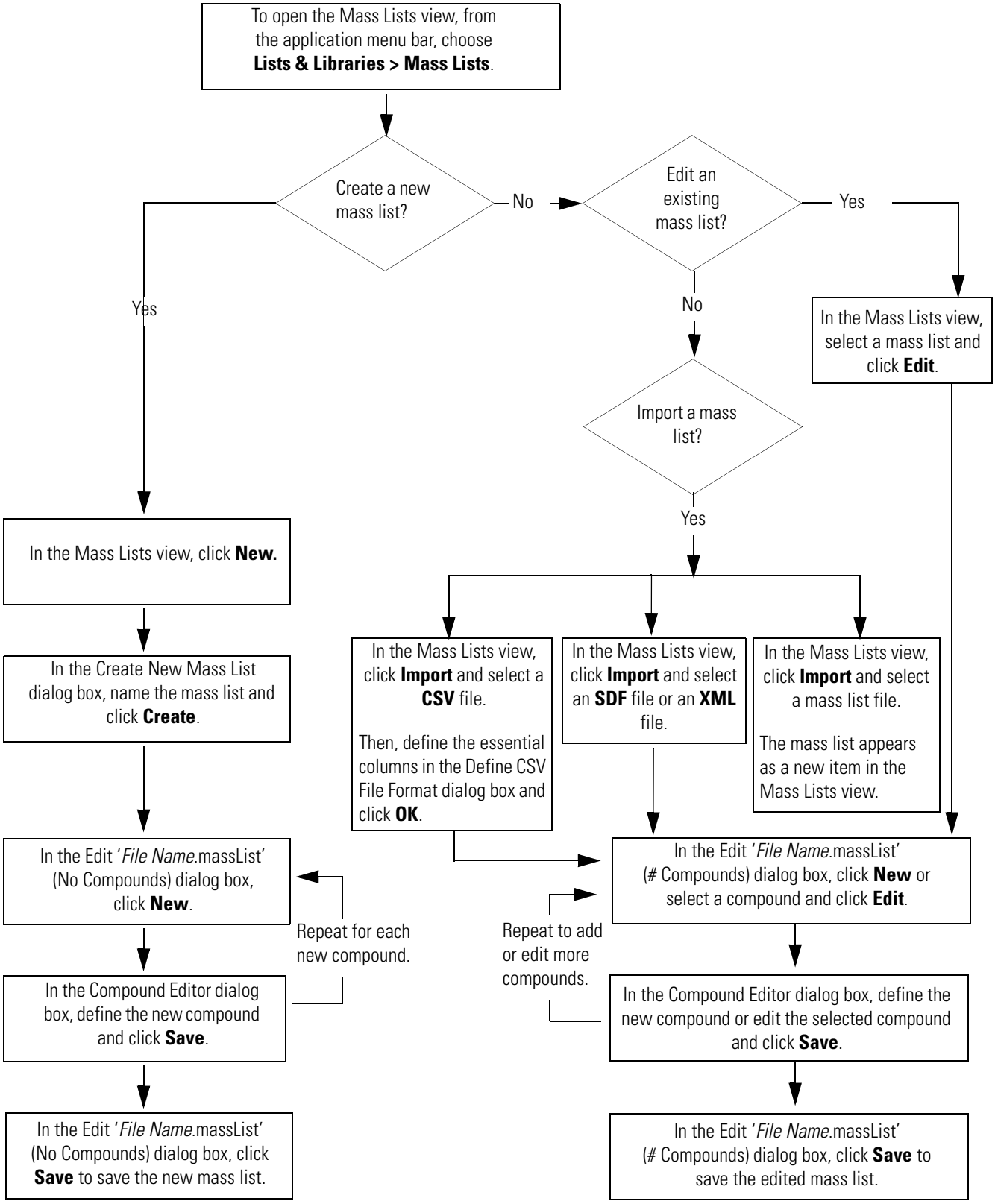
For information about creating, editing, importing, exporting, and replacing mass list files, see these topics:

- Flowchart for creating and editing mass lists
- Delete or replace mass list files
- Import a mass list from a CSV file
- Import a mass list from a massList file, an XML file, or an SDF file
- Export a mass list file
- Mass Lists view parameters

Flowchart for creating and editing mass lists

Figure 192 shows a flowchart for creating a new mass list from scratch or editing the compounds in an existing mass list.

Figure 192. Flowchart for creating, importing, and editing mass lists within the application



Delete or replace mass list files

❖ To delete mass list files or replace a mass list file

Do either of the following in the Lists & Libraries > Mass Lists view:

- To delete mass list files, select the entries to delete and click **Delete**. Then, at the prompt, click **Yes**.
- To replace a mass list file, select the entry and click **Replace**. Then, browse to the appropriate folder, select a massList file, and click **Open**.

Import a mass list from a CSV file

You can import mass lists from CSV, massList, SDF, or XML files. Follow this procedure to import a mass list from a CSV file.

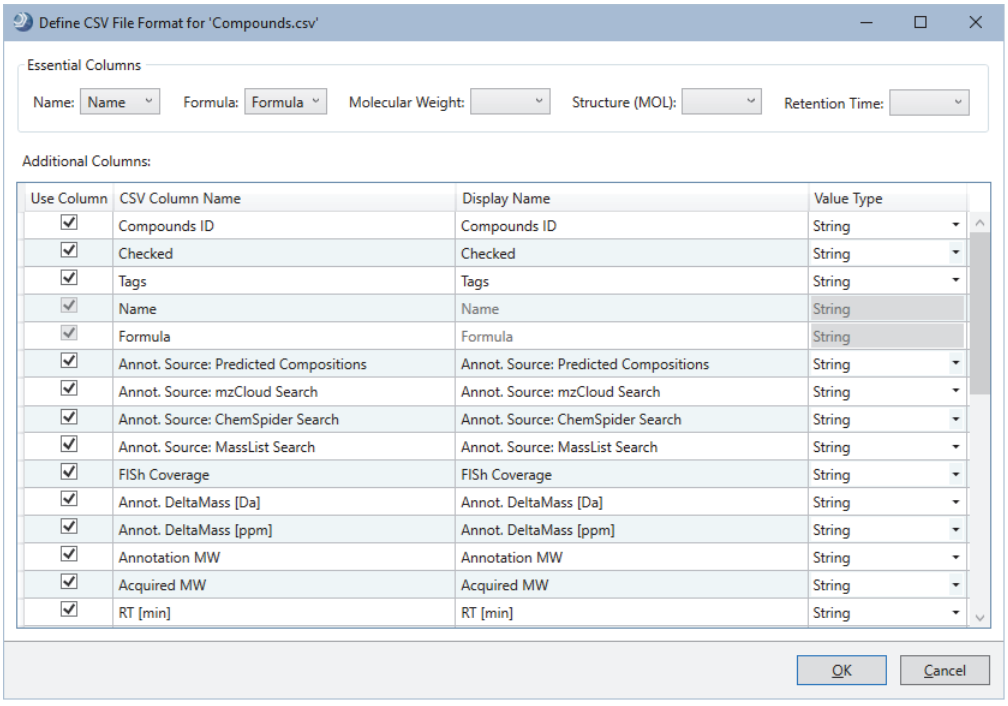
Tip You can create CSV files by exporting compound entries as plain text from the following result tables: Compounds, GC EI Compounds, or GC PCI Compounds.

❖ To import a mass list from a CSV file

1. In the Lists & Libraries > Mass Lists view, click **Import**.
2. Locate the CSV file of interest and click **Open**.

   The Define CSV Format dialog box opens.

Figure 193. Define DSV File Format for '*Filename*.csv' dialog box



Note When the column header in the CSV file matches the name of an essential column, the application recognizes it in the Essential Columns area. A red border around a column name indicates that you must define the column.

The OK button remains unavailable until you define the Name column and at least one column that provides the compound's mass.

3. Define the essential parameters in the Essential Columns area as follows:
   - To define the column in the CSV file that contains the compound names, select the column name from the Name list.
   - To define the column in the CSV file that provides the compound masses, select the column name from the Formula, Molecular Weight, or Structure lists.

     Note Double (for decimal numbers) is the value type for the Molecular Weight column.

   - To define the column in the CSV file that provides the chromatographic retention times of the compounds, select the column name from the Retention Time list.
4. Click **OK**.

   The Edit '*File Name.*massList (# Compounds)' dialog box opens.
5. To edit the mass list, see "Create and edit mass list files."

Import a mass list from a massList file, an XML file, or an SDF file

You can import mass lists from CSV, massList, SDF, or XML files.

❖ **To import a mass list from a massList file, an XML file, or an SDF file**

1. In the Libraries & Lists > Mass Lists view, click **Import**.
2. Locate the massList file, XML file, or SDF file and click **Open**.

   The Edit '*File Name.*massList (# Compounds)' dialog box opens.
3. To edit the mass list, see "Create and edit mass list files."

Export a mass list file

❖ **To export a mass list file to a specified file directory**

1. In the Libraries & Lists > Mass Lists view, select the file.
2. Click **Export**.
3. Select a folder for the file, rename the file if applicable, and click **Save**.

Mass Lists view parameters

Table 195 describes the parameters in the Mass Lists view.

Table 195. Mass Lists view parameters (Sheet 1 of 2)

Parameter	Description
Button	
New	Opens the Create Mass List dialog box for creating and naming a new and empty mass list file. After you name the file and click Create, the Edit '*File Name.*massList (# Compounds)' dialog box opens for adding compounds to the list.
Edit	Opens the Edit '*File Name.*massList (# Compounds)' dialog box for editing the selected mass list. Selecting a table row makes this button available.
Delete	Deletes the selected file from the library. Selecting a table row makes this button available.
Import	Opens a dialog box for locating and opening a CSV, a massList, an SDF, or an XML file that contains, at a minimum, a list of masses. When you select a CSV file, the Define CSV File Format 'File Name.csv' dialog box opens.
Export	Opens the Save As dialog box for renaming and saving the selected mass list file to another folder.
Replace	Replaces the selected file with the replacement file. Use this command when the replacement file has the same name as the current file. Selecting a table row makes this button available.
Table columns	
Filename	Displays the file name of the imported file.
Description	User-editable field for adding descriptive information about the mass list.
File Size	Displays the file size of the imported file.
Uploaded	Displays the date (month/day/year) and time (hour/minute) when you added the file to the library in the following format: MM/DD/YYYY HH:mm
Updated	Displays the data and time when the file was updated.

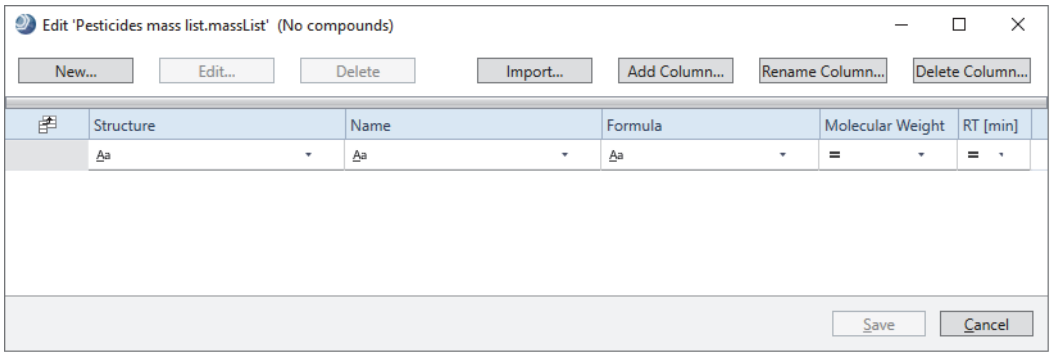
Table 195. Mass Lists view parameters (Sheet 2 of 2)

Parameter	Description
Context	Displays the source of the mass list—for example, Import from CSV or Import from XML.
State	Specifies whether the mass list is available, corrupted, or missing. If you remove a mass list from the ServerFiles folder or edit a mass list in the ServerFiles Folder, and then restart the application, the mass list's state changes to Missing or Corrupted, respectively.

Create and edit mass list files

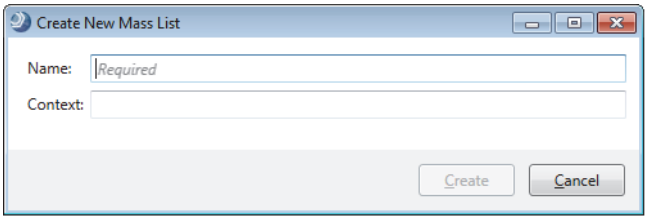
Use the Edit '*File Name*.massList (# Compounds or No Compounds) dialog box to modify the compounds list in a mass list. You can modify the mass list by adding, deleting, and editing the compounds in the list.

Figure 194. Edit '*File Name*.massList' (No Compounds) dialog box



❖ To create a new mass list from scratch or edit the compounds in an existing or imported mass list

1. From the application menu bar, choose **Lists & Libraries > Mass Lists**.
2. Do one of the following:
   - To create a new mass list from scratch, click **New**. Then, in the Create New Mass List dialog box, name the file and click **Create**.



The Edit *File Name* (No Compounds) dialog box opens with an empty mass list and the new file name appears in the table in the Mass Lists view.

- To import a mass list from an external .massList file or SDF file, click **Import**, select the file, and click **Open**.

  The Edit '*File Name* (# Compounds)' dialog box opens with editable entries for the selected mass list or an empty mass list.

- To edit an existing mass list file, select it and click **Edit**. Or, double-click it.

  The Edit '*File Name* (# Compounds)' dialog box opens with editable entries for the selected mass list or an empty mass list.

3. To modify the opened mass list, perform any of the tasks in Table 196.

Note You can add, rename, and delete nonessential columns. If you add a column, you cannot delete it until you save your changes and reopen the mass list for editing.

Table 196. Editing a mass list that is opened in the Edit '*File Name*' dialog box (Sheet 1 of 2)

Task	Procedure
Add a compound.	Click **New,** and follow the instructions in "Add and edit mass list compounds with the Compound Editor."
Delete a compound.	1. Select the compound and click **Delete**. 2. At the prompt, click **Yes**.
Import compounds from an XML file.	Click **Import**, locate the XML file, and click **Open**.
Import compounds from an SDF file.	Click **Import**, locate the SDF file, and click **Open**.
Import compounds from a CSV file.	1. Click **Import**, locate the CSV file, and click **Open**. 2. Define the essential columns as described in "Import a mass list from a CSV file." 3. Click **OK**.
Add a nonessential column.	1. Click **Add Column**. 2. In the Add Column dialog box, do the following: a. Name the column. b. (Optional) Select the data type: • String: Alphanumeric and special characters • Double: Decimal numbers • Integer: Integers c. Click **Add**.

Table 196. Editing a mass list that is opened in the Edit '*File Name*' dialog box (Sheet 2 of 2)

Task	Procedure
Rename a nonessential column.	1. Click **Rename Column**. 2. In the Old Name list, select the column. 3. In the New Name box, type the new name. 4. Click **Rename**.
Delete a nonessential column.	1. Click **Delete Column**. 2. In the Column list, select the column. 3. Click **Delete**.

4. Click **Save** to save the changes to the mass list.

Table 197 describes the buttons at the top of the Edit '*File Name*.massList' (#Compounds) dialog box.

Table 197. Edit '*File Name*.massList' (# Compounds) dialog box parameters

Feature	Description
Buttons	
New	Opens the Compound Editor dialog box for defining a new compound.
Edit	Opens the Compound Editor dialog box for editing the selected compound in the mass list. Selecting a compound makes this button available.
Delete	Deletes the selected compound from the mass list. Selecting a compound makes this button available.
Import	Opens a dialog box for locating and opening a CSV, massList, or XML file that contains, at a minimum, a list of masses. When you select a CSV file, the Define CSV File Format 'File Name.csv' dialog box opens.
Add Column	Opens the Add Column dialog box for naming and defining an additional table column.
Rename Column	Opens the Rename Column dialog box for renaming a nonessential column.
Delete Column	Opens the Delete Column dialog box for deleting a nonessential column.

Add and edit mass list compounds with the Compound Editor

Use the Compound Editor dialog box to add entries to and edit entries in a mass list.

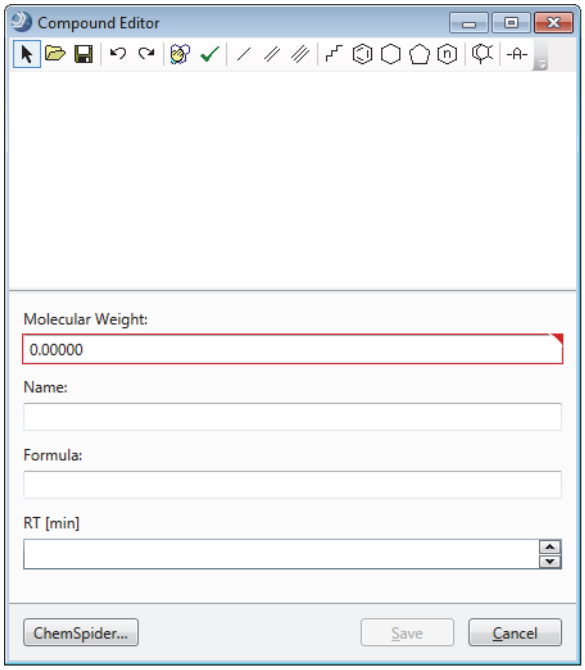
Note The application includes three similar Compound Editor dialog boxes. All three dialog boxes include the same structure drawing tools, but their data entry fields differ. The Compound Editor dialog box that opens for editing mass list compounds includes the following data entry fields: Molecular Weight, Name, Formula, and RT [min].

❖ To add a compound to or edit a compound in a mass list

1. From the Libraries & Lists > Mass Lists view, open the mass list for editing. See "Create and edit mass list files."
2. In the Edit '*File Name* (# Compounds)' dialog box, do one of the following:
   - To add a compound, click **New**.
   - To edit a compound, double-click it (or select it and click **Edit**).

   The Compound Editor dialog box opens (Figure 195). The dialog box is unpopulated for a new compound. The minimum required information is the compound's molecular weight.

Figure 195. Compound Editor dialog box for editing mass list compounds



3. To change the structure in or add a structure to the drawing area, use the structure tools, load a structure file, or click **ChemSpider** to find a structure file.

   For details, see these topics:

   - Structure drawing tools and commands
   - Load a structure from a structure file
   - Find a structure in the ChemSpider database

   Note If you are editing the structure for an existing entry in the mass list, the Molecular Weight field is unavailable, and any formula or structure that you enter must match the displayed molecular weight.

   The chemical structure appears in the drawing pane and its molecular weight and formula appear in their respective fields.

4. (Optional) In the Name box, type or edit the name of the compound.
5. (Optional) In the RT [min] box, enter a chromatographic retention time.

   The application rounds the retention time to three decimal places.

6. Click **Save**.

   The Edit '*File Name* (# Compounds)' dialog box appears.

7. Review the new or edited compound. If necessary, use the filter row to display only the new entry. See "Filter the tables on a study page or a list or library view."
8. To save the changes to the mass list that you are editing, click **Save**.

   Note If you attempt to close the dialog box without saving the changes, an Unsaved Changes prompt appears.

Spectral Libraries view

The following spectral libraries are snapshots of the mzCloud database taken in July 2021:

- mzCloud Offline for mzVault_Endogenous_2021B
- mzCloud Offline for mzVault_Endogenous-Autoprocessed_2021B
- mzCloud Offline for mzVault_Autoprocessed_2021B
- mzCloud Offline for mzVault_Reference_2021B

You can create your own custom mzVault libraries by using the mzVault 2.3 SP1 application or by exporting the spectral information from a Compound Discoverer result file from an LC study. See "Export spectral data to a new or existing mzVault library."

Tip The Search mzVault node does not require the mzVault application, so installing the mzVault 2.3 software is optional. However, Thermo Fisher Scientific recommends installing the software to do any of the following:

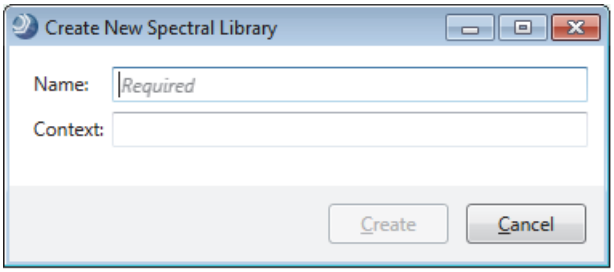
- Edit existing spectral libraries.
- Create new spectral libraries with curated spectra.
- Convert existing legacy mzVault spectral libraries.

You can create new mzVault libraries with the Compound Discoverer 3.3 application, but you are limited to exporting spectra from these result tables: Compounds and Expected Compounds.

Note You cannot edit spectral libraries in the Compound Discoverer application. The Edit button in the command bar is unavailable.

Table 198 provides instructions for managing the spectral libraries.

Table 198. Tasks for managing the spectral libraries

Task	Procedure
Open the Spectral Libraries view.	From the application menu bar, choose **Lists & Libraries > Spectral Libraries**.
Add an mzVault library.	Click **Import**, locate the library, and click **Open**.
Replace an mzVault library.	In the Spectral Libraries view, select the library. Then, click **Replace**, locate the library, and click **Open**.
Export an mzVault library.	In the Spectral Libraries view, select the library. Then, click **Export**, select a folder, and click **Save**.
Delete an mzVault library.	In the Spectral Libraries view, select the library, and click **Delete**.
Create a new but empty mzVault library.	1. In the Spectral Libraries view, click **New**. The Create New Spectral Library dialog box opens.  2. Name the file and click **Create**.

Metabolika Pathways view

Initially, the Metabolika Pathways view contains a list of the Metabolika pathways files (.metabolika) that install with the Compound Discoverer application.

Use the Metabolika Pathways view to create new pathways, edit existing pathways, import and export pathways, and replace pathways.

Tip To open the Metabolika Pathways view, from the application menu bar, choose **Lists & Libraries > Metabolika Pathways**.

For details, see these topics:

- Metabolika Pathways view parameters
- Delete, import, export, and replace Metabolika pathways

For information about creating and editing Metabolika pathways, see "Edit new and existing Metabolika pathways."

Metabolika Pathways view parameters

Table 199 describes the buttons across the top of the view and the table columns from left to right.

Table 199. Metabolika Pathways view parameter descriptions (Sheet 1 of 2)

Parameter	Description
Filter row	Use this row to filter the table as appropriate. See "Filter the tables on a study page or a list or library view."
Button	
New	Opens the Create New Metabolika Pathway dialog box for naming the new Metabolika Pathway file.
Edit	Opens Edit Metabolika Pathway '*Pathway name*' dialog box.
Delete	Deletes the selected Metabolika pathway files from the list.
Import	Opens the file browser for selecting a Metabolika pathway file.
Export	Opens the Save As dialog box for renaming the pathway, saving it to a new directory, or both.
Replace	Opens the file browser for selecting a Metabolika pathway file to replace the currently selected file.
Column	
Filename	Displays the file name of the imported file.
Description	User-editable field for adding descriptive information about the pathway.

Table 199. Metabolika Pathways view parameter descriptions (Sheet 2 of 2)

Parameter	Description
File Size	Displays the file size of the imported file.
Uploaded	Displays the date (month/day/year) and time (hour/minute) when you added the file to the list in the following format: MM/DD/yyyy HH:mm
Updated	Displays the data and time when the file was updated.
Context	Displays the source of the pathway.
State	Specifies whether the pathway is available, corrupted, or missing. If you remove a pathway file from the ServerFiles folder or edit a pathway in the ServerFiles Folder, and then restart the application, the state of the pathway changes to Missing or Corrupted, respectively.

Delete, import, export, and replace Metabolika pathways

Table 200 describes how to delete, import, export, and replace Metabolika pathways.

Table 200. Deleting, importing, exporting, or replacing Metabolika pathways

Task	Procedure
Delete Metabolika pathways from the list.	1. In the Metabolika Pathways view, select the pathways and click **Delete**. 2. At the prompt, click **Yes**.
Import Metabolika pathway files into the list.	1. In the Metabolika Pathways view, click **Import**. 2. Locate the files (.metabolika) and click **Open**.
Export Metabolika pathway files to another folder.	1. In the Metabolika Pathways view, select the pathways, and then click **Export**. 2. In the Browse For Folder dialog box, select a folder and click **OK**. The application copies the files to the selected folder.
Replace a Metabolika pathway file with another Metabolika pathway file.	1. In the Metabolika Pathways view, select the pathway and click **Replace**. 2. Locate the replacement file and click **Open**.

Edit new and existing Metabolika pathways

Use the Edit '*File Name*.metabolika' dialog box to create a new Metabolika pathway or edit an existing Metabolika pathway.

To create or edit a Metabolika pathway, see these topics:

- Create a new Metabolika Pathway file
- Edit an existing Metabolika pathway
- Modify the arrows in a Metabolika pathway
- Shortcut menu for the Metabolika pathway editor

Create a new Metabolika Pathway file

You can create new Metabolika Pathway files.

❖ To create a new Metabolika pathway

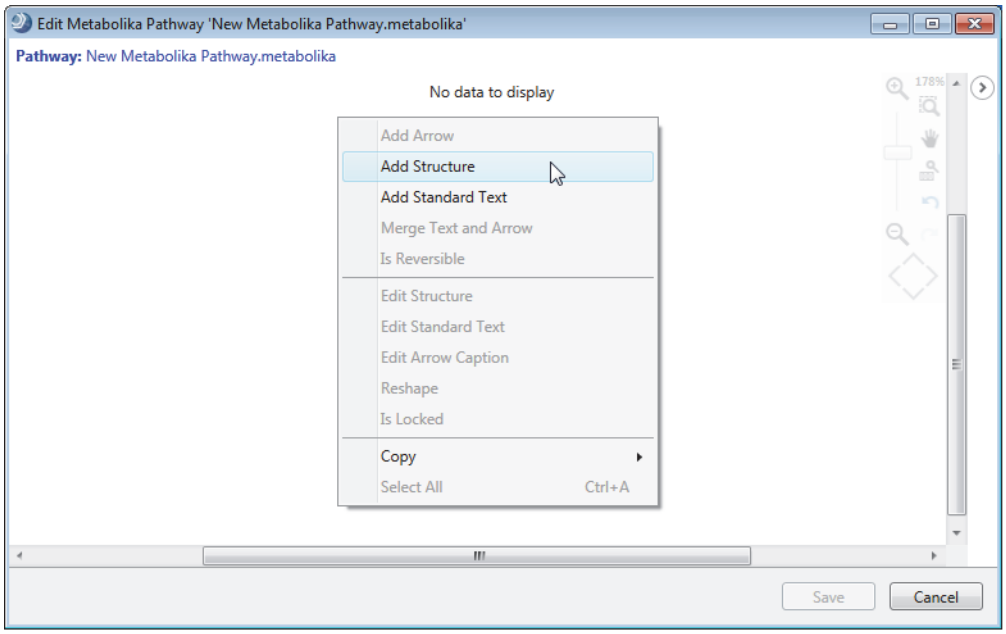
1. From the application menu bar, choose **Lists & Libraries > Metabolika Pathways**.
1. In the Metabolika Pathways view, click **New**.

   The Create New Metabolika Pathway dialog box opens.
2. Name the file and click **Create**.

   The Edit Metabolika Pathway '*File Name*.metabolika' dialog box opens.

3. In the pathway editor, right-click and choose **Add Structure**.

   Figure 196. Metabolika pathway editor with shortcut menu



   The Compound Editor opens.

4. Use the Compound Editor to add new structures. See "Add and edit Metabolika pathway structures."

5. To add an arrow to indicate the direction between reactants and products, right-click a structure and choose **Add Arrow**. To add more arrows, repeat this step.

   By default, arrows are straight unidirectional lines with one arrowhead and four anchor points (Figure 197). To change the arrow's properties, see "Modify the arrows in a Metabolika pathway."

   Figure 197. Selected arrow with four anchor points

6. To clean up the drawing, do any of the following:

   - To delete a structure or an arrow, select it and press the Delete key.
   - To delete all the drawing items, right-click and choose **Select All**. Then, press the Delete key.
   - To move a structure or an arrow, select it and hold down the left mouse button to display the move pointer. Then, drag the items to another location.

Edit an existing Metabolika pathway

❖ **To edit an existing Metabolika pathway**

1. In the Metabolika Pathways view, select the pathway and click **Edit**.

   The Metabolika pathway editor opens and displays the selected pathway or the beginning section of the pathway in the left pane and the entire pathway at a lower zoom level in the right pane. Use the tools in the upper right of the left pane to change the zoom level, and the selection window in the right pane to display a different section of the pathway in the left pane.

2. To modify the pathway, do any of the following:

   - To edit a structure, right-click it and choose **Edit Structure**.

     The Compound Editor opens.

   - To add a structure, right-click it anywhere in the left pane and choose **Add Structure**.

     The Compound Editor opens.

   - To edit the arrows, see "Modify the arrows in a Metabolika pathway."

3. To undo a change, use the CTRL+Z keys.

   You can undo up to six changes.

Modify the arrows in a Metabolika pathway

To modify the arrows in a Metabolika pathway, see the following table.

Table 201. Modifying the arrows in a Metabolika pathway (Sheet 1 of 3)

Task	Procedure
Move an arrow.	1. Select the arrow and hold down the left mouse button to display the move pointer (✥).  2. Drag the arrow to another location.
Change the angle of an arrow.	1. Select the arrow to display its anchor points, and then point to an end anchor point. 2. When this pointer (⇳) appears, drag the end of the arrow up or down as appropriate.

Table 201. Modifying the arrows in a Metabolika pathway (Sheet 2 of 3)

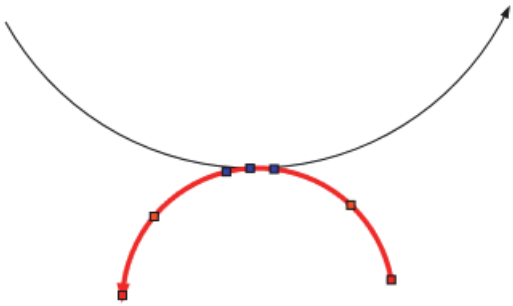
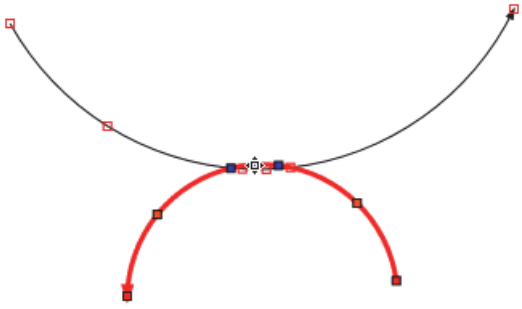
Task	Procedure
Change the curvature of an arrow.	1. Select the arrow to display its anchor points, and then point to one of its two internal anchor points. 2. When this pointer (⇕) appears, drag the pointer arrow up or down as appropriate. 
Straighten a curved arrow.	Right-click the arrow and choose **Reshape**.
Make an arrow bidirectional to represent a reversible reaction.	Right-click it and choose **Is Reversible**.
Merge arrows.	1. Reshape the arrows into curves. 2. Overlay the curved arrows, and then select one of the curves.  3. Point to any of the blue squares. 4. When this pointer (✥) appears, drag the selected curve until the red square anchor points appear on the second curve, and then release the mouse button.  5. To straighten one of the merged arrows, right-click it and choose **Reshape**.

Table 201. Modifying the arrows in a Metabolika pathway (Sheet 3 of 3)

Task	Procedure
Add an arrow caption.	1. Right-click the arrow and choose **Edit Arrow Caption**. 2. In the Plain HTML dialog box, type text or text with standard HTML tags and click **OK**. 3. To lock the caption to the arrow, right-click the arrow and choose **Is Locked**.

Shortcut menu for the Metabolika pathway editor

Table 202 describes the shortcut menu for the Metabolika pathway editor.

Table 202. Shortcut menu for the Metabolika pathway editor

Command	Function
Add Arrow	Adds a straight, unidirectional arrow.
Add Structure	Opens the Compound Editor dialog box for adding a structure.
Add Standard Text	Opens the Plain HTML dialog box for adding formatted text.
Merge Text and Arrow	Merges a selected standard text string to a selected arrow.
Is Reversible	Makes the selected arrow bidirectional.
Edit Structure	Opens the Compound Editor dialog box for editing the selected structure. Available for a selected structure.
Edit Standard Text	Use to edit standard text, which is text that is not associated with a structure or an arrow.
Edit Arrow Caption	Opens the Plain HTML dialog box for entering formatted text as an arrow caption.
Reshape	Straightens a curved arrow.
Is Locked	Locks the arrow caption to the arrow.
Copy > Selection	Copies the selected items. Press CTRL+V to paste the copied items elsewhere in the dialog box.
Copy > Structure	Copies the selected structure.
Copy > Pathway	Copies the pathway.
Select All	Selects all the drawing items in the dialog box.

Add and edit Metabolika pathway structures

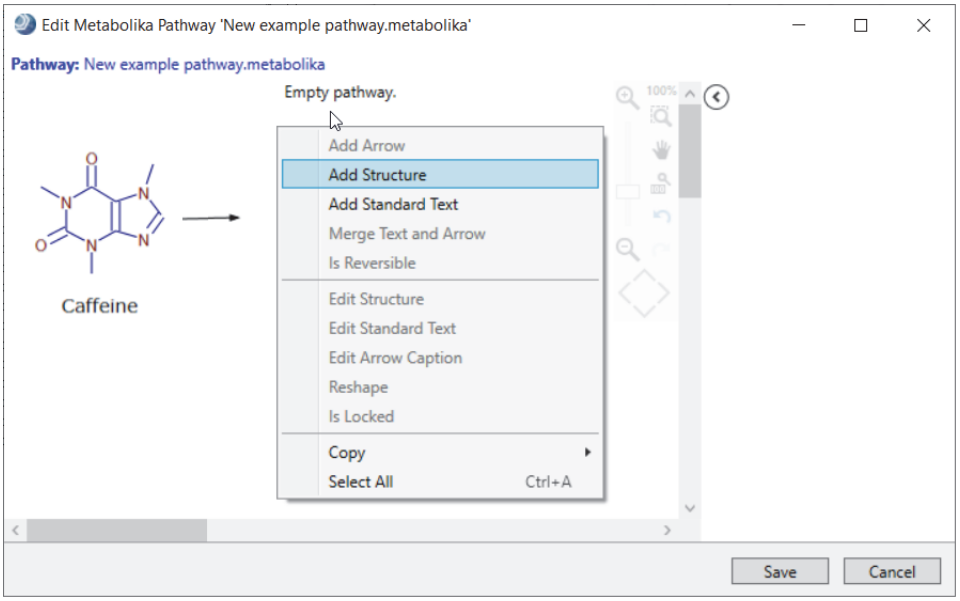
Use the Compound Editor to add structures to and edit the structures in a Metabolika pathway.

❖ To edit or add a structure to a Metabolika pathway

1. Open the Compound Editor for editing and adding Metabolika pathway structures by doing one of the following:

   - Right-click the workspace in the Edit Metabolika Pathway '*pathway name*' dialog box and choose **Add Structure**.

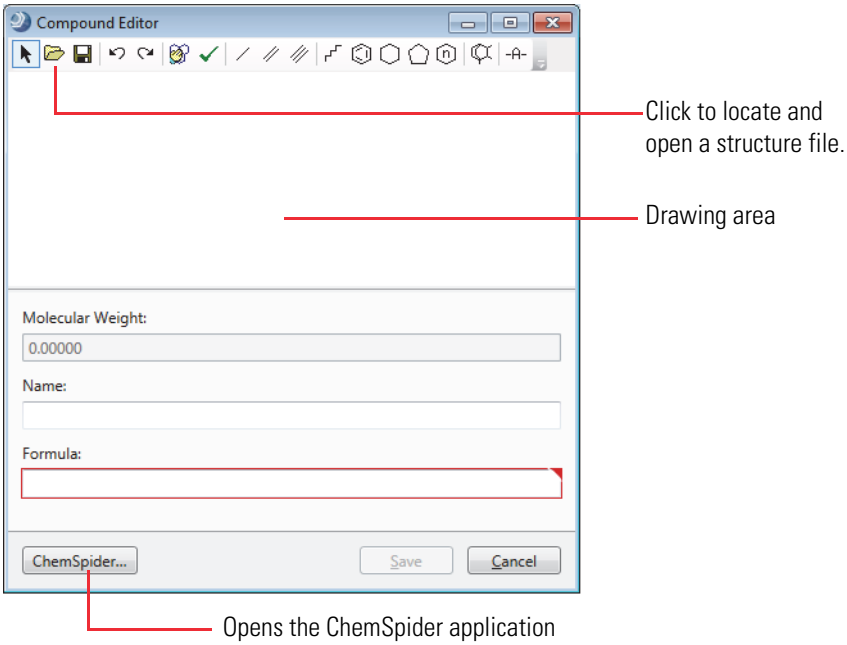
     Figure 198. Edit Metabolika Pathway '*pathway name*' dialog box with shortcut menu

   - Double-click a structure in the pathway.

   Figure 199 shows the Compound Editor dialog box for a new structure.

Figure 199. Compound Editor dialog box for editing Metabolika pathway structures



2. Do one of the following:

   - When adding a new structure, do any of the following:
     - Use the drawing tools. See "Structure drawing tools and commands."
     - Load a structure file. See "Load a structure from a structure file."
     - Use the ChemSpider application. See "Find a structure in the ChemSpider database."

     The application automatically populates the Molecular Weight and Formula boxes.
   - When editing an existing structure, you are limited to structures that match the current molecular weight and formula.

Compound Classes view

The Compound Classes view contains a library of compound class files. Each compound class file contains a list of fragment ions.

When the processing workflow includes the Compound Class Scoring node with one or more user-specified compound class lists of fragments, the application determines the probability that an unknown compound belongs to the compound classes by comparing the ions detected in the fragmentation scans to the fragments in the compound class lists.

Tip To open the Compound Classes view, choose **Lists & Libraries > Compound Classes** from the application menu bar.

The view opens as a tabbed page in the application window.

The application comes with four compound class lists:

- Omeprazole Compound Class.clib

  This file contains the fragments for the target compound in the *Compound Discoverer Metabolism Tutorial*.

- PFAS Fine Signature Fragment-lib.clib and PFAS General from FluoroMatch Suite.clib

  These files contain fragments for the PFAS family of compounds. The following processing workflow template uses these compound class files in the Compound Class Scoring node:

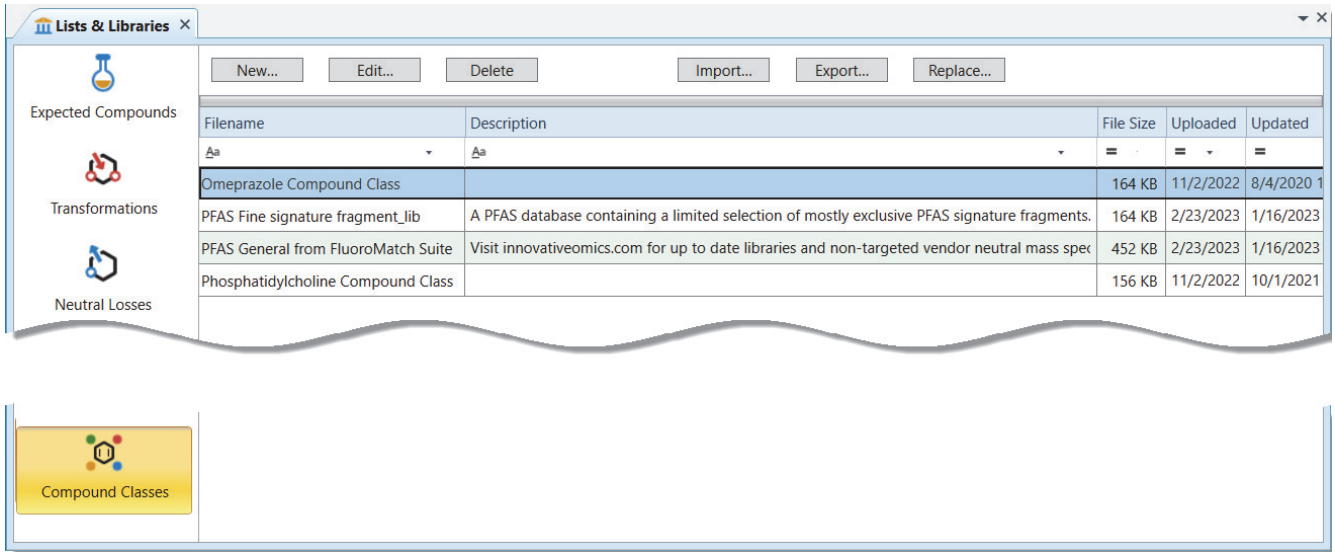
  PFAS Unknown ID w Database Searches and Molecular Networks.cdProcessingWF

  Note For information about identifying compounds in the PFAS family, see "PFAS identification."

- Phosphatidycholine Compound Class.clib

Use the Compound Classes view, the Edit '*Named Compound Class*' dialog box, and the Fragmentation Editor to create your own compound class files.

Figure 200. Compound Classes view



The process for editing the fragment structures in a compound class file is as follows:

1. From the application menu bar, choose **Lists & Libraries > Compound Classes**.

   The Compound Classes view opens.

2. In the Compound Classes view, double-click the file that you want to edit.

   The Edit Compound Class '*File name*' dialog box opens.

3. In the Edit Compound Class dialog box, double-click the fragment that you want to edit.

   The Fragment Editor opens.

4. Edit the fragment and click **Save**. Then, click **Save** to save the compound class file.

For more information about the Compound Classes view, see the following topics:

- Compound Classes view parameters
- Add new files to the Compound Classes library
- Delete, import, and export compound class files
- Edit compound class files
- Edit Compound Class dialog box parameters

Compound Classes view parameters

Table 203 describes the parameters in the Compound Classes view.

Table 203. Compound Classes view parameters (Sheet 1 of 2)

Parameter	Description
Button	
New	Opens the Create New Compound Class dialog box for naming a new and empty fragments file. After you name the file and click Create, the Edit Compound Class dialog box opens for adding fragments.
Edit	Opens the fragments list for the selected compound class file. Selecting a compound class file makes this button available.
Delete	Deletes the selected file from the library. Selecting a table row makes this button available.
Import	Opens a dialog box for locating a compound class library file (.clib). The application adds the selected file to the library.

Table 203. Compound Classes view parameters (Sheet 2 of 2)

Parameter	Description
Export	Opens the Save As dialog box for renaming and saving the selected file to another folder.
Replace	Replaces the selected file with the replacement file. Use this command when the replacement file has the same name as the current file. Selecting a table row makes this button available.
Table columns	
Filename	Displays the file name of the library file.
Description	User-editable field for adding descriptive information about the file.
File Size	Displays the file size of the file.
Uploaded	Displays the date (month/day/year) and time (hour/minute) when you added the file to the library in the following format: MM/DD/YYYY HH:mm
Updated	Displays the data and time when the file was updated.
Context	Displays the description that you entered in the Context box of the Create New Compound Class dialog box.
State	Specifies whether the compound class file is available, corrupted, or missing. If you remove or edit a compound class file from its storage folder, and then restart the application, the mass list's state changes to Missing or Corrupted, respectively.

Add new files to the Compound Classes library

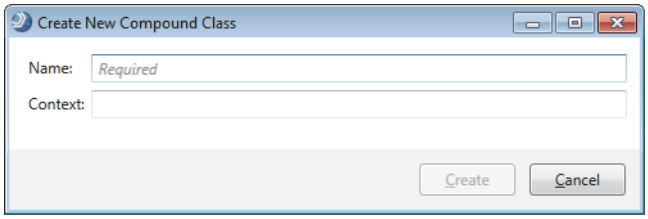
A compound class file contains a list of fragment structures. To use a compound class file, you must add it to the Compound Classes library.

❖ To add new compound class files to the Compound Classes library

1. Open the Compound Classes view by choosing **List & Libraries > Compound Classes** from the application menu bar.
2. In the Compound Classes view, click **New**.

   The Create Compound Class dialog box opens.

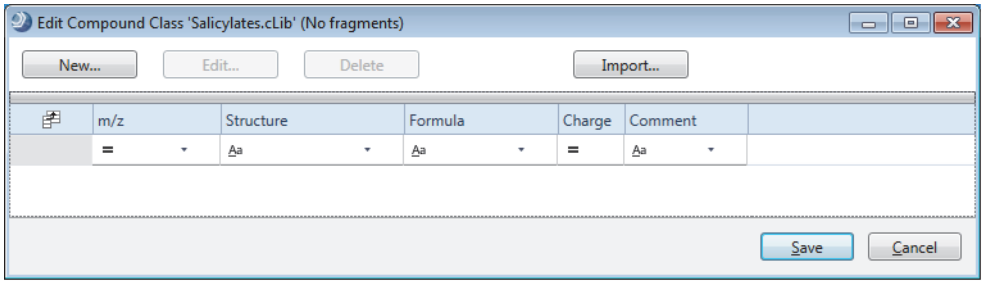
Figure 201. Create Compound Class dialog box



3. Name the compound class, optionally provide a brief description, and click **Create**.

   The named compound class appears as a new row in the Compound Classes view and the Edit Compound Class '*Name*' dialog box opens. For information about this dialog box, see "Edit Compound Class dialog box parameters."

Figure 202. Edit Compound Class *'Name'* dialog box



4. In the Edit Compound Class '*Name*' dialog box, click **New**.

   The Fragment Editor dialog box opens. Before you add any fragments to the new compound class, the dialog's title bar includes the following text: (No Fragments).

5. Define the fragments for the compound class. See Use the Fragment Editor to define fragment ions.

6. After you add the fragments of interest, click **Save.**

   The Edit Compound Class '*File name*' dialog box dialog box closes.

Delete, import, and export compound class files

In the Compound Class view of the Lists & Libraries page, you can directly delete, import, or export compound class files (.clib) by using the appropriate command in the command bar at the top of the view below the title bar.

Table 204. Deleting, importing, and exporting compound class files

Task	Procedure
Delete a compound class file from the list.	1. In the Compound Classes view, select the compound class of interest and click **Delete**. 2. At the prompt, click **Yes**.
Import a compound class file.	1. In the Compounds Class view, click **Import**. 2. Browse to and select a compound class library file (.clib). 3. Click **Open**. The application uploads the file to your local hard drive in the ProgramData\Thermo\Compound Discoverer X.X\ ServerFiles folder. A new entry appears in the library. The entry displays the following information about the compound class: name, description, # fragments, date uploaded, date updated, and file size.
Export a compound class file.	1. In the Compounds Class view, select the compound class of interest and click **Export**. 2. In the Save As dialog box, browse to a storage location for the file, change the file name when applicable, and click **Save**.

Edit compound class files

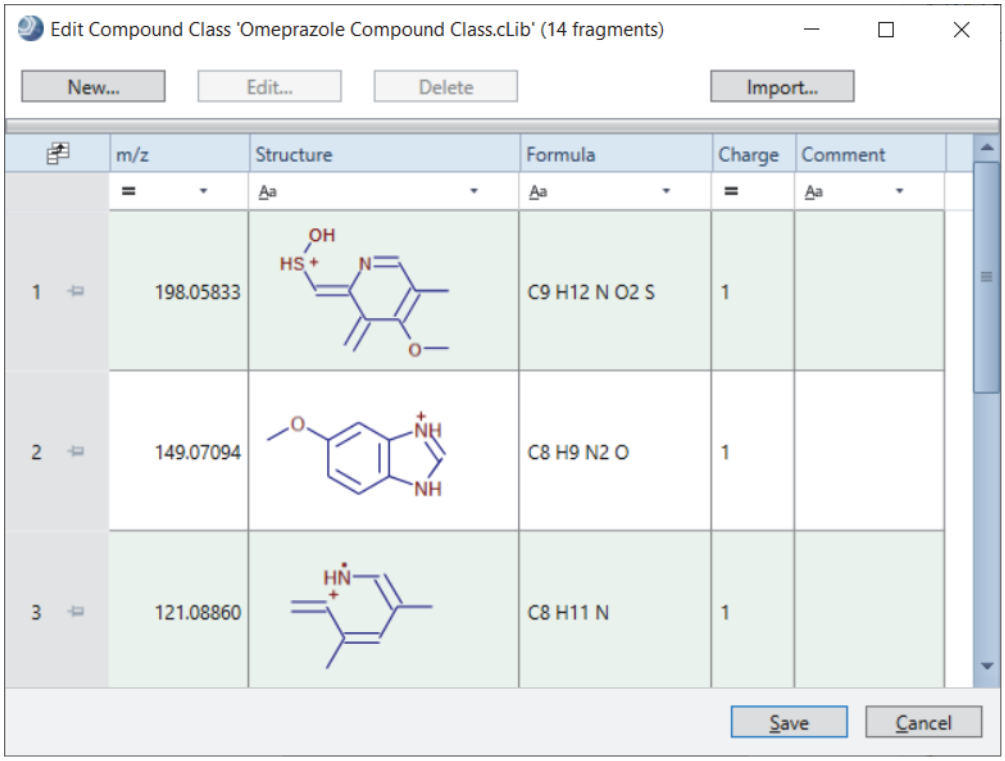
Use the Edit Compound Class '*File name*' dialog box to edit compound class files and the Fragment Editor to edit the fragments in the files.

❖ To edit a compound class file

1. In the Compound Classes view of the List & Libraries page, double-click the compound class file that you want to edit. Or, select the file and click **Edit**.

   The Edit Compound Class '*File name*' dialog box opens with a list of fragments.

Figure 203. Edit Compound Class dialog box for the Omeprazole Compound Class file



2. In the Edit Compound Class '*File name*' dialog box, do the following as applicable:
   - To add a new fragment by using the Fragment Editor, click **New**. Then, use the Fragment Editor to define the fragment (see Use the Fragment Editor to define fragment ions).
   - To add new fragments by importing their structures from a CSV file or an SDF file, click **Import**.
   - To edit a fragment, select it and click **Edit**. Then, use the use the Fragment Editor to edit the fragment (see Use the Fragment Editor to define fragment ions).
   - To delete a fragment, select it and click **Delete**.
3. Click **Save** to save your edits and return to the library.

Edit Compound Class dialog box parameters

Table 205 describes the buttons and columns in the compound class editor.

For information about using the compound class editor, see these topics:

- Add new files to the Compound Classes library
- Edit compound class files

Table 205. Edit '*Name*' Compound Class dialog box parameters

Parameters	Description
Buttons	
New	Opens the Fragment Editor for defining a fragment. See "Use the Fragment Editor to define fragment ions."
Edit	Opens the Fragment Editor with the definition of the selected fragment.
Delete	Deletes the selected fragment.
Import	Opens the Open dialog box for selecting a CSV file or an SDF file.
Table columns	
m/z	Displays the *m/z* value of the fragment.
Structure	Displays the structure of the fragment.
Formula	Displays the formula of the fragment.
Charge	Displays the charge of the fragment.
Comment	Displays the description that you typed in the Create Compound Class dialog box.

Use the Fragment Editor to define fragment ions

Use the Fragment Editor to define fragments for a compound class.

Note For information about using the drawing tools, see "Structure drawing tools and commands."

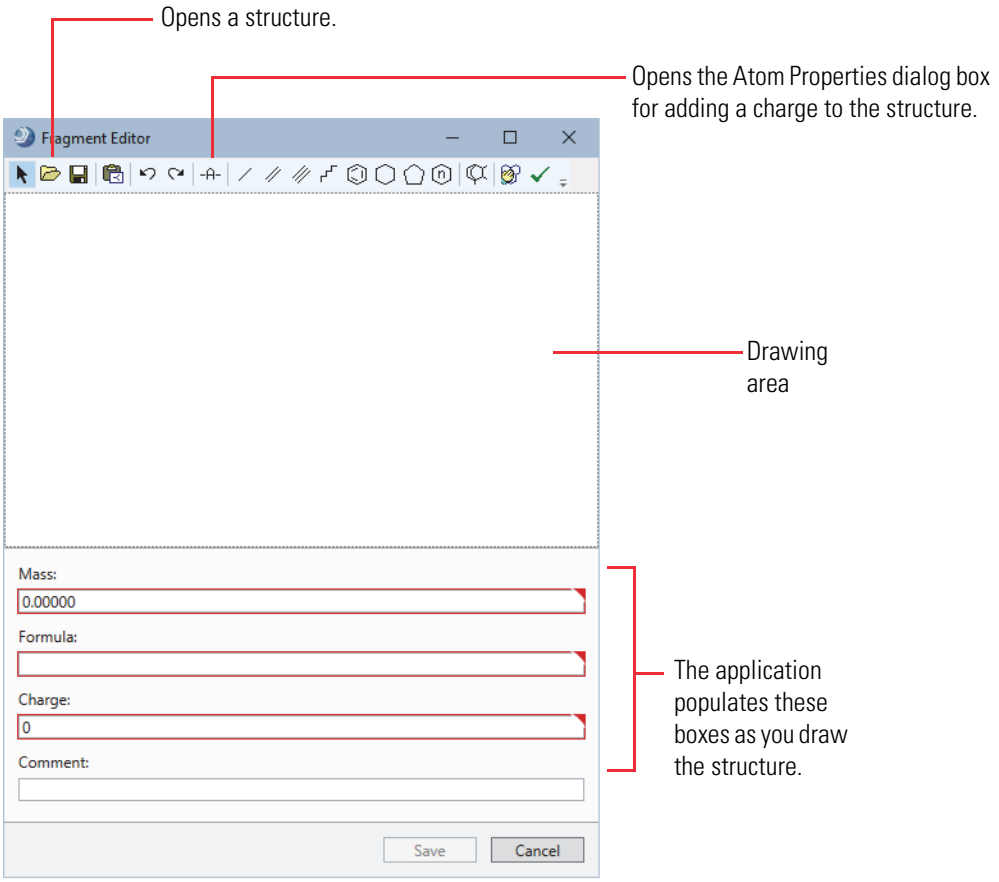
❖ To open the Fragment Editor dialog box

1. Open the Compound Classes view from the application menu by choosing **Lists & Libraries > Compound Classes**.
2. In the Compound Classes view, do one of the following:
   - To edit the fragments list in a existing compound class file, select a compound class file and click **Edit**. Then, in the Edit Compound Class *'name'* (# fragments) dialog box, select a fragment and click **Edit**.
   - To create a new compound class file, click **New**. In the Create Compound Class dialog box, name the library, type a description, and click **OK**. Then, in the Edit '*Named Compound Class*' (No Fragments) dialog box, click **New**.

   The Fragment Editor dialog box opens.

Figure 204 shows the Fragment Editor dialog box.

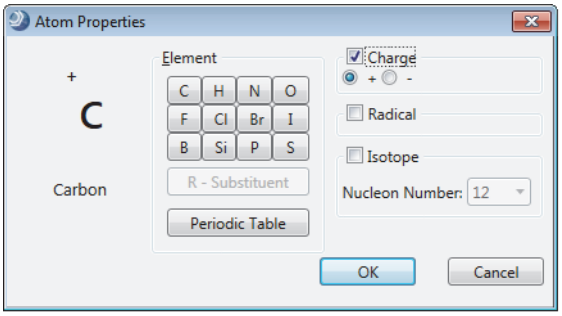
Figure 204. Fragment Editor dialog box



3. Do either of the following:
   - Use the drawing tools to add a structure to the drawing area. See "Structure drawing tools and commands."
   - Open a structure file. See "Load a structure from a structure file."
4. Add a charge to the structure as follows:
   a. Select the atom where you want to add a charge.
   b. Click the **Atom Properties** icon, .

      The Atom Properties dialog box opens.

Figure 205. Atom Properties dialog box with an available Charge check box



c. In the Atom Properties dialog box, select the **Charge** check box.

d. Select the positive (+) or negative (–) option.

e. Click **OK**.

Load a structure from a structure file

You can load a structure from a structure file from any of the compound editors or the fragment editor.

❖ **To load a structure from a structure file**

1. In the editor's toolbar, click the **Load Structure from Disk** button, .

   The Open Structure dialog box opens.

2. In the Known Structure Formats list, select the format of the structure file: **MOL Format (.mol)**, **Compressed Structure (.mcs)**, or **Template (.tml)**.

3. Locate the structure file and click **Open**.

   The chemical structure appears in the drawing pane, and the application automatically populates the Elemental Composition and Molecular Weight boxes.

If the structure is not visible or it is only partially visible in the pane, right-click the pane and choose **Select All**. Then, while pressing the SHIFT key, drag the structure into the pane.

Find a structure in the ChemSpider database

You can access the ChemSpider database from the Compound Editor dialog box or the Compound Annotation Editor dialog box and search for a compound entry with a structure file.

Note For an LC study, you can also access the ChemSpider database from the mzLogic Analysis view.

Tip For information about the editors, see "Add and edit expected compounds with the Compound Editor." For information about the mzLogic Analysis view, see "mzLogic Analysis view."

Note The search accepts uncharged and charged structures.

❖ To load a structure into the drawing area of the editor or mzLogic Analysis view

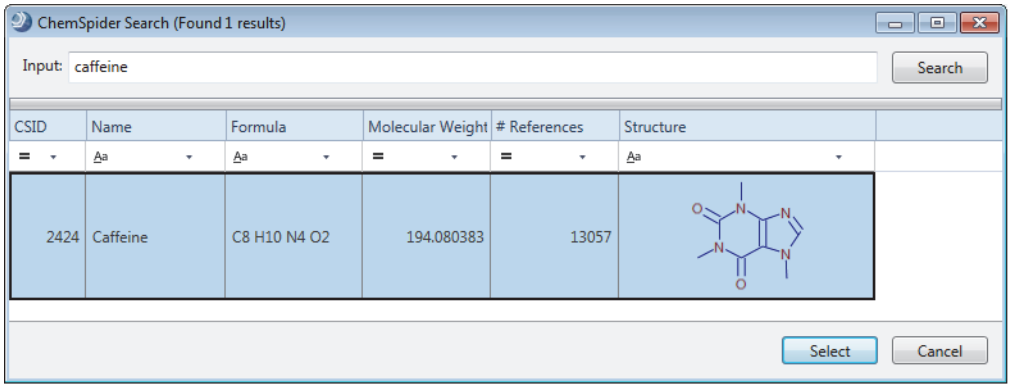
1. Click **ChemSpider**.

   The ChemSpider Search dialog box opens.

2. In the Input box, enter a name, formula, molecular weight, or CSID.

3. Click **Search**.

4. Select a compound from the search results.



5. Click **Select**.

   The chemical structure appears in the drawing pane and the molecular weight, name, and formula of the compound appear in their respective fields.

Structure drawing tools and commands

The Compound Editor, the Compound Annotation Editor, and the Fragment Editor include a set of drawing tools.

Use the toolbar for these structure editors and the shortcut menu for the drawing area to draw, manipulate, and save structures as described in the following topics:

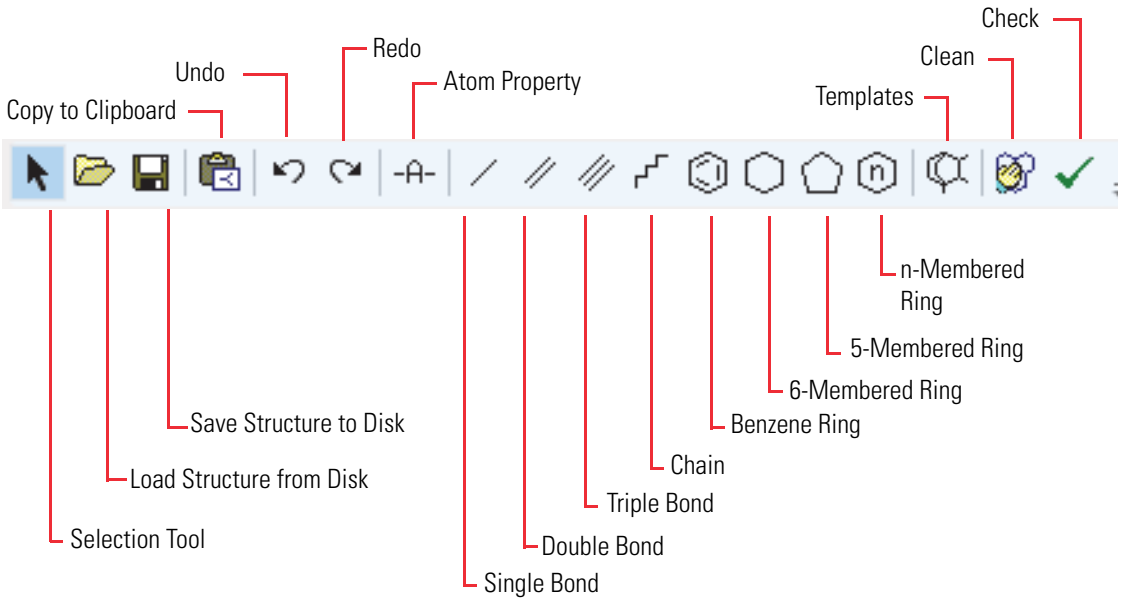
- Toolbar for the structure editors
- Shortcut menu commands for the drawing area of the structure editors
- Use the structure icons in the toolbar
- Create template structures and adding them to a drawing
- Check the validity of a structure
- Manipulate structures
- Select atoms and bonds
- Move structures
- Save a structure to a structure file
- Edit atom properties

Note The application has three different Compound Editor dialog boxes and one Fragment Editor dialog box that all have the same structure drawing tools. You can open these dialog boxes from the following Lists & Libraries views: Expected Compounds, Mass Lists, Metabolika Pathways, and Compound Classes.

Toolbar for the structure editors

The Compound Editor, Compound Annotation Editor, and Fragment Editor dialog boxes have the same set of toolbar icons.

Figure 206. Editor toolbar



Shortcut menu commands for the drawing area of the structure editors

The structure editors include a drawing area for adding a two-dimensional structure.

Table 206 describes the drawing area's shortcut menu commands.

Table 206. Shortcut menu commands for the drawing area

Menu command	Description
Selection Tool	Selects a portion of the structure.
Lasso Selection	Selects an non-rectangular portion of the structure.
Rectangle Selection	Selects a rectangular portion of the structure.
Cut	Removes the selected portion of a structure.
Copy	Copies the selected portion of a structure to the Clipboard.
Paste	Copies a structure from the Clipboard to the drawing area.
Delete	Deletes the selected portion of a structure.
Select All	Selects everything in the drawing area.
Resize	Resizes the selected portion of a structure.
Rotate	Rotates the structure around the selected axis of rotation.
Mirror	Reflects the structure along its vertical or horizontal axis.

Use the structure icons in the toolbar

The structure editors include a set of structure icons.

❖ To begin drawing a chemical structure

Tip Point to a drawing icon to display its description.

1. Click any of these structure icons,  . Or, select a template structure. See "Create template structures and adding them to a drawing."

   The cursor changes shape to represent the current drawing mode.

2. Click the drawing area where you want to place the selected structural feature.

   Until you click another structure icon, you can continue to add the same structural feature each time you click the drawing area.

3. Edit the atoms and bond properties. See these topics:

   - Edit bond properties
   - Edit atom properties

Create template structures and adding them to a drawing

Use the template tool on the structure editor toolbar to draw closely related chemical structures.

❖ To create, save, and open template structures

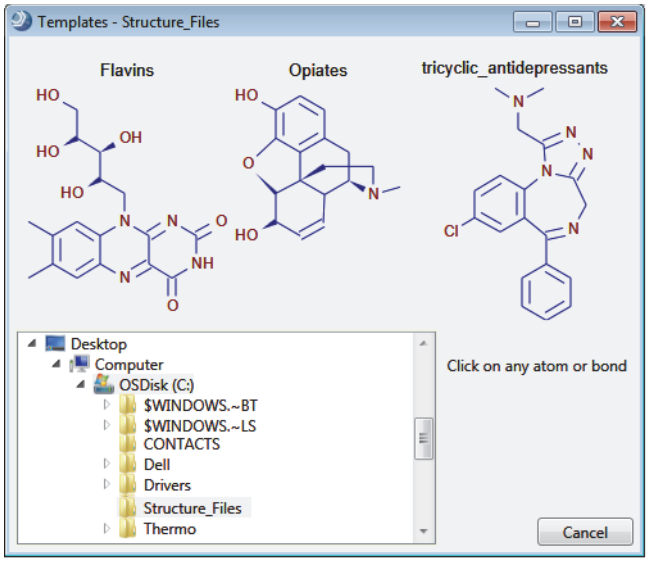
1. Open a structure file, paste a structure (InChi or MOL string), or draw a structure in the drawing area of the structure editor.
2. In the toolbar, click the **Save Structure to Disk** button,  .
3. In the Save Structure dialog box, do the following:
   a. Browse to the folder where you want to store the file.
   b. Name the file.
   c. In the Save As Type list, select **Template (*.tml)**.
   d. Click **Save**.
4. To add a template structure to the drawing area, click the **Templates** icon,  .

   The Templates dialog box opens.

5. In the Explorer view of the Templates dialog box, browse to and select the folder where you store your structure files.

   The title bar of the Templates dialog box changes from Templates to Templates – *Folder name*, and the 2D structures appear above the Explorer view. The application displays all of the structures in the folder. It does not differentiate between MOL files and Template files.

   Figure 207. Templates dialog box with a view of the stored structures



6. On the structure that you want to open, click any atom or bond.

   The templates cursor,  , appears in the drawing area of the Compound Editor dialog box.

7. To place the selected structure in the drawing area, click the drawing area.

Check the validity of a structure

The structure editors do not prevent you from creating and saving invalid structures. To check the validity of a structure as you create it or before you save it, use the check structure tool.

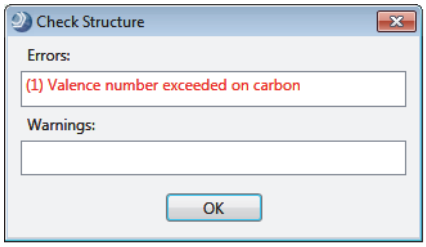
Note The check structure tool does not perform quantum mechanical or thermodynamical calculations that address possible structural stability.

❖ To check a structure

1. Click the **Check** icon,  .

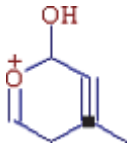
   The check structure tool searches for formal errors and unusual structural features. If a structure is formally incorrect or if the check structure tool finds its validity questionable, the Check Structure message lists the errors and warnings.

Figure 208. Check Structure message



2. Click **OK**.

The application automatically selects the atoms and bonds that it considers incorrect. The application considers structures that are not connected as mixtures and reports them as errors, but it does not select the mixtures.



Manipulate structures

You can resize, rotate, mirror, clean, and verify structures in the drawing area of a structure editor. After finishing a structure drawing, always check for errors before proceeding.

Table 207 describes how to manipulate structures.

Table 207. Manipulating structures (Sheet 1 of 2)

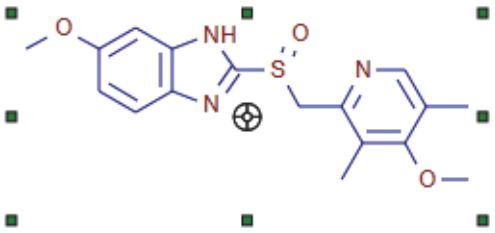
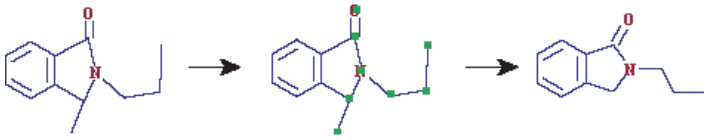
Task	Procedure
Resize a structure	1. Select the structure or part of the structure that you want to resize. 2. Right-click and choose **Resize**. 3. Drag one of the small rectangles on the edge of the structure and release the mouse button. Dragging one of the diagonal rectangles keeps the aspect ratio constant during structure resizing.
Rotate a structure	1. Select the structure or part of the structure that you want to rotate. 2. Right-click and choose **Rotate**. A small circle with a cross in the middle, ⊕, appears. The circle indicates the center of rotation. 3. Move the center of rotation by dragging the circle.  4. Rotate the selected structure around the center of rotation by dragging any of the small rectangles on the edges of the structure.

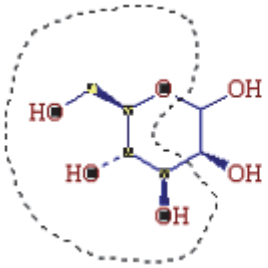
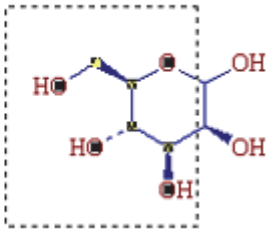
Table 207. Manipulating structures (Sheet 2 of 2)

Task	Procedure
Mirror a structure	1. Select the structure or part of the structure that you want to mirror. 2. Right-click and choose **Mirror**. 3. Click one of the small rectangles on the edge of the structure. • The top and bottom rectangles flip the selected structure along a horizontal axis. • The left and right rectangles flip the selected structure along a vertical axis.
Clean a structure	1. Do one of the following: • Select an entire structure. • Select only the atoms that you want to clean. The selected atoms must be connected. 2. Click the **Clean** icon,  . The cleaning tool helps you create a professional look for your structures.  **IMPORTANT** In some complicated cases, the Clean function can lead to structures that you might not find satisfactory. If this occurs, click the **Undo** icon,  .

Select atoms and bonds

In the structure editors, you can select individual atoms and bonds, a contiguous portion of a structure, an entire structure, or groups of atoms and bonds that are not adjacent to each other.

Table 208. Selecting atoms and bonds

Task	Procedure
Select an individual atom or bond.	Click the **Selection Tool** icon, and then click the individual atom or bond.
Choose a selection mode.	Right-click anywhere in the drawing area of the Compound Editor dialog box and choose **Lasso Selection** or **Rectangle Selection**.  Lasso Selection  Rectangle Selection
Select a group of adjacent atoms.	Do one of the following: • Right-click and choose **Rectangle Selection**. Then drag the cursor to form a rectangle around the atoms. • Right-click and choose **Lasso Selection**. Then draw a free-form shape around the atoms.
Select the entire structure.	Do one of the following: • Right-click the drawing area and choose **Select All**. • Click the **Selection Tool** icon, and then double-click anywhere in the drawing area, except on atoms or bonds.

Move structures

In the structure editors, you can move all or part of a structure or all the structures.

Table 209. Moving structures

Task	Procedure
Move a structure.	1. Select the atoms or bonds that you want to move. 2. Drag the selected structures to a new location.
Move all the structures in the drawing area.	1. Right-click the drawing area and choose **Select All**. 2. Click any atom or bond in the drawing area, and then drag the structures to a new location.

Edit bond properties

In any of the structure editors, use the bond icons to change the bond multiplicity.

❖ **To change the multiplicity of a bond**

Click  ,  , or  , and then click the bond that you want to change.

Edit atom properties

Use the Atom Properties dialog box to change the isotope of an atom or the entire element. For more information about modifying compound structures, see "Structure drawing tools and commands."

IMPORTANT The application does not support compounds with a radical. It also does support the R-Substituent feature.

❖ **To edit the element or nucleon number for a single atom in a structure**

1. Open the structure that you want to edit.

Note For LC studies, the editor that opens depends on whether you are editing a compound definition, a compound annotation, or a fragment definition:

- The Compound Editor dialog box opens when you add a new compound to or edit a compound in the expected compounds list or a mass list.
- The Compound Annotation Editor dialog box opens when you edit the annotations for a compound in the Compounds table, the Expected Compounds table, or a Structure Proposals table.
- The Fragment Editor dialog box opens when you add a new fragment to or edit a fragment in the Edit Compound Class dialog box.

2. Click the **Selection Tool** icon, .
3. Do one of the following:
   - Double-click the atom that you want to change.

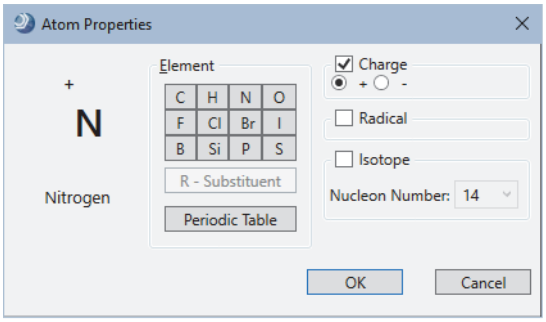
   –or–

   - Select the atom that you want to change and click the **Atom Properties** icon, .

   The Atom Properties dialog box opens with the properties of the selected atom displayed.

> **Tip** In the Compound Editor dialog box, you can save compounds with charges. You can also save compounds with radicals, but the application ignores radicals for data processing.

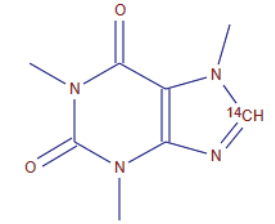
Figure 209. Atom Properties dialog box, showing the properties for a charged nitrogen atom



4. To change the element, do the following:
   - To change the atom to an element that is in the Element area, click the appropriate Element button.
   - To change the atom to an element not listed in the Element area, click **Periodic Table**. Then, in the Periodic Table dialog box, select an element and click **OK**.
5. To add a charge, select the **Charge** check box, and then select the **+** (positive) or **–** (negative) option.
6. To specify a less abundant isotope of the element, select the **Isotope** check box, and then select the appropriate value in the Nucleon Number list.

Tip For example, to create a compound that is labeled with one carbon-14 atom, double-click the labeling site—the atom that you want to change. In the Atom Properties dialog box, select the **Isotope** check box, and then select **14** in the Nucleon Number list.

The application displays carbon-14 as [14]C—that is, the elemental composition of carbon-14 labeled caffeine is displayed as C7 [14]C H10 N4 O2.



7. When you finish editing the selected atom, click **OK**.

   Changes you make in the Atom Properties dialog box affect only the selected atom.

Save a structure to a structure file

After you draw or modify a structure, you can save the structure as a structure file (in MOL format or as a compressed structure) or as a template file.

❖ To save a structure as a structure file

1. Click the **Save Structure to Disk** button in the toolbar, .
2. In the Save Structure dialog box, do the following:
   a. Browse to the directory where you want to store the file.
   b. Name the structure file.

      You can save structures under their actual names, regardless of length (for example, 1-Amino-2-hydroxyindane.mol).
   c. In the Save As Type list, select a file type.
   d. Click **Save**.

Copy and paste InChi strings and MOL strings

You can copy InChi or MOL strings to the Clipboard, and then paste them to the workspace of the compound editor dialog boxes. You can also copy structures from the workspace of compound editors to the Clipboard in these formats: InChi, MOL, or InChi Key string.

Use the License Manager

The following topics describe how to use the License Manager to activate or deactivate the software license and to install new processing workflow nodes as they become available:

- Open the License Manager
- License Manager command bar
- Activate the software license
- Deactivate the software license for transfer to another computer
- Install or update a processing workflow node
- Obtain and install the KEGG license

Note After you install the Compound Discoverer application on your computer, you can use the application without activating the license for up to 60 days.

After you activate the software license on one computer, you can deactivate the license and transfer it to another computer.

Open the License Manager

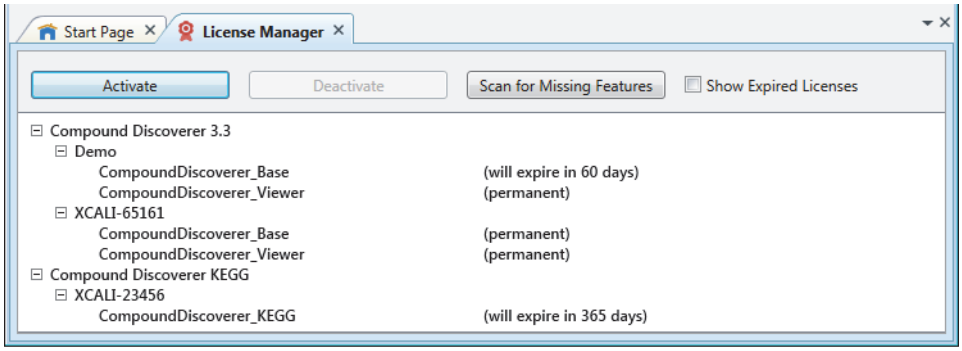
Access the License Manager page from the Help menu.

❖ **To open the License Manager page**

From the menu bar, choose **Help > License Manager**.

The License Manager opens as a tabbed document in the application window.

Figure 210. License Manager page



License Manager command bar

Table 210 describes the License Manager command bar.

Table 210. License Manager command bar

Command or feature	Description
Activate	Opens the License Activation dialog box where you can apply a new activation code and activate the license on the current computer.
Deactivate	Opens the License Deactivation dialog box for deactivating the software license.
Scan for Missing Features	Activates a scan for newly installed processing workflow nodes.
Show Expired Licenses	Selecting this check box displays any expired licenses.

Activate the software license

To activate your Compound Discoverer 3.3.x software license, see these topics as necessary:

1. Enter the product ID and the activation code
2. Follow one of these topics:
   - Activate the license on an online computer
   - Activate the license on an offline computer

Enter the product ID and the activation code

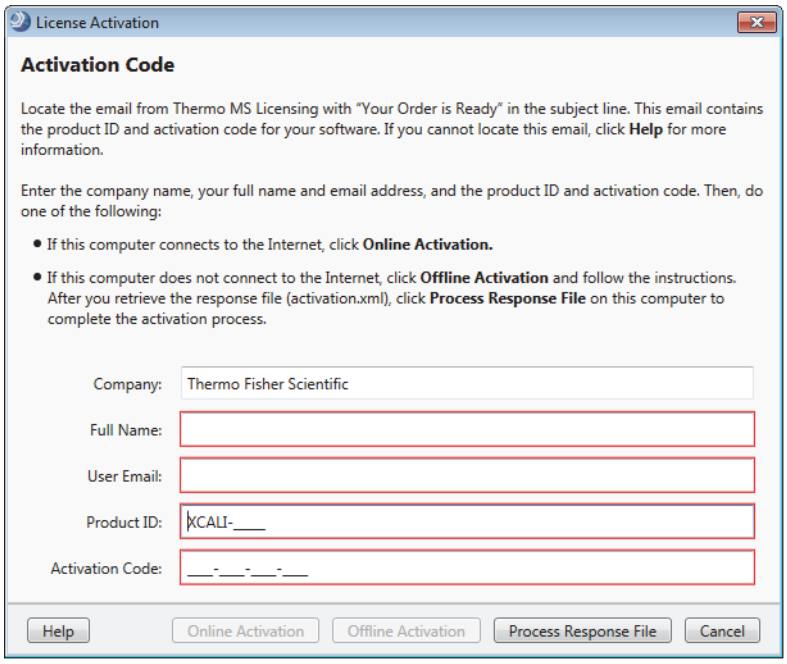
To activate your Compound Discoverer 3.3 license, you must know the product ID (XCALI-*XXXXX*) and the activation code. Within one week of ordering the software, you should receive an email from Thermo MS Licensing with the subject line "Your Order Is Ready." This email contains the product ID and activation code information.

❖ To enter the licensing information

1. On the License Manager page, click **Activate**.

   The License Activation dialog box opens to the Activation Code view.

   Figure 211. License Activation dialog box opened to the Activation Code view



2. If you have not already received your activation code, do the following:

   a. Check your Junk Email folder.

   b. If the email is not in your Junk Email folder, log in to your account at the following URL. In the left navigation pane, under Software & Services, click **Order History**. Then, in the list of ordered products, click the order number.

      https://thermo.flexnetoperations.com

   c. If you cannot find your account, send an email message to Licensing at ThermoMSLicensing@thermofisher.com.

      Provide the following information in the body of the message:

      - Software application: Compound Discoverer
      - Sales order number or purchase order number:_____
      - End user name:_____
      - End user email:_____

3. In the License Activation dialog box (Figure 211), enter the following:
   - Your company name
   - Your full name
   - Your contact email address
   - The product ID for the Compound Discoverer 3.3 application.

     There are five possible product IDs. Four of the product IDs are for software upgrades (see Table 211).
   - The activation code. You can type or paste the activation code.

     Table 211. Product IDs for the Compound Discoverer 3.3 software

Material Order No.	Product ID	Description
OPTON-31055	XCALI-65161	SW, Compound Discoverer 3.3 SP2 (single license)
OPTON-31056	XCALI-65161	SW, Compound Discoverer 3.3 SP2 (2 or more licenses)
OPTON-31060	XCALI-65162	SW, Compound Discoverer (CD) 3.3 SP2 upgrade from CD 1.0, CD 2.0, CD 2.1
OPTON-31061	XCALI-65163	SW, Compound Discoverer 3.3 SP2 upgrade from Compound Discoverer 3.0, 3.1, and 3.2
OPTON-31062	XCALI-65164	SW, Compound Discoverer 3.3 SP2 and Mass Frontier 8.0 SR1 with Curator
OPTON-31063	XCALI-65165	SW, Compound Discoverer 3.3 SP2 and Mass Frontier 8.0 SR1 with Curator (2 or more licenses)

4. Depending on whether you are activating the license on an online or offline computer, continue with the appropriate topics:
   - Activate the license on an online computer
   - Activate the license on an offline computer

Activate the license on an online computer

Follow these instructions if your processing computer has an Internet connection.

❖ To activate the software license on an online computer

1. If you have not already entered the licensing information, enter it in the Activation Code view of the License Activation dialog box.

2. Click **Online Activation** to process the activation code.
3. At the confirmation prompt, click **OK**.
4. At the "new features" prompt, click **OK**.

This completes the online license activation process.

Activate the license on an offline computer

Follow these instructions if your processing computer is not connected to the Internet.

Note Activating the license on an offline computer is a three-step process that requires access to an online computer.

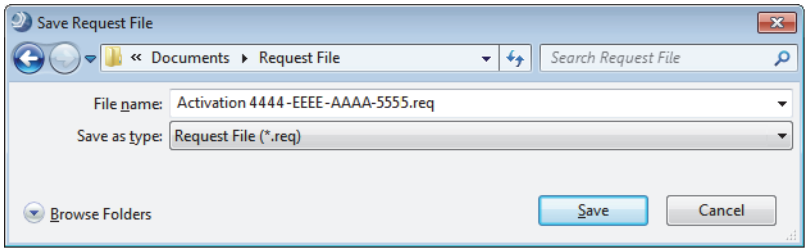
1. Create an activation request file (Activation-*Activation Code*.req) on the offline computer.
2. Transfer the activation request file to an online computer where you upload it to the licensing portal to obtain a response file (activation.xml).
3. Transfer the response file (activation.xml) to the offline computer, and then process it by clicking Process Response File in the License Activation dialog box.

❖ To activate the software license on an offline computer

1. If you have not already entered the licensing information in the Activation Code view of the License Activation dialog box, enter it now.
2. In the License Activation dialog box, click **Offline Activation**.

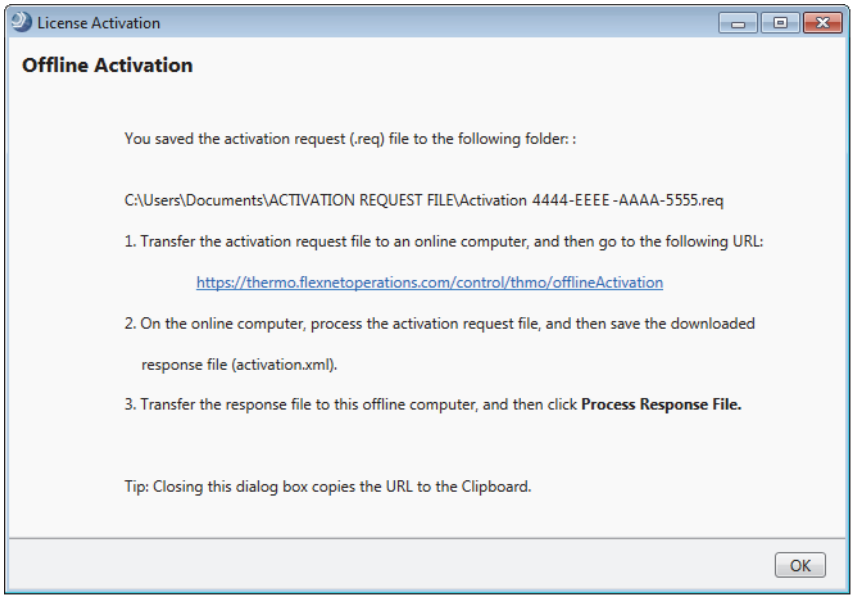
   The Save Request File dialog box opens.
3. Save the activation request file (Activation-*Activation Code*.req).

Figure 212. Save Request File dialog box with activation code



The Offline Activation instructions appear.

Figure 213. Offline activation instructions



4. Click **OK**.

   The Activation Code view of the License Activation dialog box reappears.

   Tip When you close the Offline Activation dialog box, the application automatically saves the URL to the Clipboard, so that you can save the URL to a file for use on an online computer.

5. (Optional) Save the URL to a file.

6. Keep the License Activation dialog box open on this offline computer.

   IMPORTANT If you accidentally close the License Activation dialog box, start over at step 1.

7. To download the response file (activation.xml) from the licensing server, do the following on an online computer:

   a. Transfer the activation request file ((Activation-*Activation Code*.req) to the online computer.

   b. Go to the following URL (case sensitive):

      https://thermo.flexnetoperations.com/control/thmo/offlineActivation

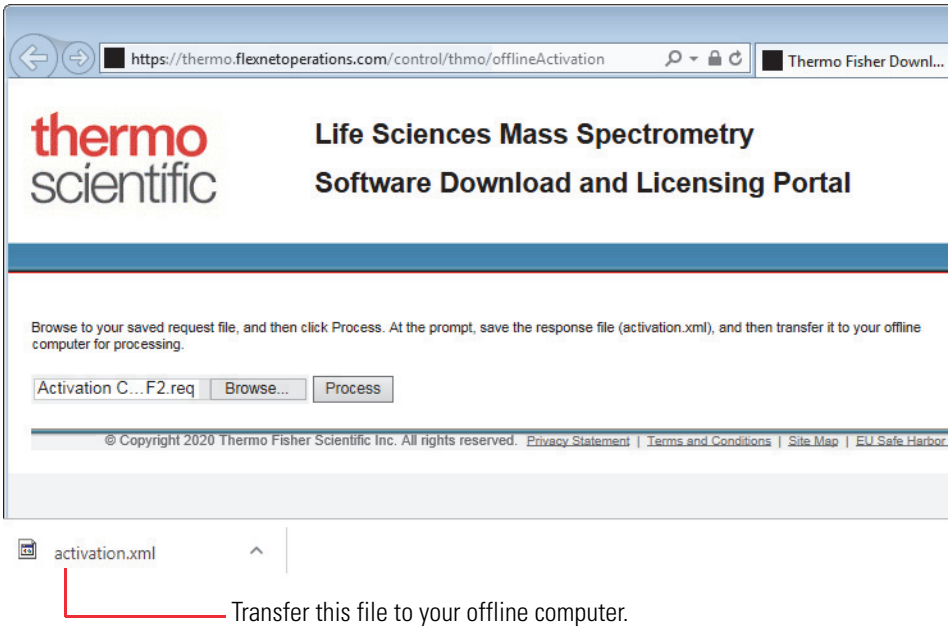
      The Life Sciences Mass Spectrometry Software Download and Licensing Portal opens.

   c. Click **Choose File** or **Browse**, browse to and select the request file (**Activation *Activation Code*.req**), click **Open**, and then click **Process**.

Note Whether the page includes a Choose File button or a Browse button depends on the web browser.

The server downloads the activation file.

Figure 214. Software licensing portal with a view of a downloaded response file



d. Save the response file (activation.xml).

8. To activate the license on the offline computer, do the following:
   a. Transfer the response file (activation.xml) to this computer.
   b. In the License Activation dialog box that you left open, click **Process Response File**.

      The Open Response File dialog box opens.
   c. Browse to and select the response file (activation.xml), and then click **Open**.
   d. At the "license response processed" prompt, click **OK**.
   e. At the "new features" prompt, click **OK**.

This completes the offline license activation process. The License Manager indicates that the license for the specified product (XCALI-*XXXXX*) is permanent.

Deactivate the software license for transfer to another computer

To transfer the software license to another computer, you must first deactivate the license on the current computer.

Follow the appropriate topic:

- Deactivate the software license on an online computer
- Deactivate the software license on an offline computer

Deactivate the software license on an online computer

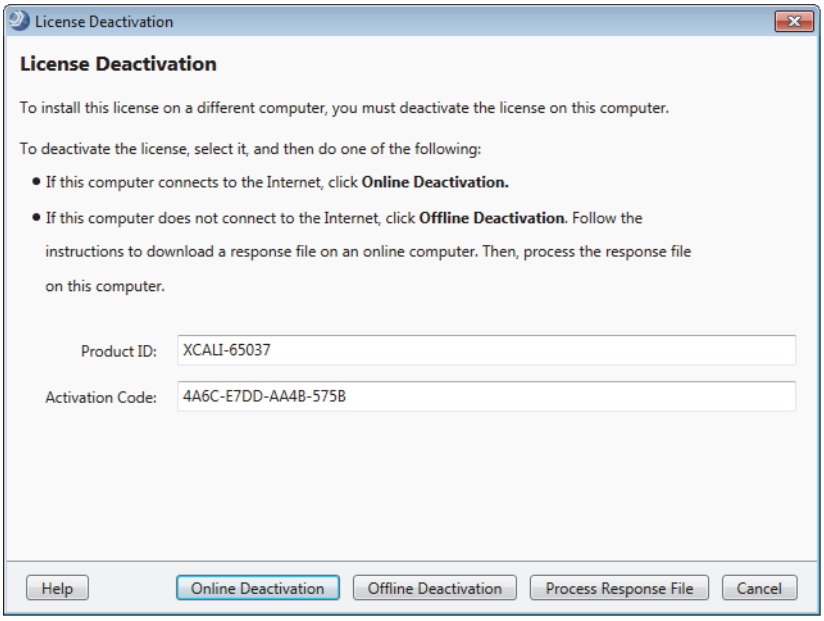
Follow this procedure if your computer has Internet access.

❖ To deactivate the software license on an online computer

1. On the License Manager page, select the software product that you want to deactivate, and then click **Deactivate**.

   The License Deactivation dialog box opens. The Product ID box is populated with the selected product's ID, and Activation Code box is populated with the activation code for your license.

   Figure 215. License Deactivation dialog box populated with the product ID and activation code

2. If the computer is connected to the Internet, click **Online Deactivation**.
3. At the confirmation prompt, click **Yes**.

   The license deactivation process is complete, and the product ID disappears from the License Manager page.

Deactivate the software license on an offline computer

If your processing computer is not connected to the Internet, follow these instructions to deactivate the software license.

Note Deactivating the license on an offline computer is a three-step process that requires access to an online computer.

1. Create a deactivation request file (Deactivation-*Activation Code*.req) on the offline computer. This step only starts the license deactivation process.
2. Transfer the deactivation request file (Deactivation-*Activation Code*.req) to an online computer where you upload it to the licensing portal to obtain a response file (activation.xml).
3. Transfer the response file to the offline computer, and then process it to complete the deactivation process.

❖ To deactivate the software license on an offline computer

1. On the offline computer, create the deactivation request file as follows:
   a. On the License Manager page, select the software license that you want to deactivate, and then click **Deactivate**.

      The License Deactivation dialog box opens. The Product ID box is populated with the selected product's ID, and Activation Code box is populated with the activation code for your license.

   b. Click **Offline Deactivation**.
   c. At the confirm deactivation prompt, click **Yes**.

      The Save Request File dialog box opens. The File Name box displays the following text: Deactivation *Activation Code*.req.

   d. Save the deactivation request file.
   e. At the prompt, which displays the location of the saved request file, click **OK**.

      The license state changes to Deactivation in Progress, and the URL is copied to the Clipboard.

   f. (Optional) Copy the URL to a file.
2. From the online computer, retrieve the response file (activation.xml) as follows:
   a. Transfer the deactivation request file and the file with the URL to this computer.
   b. Go to the following URL (case sensitive):

      https://thermo.flexnetoperations.com/control/thmo/offlineActivation

      The Life Sciences Mass Spectrometry Software Download and Licensing Portal opens.

c. Click **Choose File**, browse to and select the **Deactivation *Activation Code*.req** file, click **Open**, and then click **Process**.

   The server downloads the response file.

d. Save the response file (activation.xml).

3. Complete the deactivation process on the offline computer as follows:

   a. Transfer the response file (activation.xml) to this computer.

   b. On the License Manager page, select the license that you are in the process of deactivating, and click **Deactivate**.

      The License Deactivation dialog box opens.

   c. Click **Process Response File**.

      The Open Response File dialog box opens.

   d. Select the response file (activation.xml) and click **Open**.

      The license disappears from the License Manager page.

Install or update a processing workflow node

The application uses a node-based workflow to process raw data files. Following set guidelines, you can create your own custom workflow nodes. In addition, Thermo Fisher Scientific might occasionally provide custom workflow nodes on its customer website.

❖ To install a new processing workflow node

1. Download the executable files and store them in the appropriate folder on the computer where you are running the application.
2. Open the License Manager page.
3. Click **Scan for Missing Features**.
4. Close and reopen the application.
5. Choose **Help > About**.

   The About Compound Discoverer dialog box opens with the Patent and Legal Notices page displayed.

6. Expand the Nodes list and verify that it lists the new node.

Obtain and install the KEGG license

To use the Map to KEGG Pathways workflow node in the Compound Discoverer application, you must install a valid KEGG license on your processing computer. To license the KEGG Pathways module, you must contact Pathway Solutions for the activation key. After you obtain the activation key from Pathway Solutions, you must install it on your processing computer by using the Compound Discoverer License Manager.

Note You must contact Pathway Solutions for a KEGG license. Kanehisa Laboratories does not provide KEGG licenses for the Compound Discoverer application.

For details, see these topics:

- Contact Pathway Solutions to obtain a KEGG Pathways activation key
- Install the KEGG license

Contact Pathway Solutions to obtain a KEGG Pathways activation key

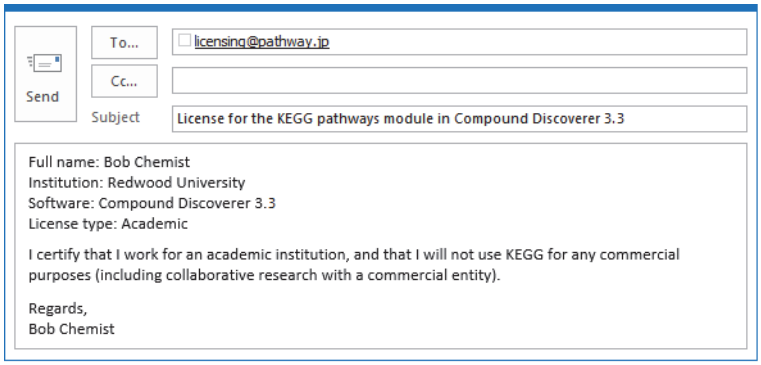
To obtain the activation key for the KEGG Pathways module, contact Pathway Solutions at the following email address: licensing@pathway.jp

Include the following information in your email:

- Your full name: First and last name
- Institution: Institution name
- Software: Compound Discoverer
- Version number: 3.3
- License type: Commercial or academic*

*If you are applying for an academic license, you must include the following statement in your email:

> I certify that I work for an academic institution, and that I will not use KEGG for any commercial purposes (including collaborative research with a commercial entity).



Install the KEGG license

After you receive the KEGG activation key from Pathway Solutions, follow this procedure to install it.

❖ To install the KEGG license

1. From the menu bar of the Compound Discoverer application, choose **Help > License Manager**.
2. Click **Activate**.
3. In the License Activation dialog box, enter the name of your company, your full name, your email address, the product ID number (XCALI-23456), and the activation code that you received from Pathway Solutions.
4. Follow the instructions for online or offline activation as appropriate.

   After you install the license, it might appear under Compound Discoverer_KEGG. If the License Manager displays an expiration date, the license is valid.

14

Compound Discoverer configuration options

To set up the configuration options for the Compound Discoverer application, do the following as needed:

- Open the Configuration page
- Select the maximum number of parallel processing jobs
- Select where to store temporary data
- Turn off the auto-save feature for studies
- Hide the workflow node numbers
- Set up the global color palette
- Specify the default mzCloud mass tolerance settings
- Set up a BioCyc account and optionally purchase a subscription
- Specify the fragmentation databases

Open the Configuration page

Use the Configuration page to set up the global configuration options for the application.

❖ **To open the Configuration page**

From the menu bar, choose **Help > Configuration**.

Select the maximum number of parallel processing jobs

Use the Parallel Option view of the Configuration page to specify the maximum number of analyses (jobs) that the application can process in parallel.

❖ **To change the maximum number of parallel jobs**

1. In the application menu bar, choose **Help > Configuration**.

2. In the left pane of the Configuration page, select **Parallel Options** under Server Settings.

   The Parallel Options view opens.

3. In the Maximum Number of Processing Workflows in Parallel Execution box, type or select an integer from **1** to **4**.

   The default value is equal to half the number of CPU cores in the processing computer.

4. Click **Save Current Settings**.

Select where to store temporary data

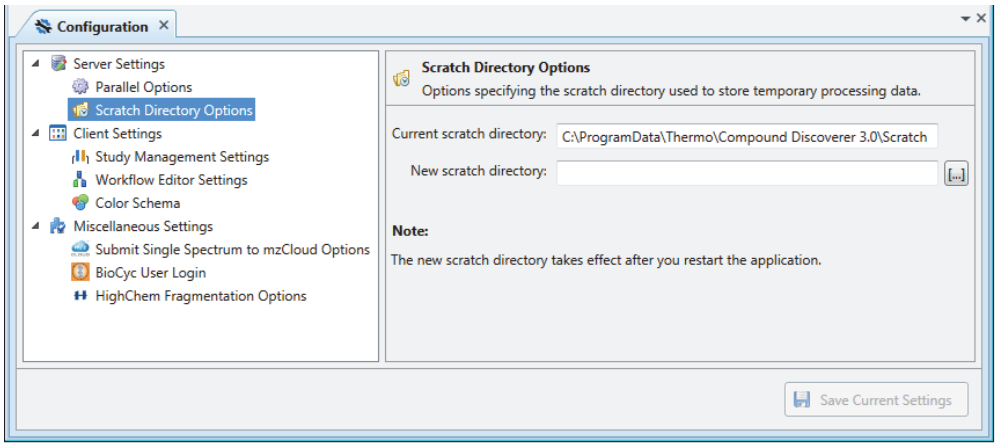
Use the Scratch Directory Options view of the Configuration page to change the folder where the application stores temporary data during data processing.

❖ To change the scratch directory

1. In the application menu bar, choose **Help > Configuration**.
2. In the left pane of the Configuration page, choose **Scratch Directory Options** under Server Settings**.**

   The Current Scratch Directory box lists the current location of the scratch folder.

   Figure 216. Scratch Directory Options view



3. Click the browse button next to New Scratch Directory and locate the new directory.
4. Click **Save Current Settings**.
5. Restart the application.
6. Reopen the Scratch Directory Options view and make sure that the Current Scratch Directory box lists the new scratch directory.

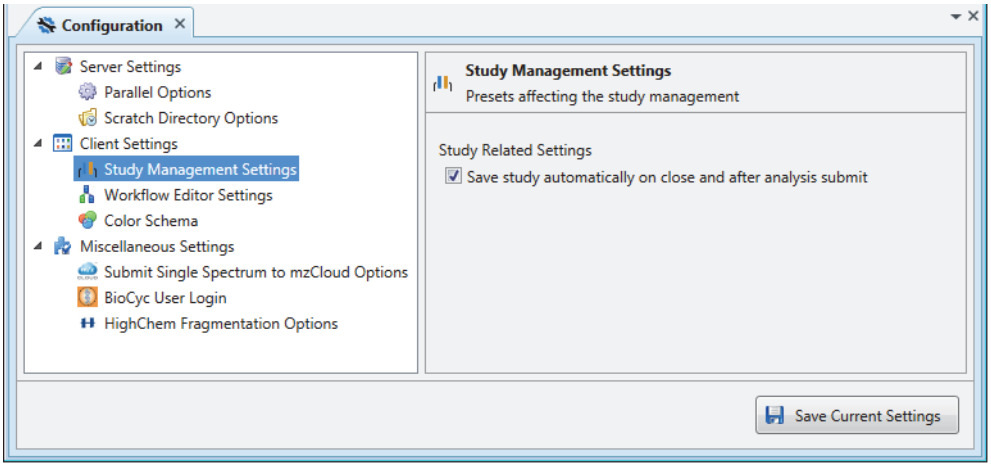
Turn off the auto-save feature for studies

If you want the application to automatically save changes that you make to studies, including the list of result files on the Analysis Results page, do not turn off the auto-save feature.

❖ To turn off the auto-save feature

1. In the application menu bar, choose **Help > Configuration**.
2. In the left pane of the Configuration page, under Client Settings, choose **Study Management Settings**.

   Figure 217. Study Management Settings view with the default setting



3. Clear the **Save Study Automatically On Close and After Analysis Submit** check box.
4. Click **Save Current Settings**.
5. Restart the application.

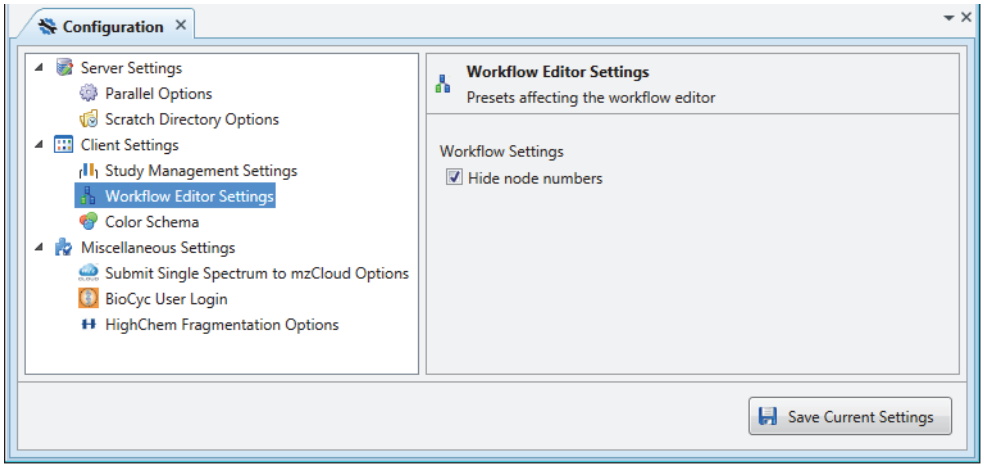
Hide the workflow node numbers

When you create a processing workflow by dragging the workflow nodes into the Workflow Tree pane, the application automatically adds an integer to each workflow node. Use the Workflow Editor Settings view to hide these numbers.

❖ To hide the workflow node numbers

1. In the application menu, choose **Help > Configuration**.
2. In the left pane of the Configuration page, under Client Settings, choose **Workflow Editor Settings**.
3. Under Workflow Settings, select the **Hide Node Numbers** check box.

Figure 218. Workflow Editor Settings view

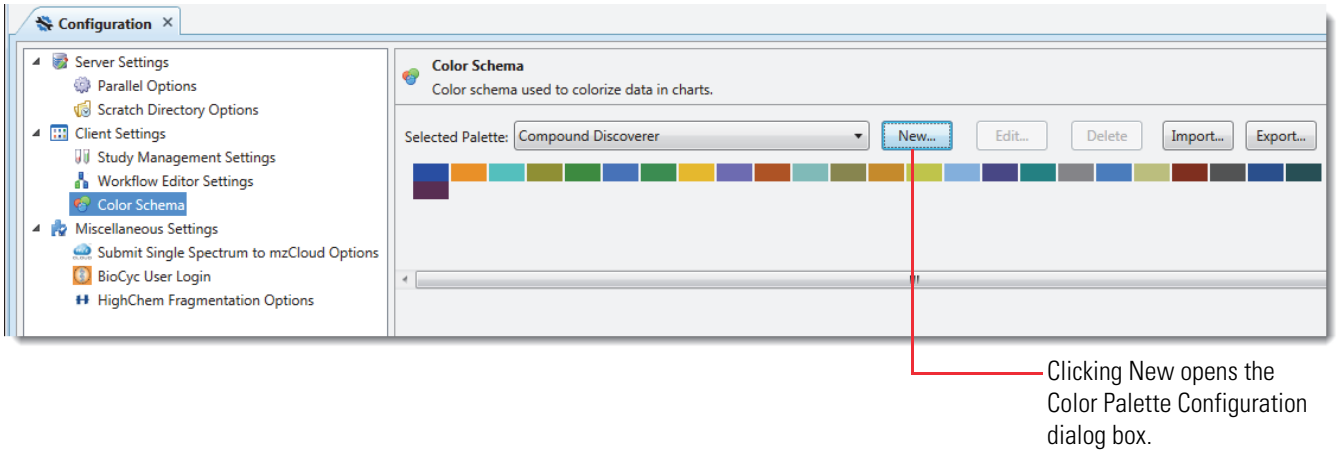


4. Click **Save Current Settings**.

Set up the global color palette

Use the Color Schema view of the Configuration page to select one of the standard global color palettes or create a custom color palette. The colormap selection affects the sample group colors in the following views: Chromatograms, Trend Charts, Principal Component Analysis, and Descriptive Statistics. The selection does not affect the color-coding in the result tables.

Figure 219. Color Schema view



For details about setting up the global color palette, see the following topics:

- Open the color schema view of the configuration page
- Select a standard color palette
- Create new custom color palettes

- Delete custom color palettes
- Import custom color palettes
- Export custom color palettes
- Edit custom color palettes
- Add colors to a custom palette
- Insert colors in a custom palette
- Replace a color in a custom palette
- Remove a color from a custom palette
- Select a color in the gradient color chart

Open the color schema view of the configuration page

❖ **To open the Color Schema view**

1. From the menu bar, choose **Help > Configuration**.
2. In the left pane of the Configuration page, under Client Settings, choose **Color Schema**.

Select a standard color palette

For visualizing chart data, you can select from four standard color palettes on the Color Schema view of the Configuration page.

❖ **To select a standard color palette**

1. Open the color schema view of the configuration page.
2. In the Selected Palette list, select from four palettes.
   - Compound Discoverer

     
   - Proteome Discoverer

     
   - 60 Distinct Colors

     
   - Deuteranopia, Protanopia, and Tritanopia

     
3. Click **Save Current Settings**.

Create new custom color palettes

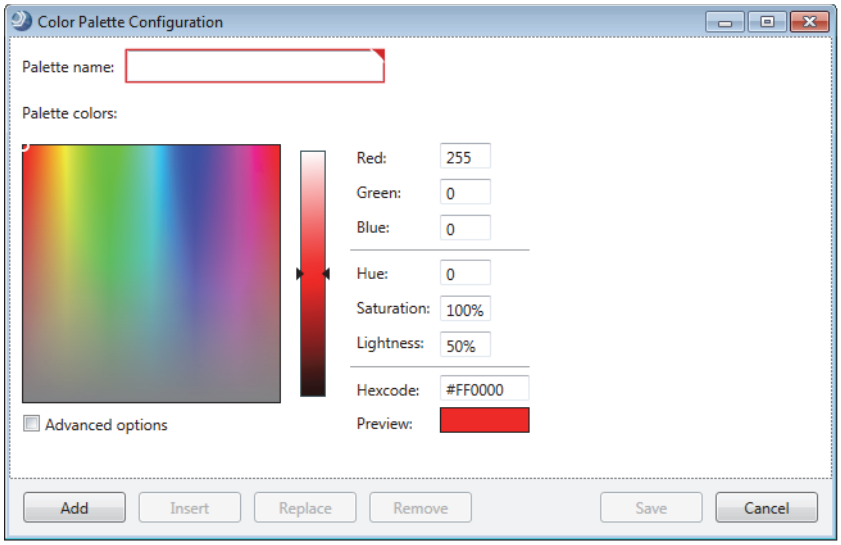
When you create a custom color palette, you can select any of the colors in the color chart.

❖ To create a custom color palette

1. Open the color schema view of the configuration page.
2. Click **New**.

   The Color Palette Configuration dialog box opens.

   Figure 220. Color Palette Configuration dialog box



3. Name the custom color palette.
4. Add selected colors to the custom color palette. See "Edit custom color palettes."
5. Click **Save**.

   The custom color palette appears as the selected palette in the Selected Palette list of the Color Schema view.
6. To apply the new color palette, click **Save Current Settings**.

Delete custom color palettes

A custom color palette is any palette other than one of the four standard palettes.

❖ To delete a custom color palette

1. Open the color schema view of the configuration page.
2. Select the custom color palette in the Selected Palette list.
3. Click **Delete**.

Import custom color palettes

❖ **To import a custom color palette**

1. Open the color schema view of the configuration page.
2. Click **Import**.
3. Locate the color palette file (XML) and click **Open**.

   The import color palette appears in the Selected Palette list.

Export custom color palettes

After you create a custom color palette, you can export it as an XML file.

❖ **To export a custom color palette**

1. Open the color schema view of the configuration page.
2. Select the custom color palette that you want to export in the Selected Palette list.
3. Click **Export**.
4. Name the palette and click **Save**.

Edit custom color palettes

❖ **To edit a custom color palette**

1. Open the color schema view of the configuration page.
2. Select the custom color palette that you want to edit in the Selected Palette list.
3. Click **Edit**.

   The Color Palette Configuration dialog box opens.
4. Do any of the following:
   - Add a color to the custom color palette. See "Add colors to a custom palette."
   - Insert a color into the custom color palette. See "Insert colors in a custom palette."
   - Replace a color in the custom color palette. See "Replace a color in a custom palette."
   - Remove a color from the custom color palette. See "Remove a color from a custom palette."
5. Click **Save**.

   The name of the custom palette appears in the Selected Palette list.

Add colors to a custom palette

After you open a custom color palette for editing, you can add colors to it.

❖ **To add a color to a custom color palette**

1. Open the color schema view of the configuration page.
2. Select the custom color palette that you want to edit from the Selected Palette list.

   The Color Palette Configuration dialog box opens.
3. To add a color to a custom color palette, select the color in the gradient color chart.
4. Click **Add**.

   In the Palette Colors area, the new color appears to the right of the current colors.
5. When you finish editing the color palette, click **Save**.

Insert colors in a custom palette

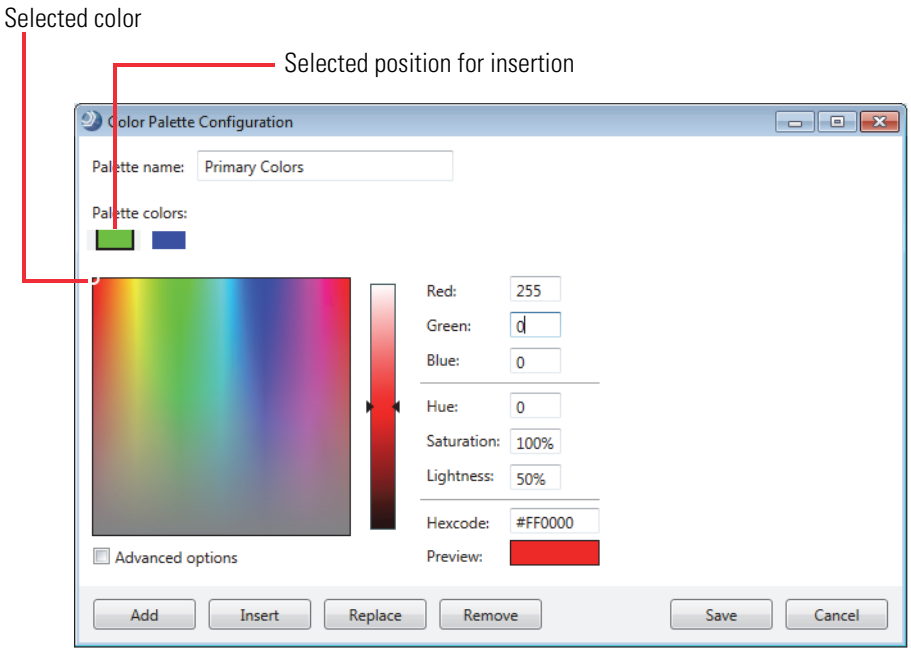
After you open a custom color palette for editing, you can insert colors.

❖ **To insert a color in a custom color palette**

1. Open the color schema view of the configuration page.
2. Select the custom color palette that you want to edit from the Selected Palette list.

   The Color Palette Configuration dialog box opens.
3. To insert a color in a custom color palette, select its insertion point—the color to the right of the intended position—in the Palette Colors area.
4. Select the new color in the gradient color chart.

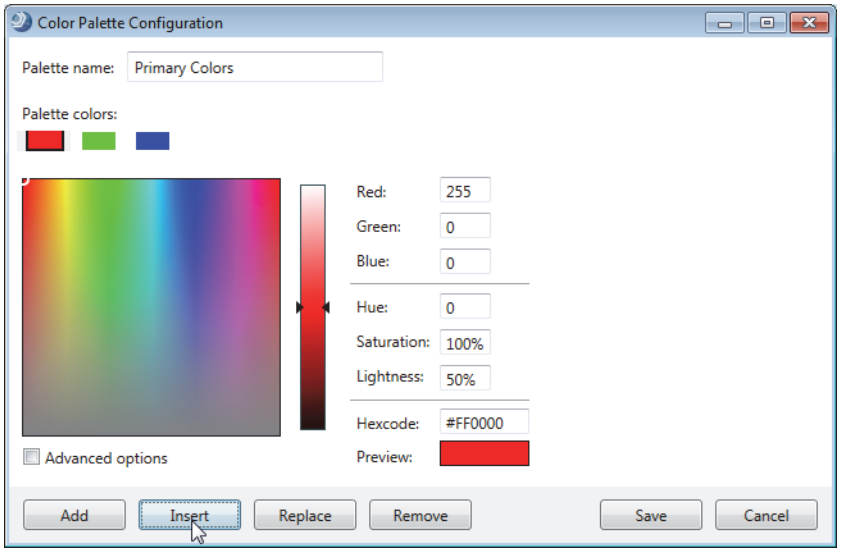
Figure 221. Color Palette Configuration dialog box with the basic options view



5. Click **Insert**.

   In the Palette Colors area, the new color appears to the left of the currently selected color.

   Figure 222. Custom color palette with the color red inserted to the left of the color green



6. When you finish editing the color palette, click **Save**.

Replace a color in a custom palette

After you open a custom color palette for editing, you can replace the colors.

❖ **To replace a color with another color**

1. Open the color schema view of the configuration page.
2. Select the custom color palette that you want to edit from the Selected Palette list.

   The Color Palette Configuration dialog box opens.
3. To replace a color with another color, select the color to replace in the Palette Colors area.
4. Select a color in the gradient color chart.
5. Click **Replace**.
6. When you finish editing the color palette, click **Save**.

Remove a color from a custom palette

After you open a custom color palette for editing, you can remove one or more colors.

❖ **To remove a color from a custom color palette**

1. Open the color schema view of the configuration page.
2. Select the custom color palette that you want to edit from the Selected Palette list, and then click **Edit**.

   The Color Palette Configuration dialog box opens.
3. Select the color in the Palette Colors area.
4. Click **Remove**.
5. When you finish editing the color palette, click **Save**.

Select a color in the gradient color chart

The Color Palette Configuration dialog box that opens when you click either New or Edit in the Color Schema view of the Configuration page includes a gradient color chart.

❖ **To select a color for a custom color palette in the gradient color chart**

1. Open the color schema view of the configuration page.
2. Do one of the following:
   - To add a color to a new custom color palette, click **New**.

     The Color Palette Configuration dialog box opens. The Palette Name box is empty.

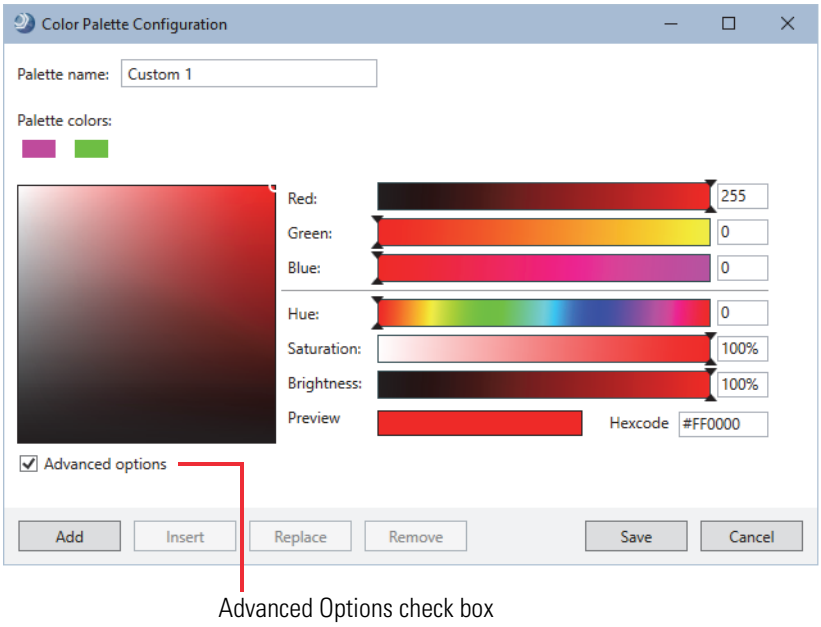
- To edit an existing custom color palette, select it in the Selected Palette list, and then click **Edit**.

  The Color Palette Configuration dialog box opens. The Palette Name box displays the name of the custom color palette that you selected.

3. Do any of the following:

   - Click a color in the hexadecimal color gradient chart.
   - Enter an RGB formula or an HSB formula by typing numeric values or using the slider.
   - Select the **Advanced Options** check box and use the separate sliders for red, green, blue, hue, saturation, and brightness.

     Figure 223. Advanced Options view of the Color Palette Configuration dialog box



   - Enter the hexadecimal code.

Specify the default mzCloud mass tolerance settings

Use the Submit Single Spectrum to mzCloud Options view to set up the mass tolerance settings for a manual mzCloud search. See "Search the mzCloud database for a matching fragmentation spectrum."

❖ To set up the mass tolerance settings for a manual mzCloud search

1. In the application menu bar, choose **Help > Configuration**.
1. In the left pane of the Configuration page, under Miscellaneous settings, choose **Submit Single Spectrum to mzCloud Options**.

2. Do any of the following:
   - For the mass tolerance of scans acquired in the Orbitrap mass analyzer, select the units, and then type an appropriate value in the FT Mass Tolerance box.
   - For the mass tolerance of scans acquired in the ion trap mass analyzer, select the units, and then type an appropriate value in the IT Mass Tolerance box.
   - If your processing workflows (for LC studies) include the Search mzCloud node, select the **Use mzCloud Node Settings** check box to use the node settings. See "Search mzCloud node."
3. Click **Save the Current Settings**.

Table 212 describes the options for submitting single scans to the mzCloud database.

Table 212. Submit Single Spectrum to mzCloud Options view

Parameter	Description
FT Mass Tolerance	Specifies the mass tolerance for scans acquired with an FT mass analyzer. Default: 12 ppm
IT Mass Tolerance	Specifies the mass tolerance for scans acquired with an ion trap mass analyzer. Default 0.4 Da
Use mzCloud Node Settings	When this check box is selected, the application uses the settings in the Search mzCloud processing workflow node if the analysis included this node. Default: Selected

Set up a BioCyc account and optionally purchase a subscription

Follow the instructions in the BioCyc User Login view on the Configuration page to set up your BioCyc user account, subscription, or both.

To obtain access to all the BioCyc databases, you must do one of the following:

- If you do not have a BioCyc user account, you must create a new BioCyc account on the Sign Up page of the BioCyc website, and then enter, test, and save your account information in the BioCyc User Login view. When you create a new account, you automatically have 30 days of trial access to all the BioCyc databases.
- If you already have an existing account, you can request a 30-day trial access period to all the BioCyc databases. Or, you can purchase an individual subscription or an institutional subscription. If you do not request a 30-day trial access period or purchase a subscription, you will have access to only the EcoCyc and MetaCyc databases.

To obtain access to all the BioCyc databases, do the following:

1. Open the BioCyc User Login view.
2. Do the following as needed:
   - Create a BioCyc user account
   - Purchase a subscription or request a free 30-day trial period
   - Enter, test, and save your BioCyc user account information

Note To access the BioCyc website where you set up a user account, purchase a subscription, or request 30 days of free trial access to all the BioCyc database, you must have Internet access.

Open the BioCyc User Login view

Use the BioCyc User Login view of the Compound Discoverer application to test and save your BioCyc credentials.

❖ To open the BioCyc User Login view

1. From the application window, choose **Help > Configuration**.

   The Configuration page opens.

2. In the left pane, under Miscellaneous settings, select **BioCyc User Login**.

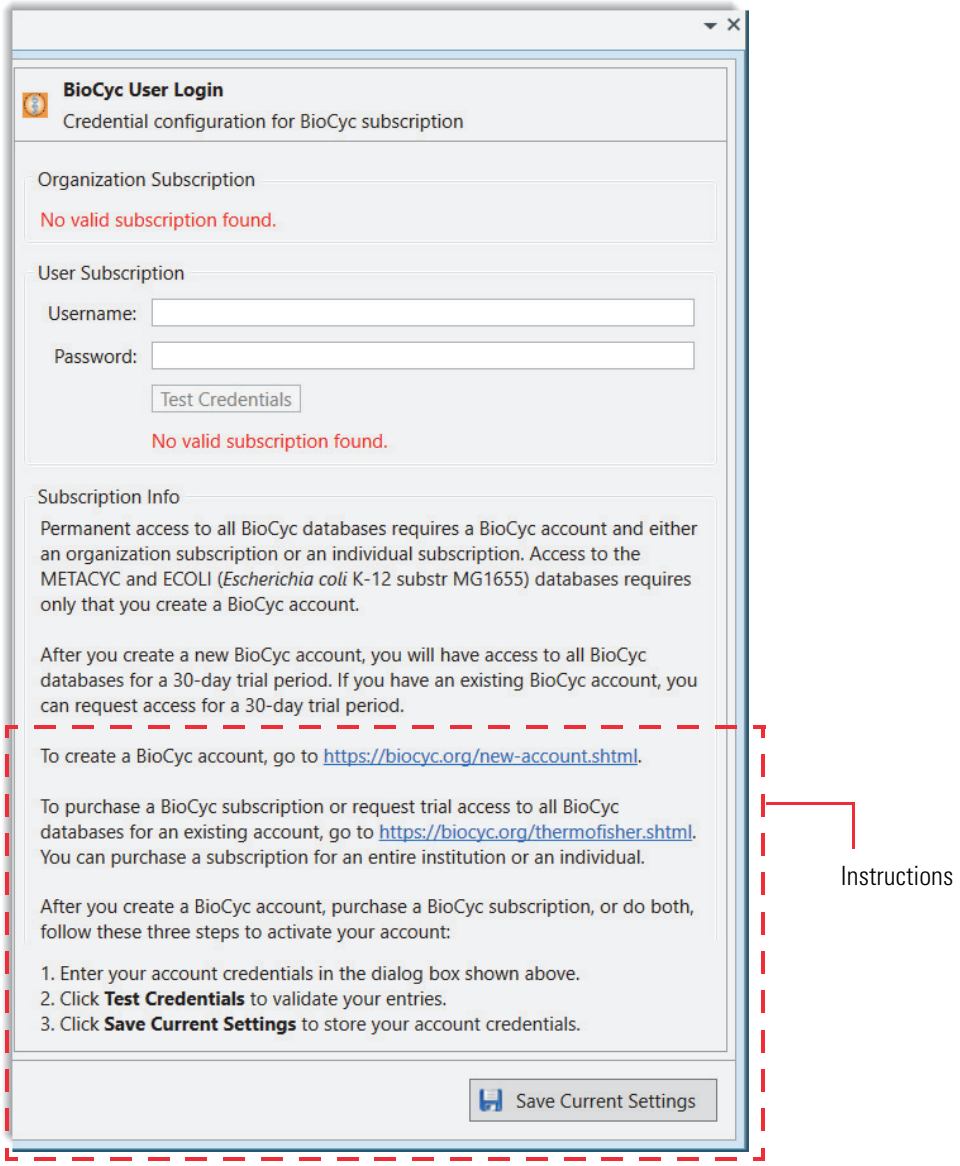
   The BioCyc User Login view appears at the right.

   - If you have an organization subscription, the Organization Subscription area displays the organization name in green. Otherwise, the area displays the following text in red: No Valid Subscription Found.
   - If you have already set up a BioCyc user account—that is, you have entered and tested your credentials and saved the settings—the Username box displays your email address. Otherwise, the following text appears in red under User Subscription:

     No Valid Subscription Found.

   Figure 224 shows the default BioCyc User Login page for a user without an organization subscription and who has not entered and tested their BioCyc user account information.

Figure 224. BioCyc User Login page for a user without a subscription



3. Do one of the following:

   - If you do not have a BioCyc user account, go to "Create a BioCyc user account."

     If the Username box is empty, you do not have a BioCyc user account or you have not entered, tested, and saved your user account information.

   - If you have a BioCyc user account, but you do not have access to all the BioCyc databases that you want access to, go to "Purchase a subscription or request a free 30-day trial period."

Create a BioCyc user account

You must have Internet access to set up a BioCyc user account. You can access the Sign Up page of the BioCyc website from the BioCyc User Login view of the Compound Discoverer application.

❖ **To create a new BioCyc account**

1. Open the BioCyc User Login view, if you closed it.
2. Go to https://biocy.org/new-account.shtml.

   The Sign Up page of the BioCyc website opens.
3. Follow the instructions on the Sign Up page of the BioCyc website to create your new user account.
4. Go to "Enter, test, and save your BioCyc user account information."

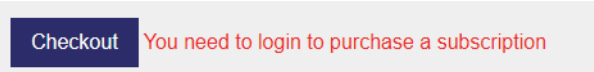
Purchase a subscription or request a free 30-day trial period

To access all the BioCyc databases, you must have a user account and one of the following: a paid subscription or an unexpired free trial period that provides access to all the BioCyc databases.

❖ **To purchase a subscription or request a free 30-day trial period**

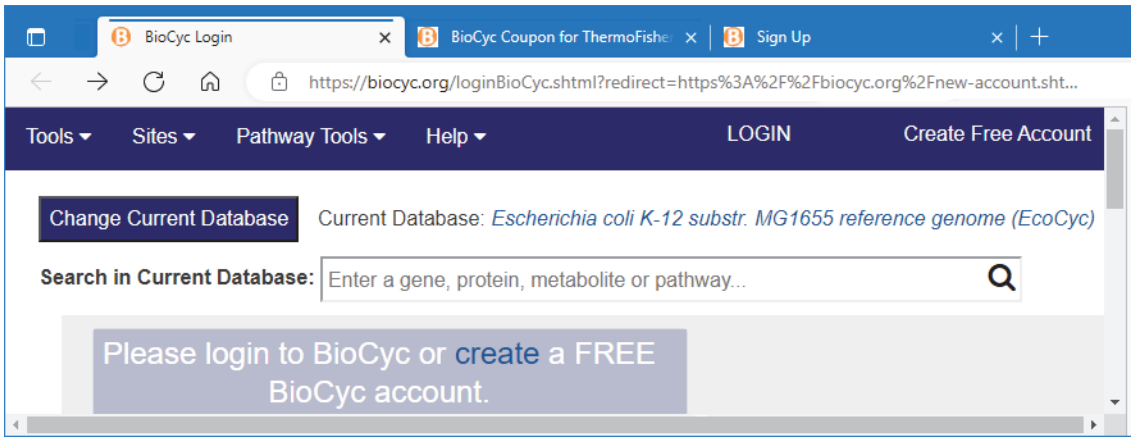
1. Open the BioCyc User Login view, if you closed it.
2. Go to https://biocyc.org/thermofisher.shtml.
3. Follow the instructions on this page to purchase an individual subscription or an institutional subscription or to request a 30-day free trial period.

   You must be logged in to the BioCyc website to purchase a subscription. If the following message appears when you click Checkout, log in as requested.

   You can log in to the BioCyc website by clicking LOGIN at the top of most of the Web site pages. See Figure 225.

Figure 225. BioCyc Login page (top portion)



Enter, test, and save your BioCyc user account information

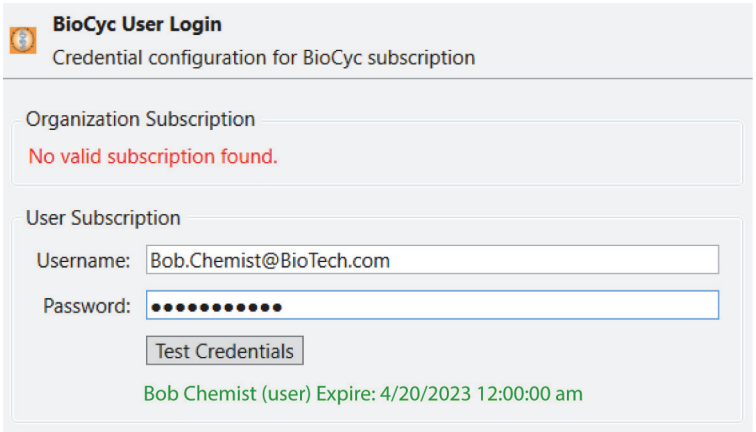
After you create your BioCyc user account on the Sign Up page of the BioCyc website, you must enter, test, and save your account information in the BioCyc User Login view of the Compound Discoverer application.

❖ To enter, test, and save your account information

1. Open the BioCyc User Login view, if you closed it.
2. In the User Subscription area of the BioCyc User Login view, enter your user name (email address) and password.
3. Below the Password box, click **Test Credentials**.
4. At the bottom right of the BioCyc User Login view, click **Save Current Settings**.

   Figure 226 shows the subscription information for a new user account with unexpired access to all the BioCyc databases.

   Figure 226. Settings for a new user account with unexpired access to all the BioCyc databases



Specify the fragmentation databases

Use the HighChem Fragmentation Options view to select the fragmentation databases.

Currently, there is only one available fragmentation database. This view is reserved for future use.

❖ To open the HighChem Fragmentation Options view

In the left pane of the Configuration page, under Miscellaneous Settings, select **HighChem Fragmentation Options**.

Common operations for manipulating data tables

The following topics describe the common operations that you can perform on the tables in the Lists and Libraries view, on the pages of a study, and in result files:

- Move table rows up or down
- Sort data tables
- Freeze table rows
- Group table rows
- Change the position of table columns
- Freeze table columns
- Show or hide table columns
- Copy table entries to the clipboard
- Filter the tables on a study page or a list or library view
- Set up a custom filter with multiple conditions

Move table rows up or down

Use the following procedure to move through the rows in a data table.

❖ **To move up or down through the rows of a result or library table**

To move down, press the **Tab** key.

To move up, hold down the **SHIFT** key and press the **Tab** key.

Sort data tables

To sort the data tables, see these topics:

- Sort table entries by one or more columns
- Sort table entries by a column with a distribution map

Sort table entries by one or more columns

❖ **To sort the rows based on the contents of one or more columns**

1. Click a column header to sort the rows between ascending order (A, B, C …) and descending order (Z, Y, X …), based on the contents of the column.

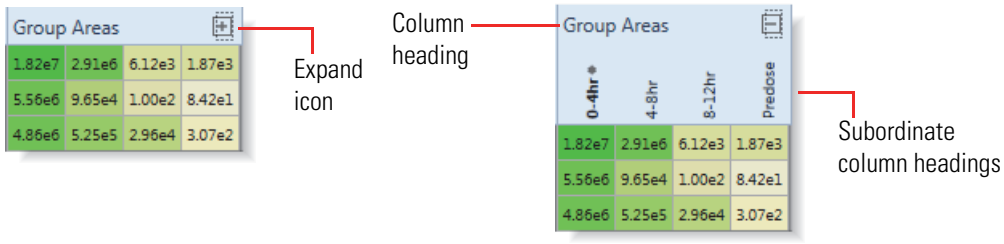
   Note The application treats formulas the same as text strings and sorts them by the order of the characters in the formula string, not by the actual number of elements in the formula.

2. To sort the data by a second column, hold down the CTRL key and click the second column heading.

Sort table entries by a column with a distribution map

❖ **To sort a table by a column that contains a distribution map**

1. Click the expand icon to display the vertical headings of the subordinate columns.



2. Select the heading of the subordinate column that you want to sort by.

   The selected subordinate column heading appears in bold text.

3. Click the column heading to sort the table rows.

Freeze table rows

Use the following procedure to freeze table rows.

❖ To affix rows at the top of the table

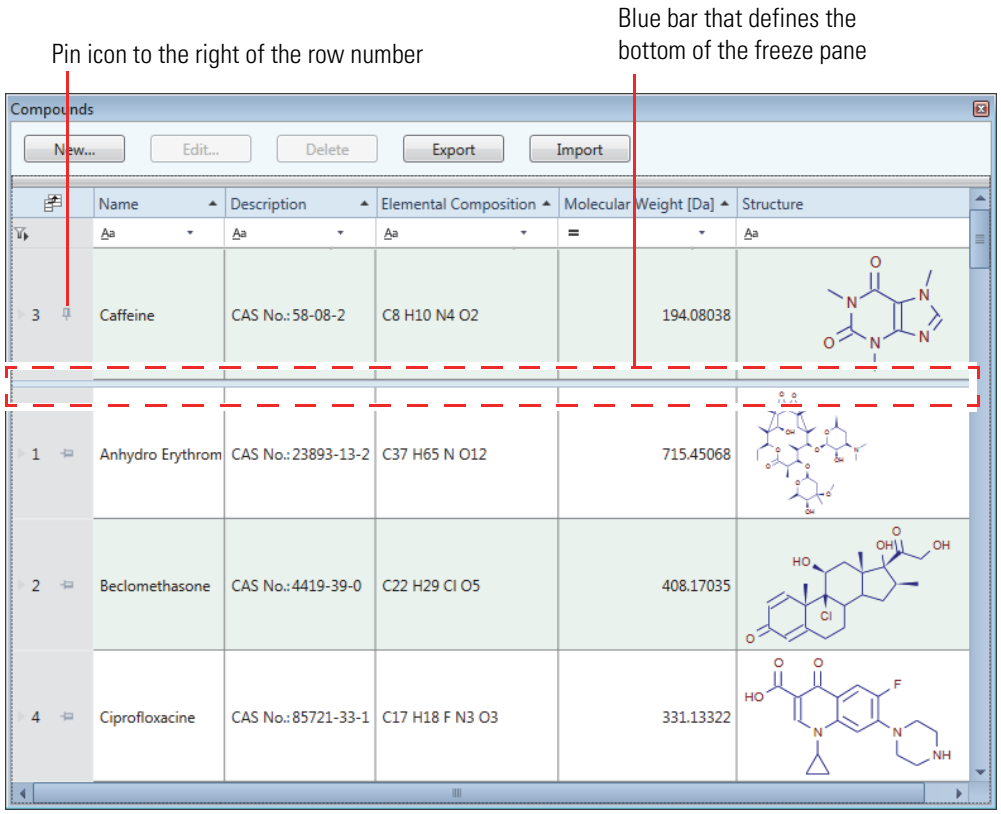
Click the pin icon, ⊣, next to the row number of the row that you want to freeze.

The row moves to the top of the table, its pin icon changes to the pinned position, ⊣, and a blue bar that defines the bottom of the freeze pane appears below the fixed row.

As you fix additional rows, they move up to the freeze pane in the order selected and their icons change to pinned, ⊣. The row just above the blue bar is the last fixed row.

When you scroll the table, the freeze pane remains at the top. Figure 227 shows a compound library with caffeine in the freeze pane.

Figure 227. Compound library with a freeze pane



Group table rows

For a table on a study page, use the Enable Row Grouping shortcut menu command to group items by a column heading.

❖ To group and ungroup the table rows on a study page

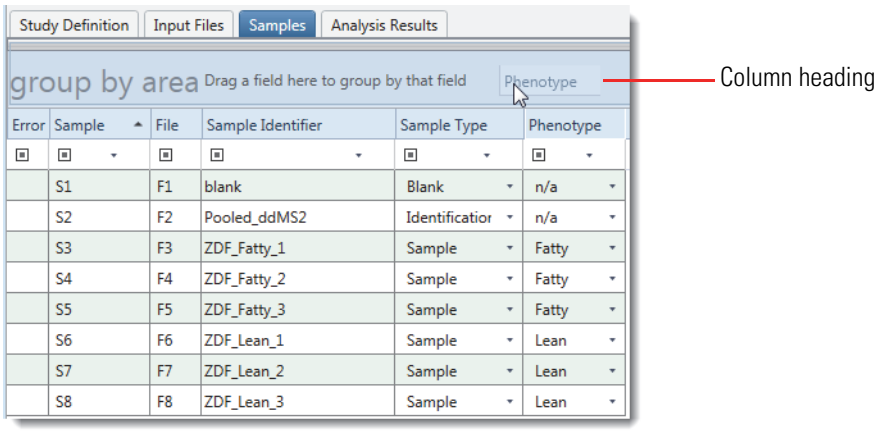
1. Right-click the page and choose **Enable Row Grouping**.

   The Group by Area bar appears above the table heading row.

2. Drag the column heading that you want to group by into the Group by Area bar.

   Figure 228 shows the column heading for a study factor being dragged to the Group by Area bar.

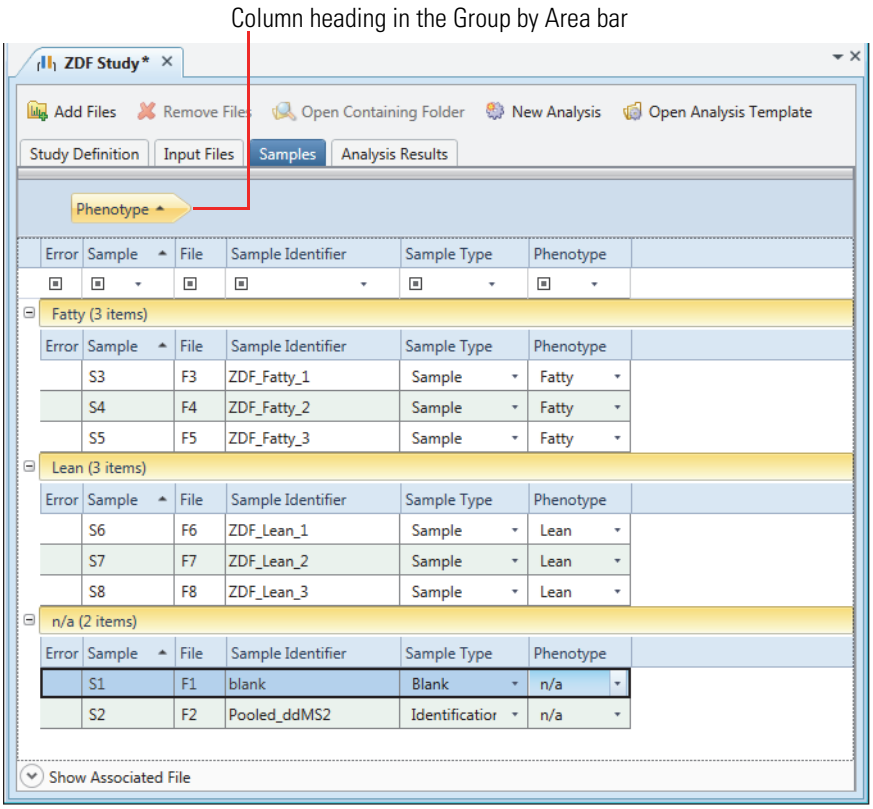
   Figure 228. Group by Area bar above the table heading row



3. To ungroup the table rows, drag the column heading out of the Group by Area bar.

   Figure 229 shows the study factor (Phenotype) column heading inside the Group by Area bar, and the table rows grouped by the study factor value (Lean, Fatty, or n/a).

Figure 229. Samples table grouped by phenotype



4. To turn off the group by row feature, right-click the page and choose **Disable Row Grouping**.

Change the position of table columns

You can save the layout changes to a result table. Changes to the table layout in any of the Lists & Libraries views are temporary.

To change the position of table columns, see the following topics:

- Change the column order
- Stack two table columns into one column

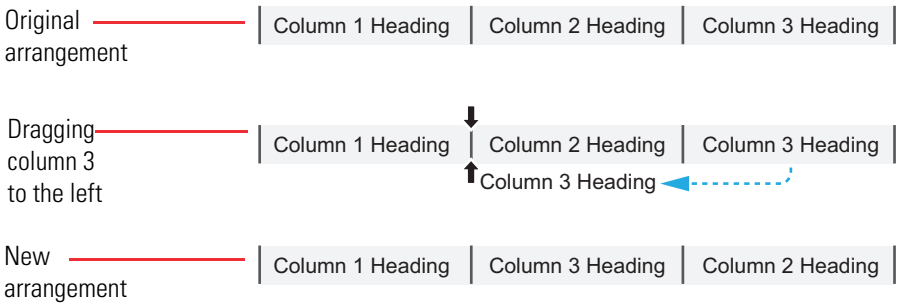
Change the column order

❖ **To change the order of the columns in a table**

1. To move a column to the left of its current position, drag the column header to the left. Release the mouse button when the cursor ( ) appears over the column delineator.

Note If you release the mouse button when the column-stacking cursor (➡ ⬅) appears instead of when the column-reordering cursor (⬍) appears, the application stacks the two columns. See Stack two table columns into one column.

Figure 230. Moving a column to the left



2. To save the current layout for a result file, choose **File > Save** from the menu bar.

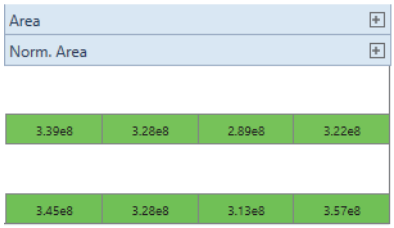
Note To save the current layout to a layout file that you can apply to other result files, choose **Window > Save Layout**. Then, in the Save Result Layout dialog box, name the layout and click **OK**.

Stack two table columns into one column

Stacking table columns can make it easier to compare the results in two table columns.

Figure 231 shows an example where the Area and Norm. Area columns of a compounds table are stacked.

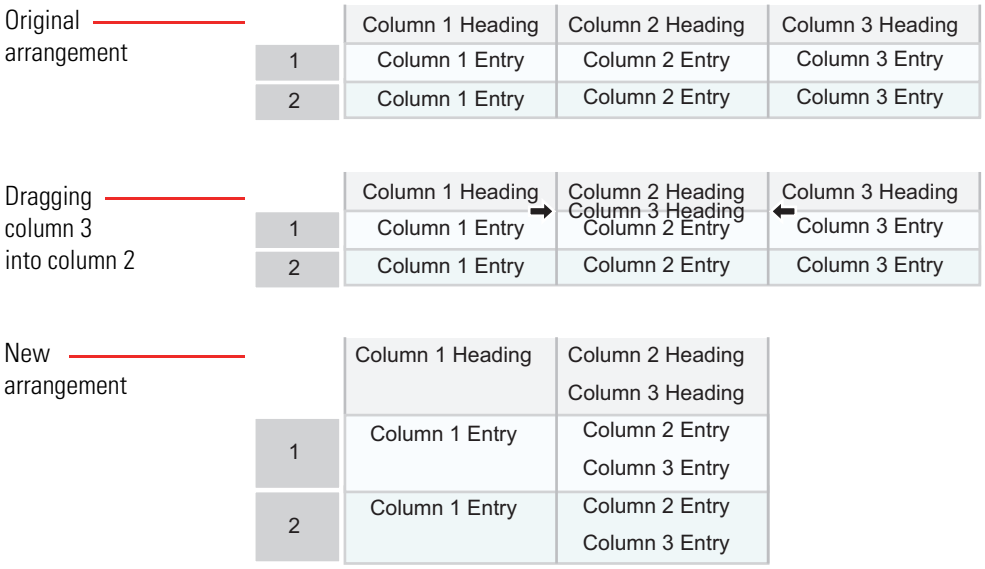
Figure 231. Stacked columns



❖ To stack two table columns into one column

1. Drag the column header of the column that you want to stack below the column header of the column that you want on top. Release the mouse button when the cursor (➡ ⬅) appears over the column heading.

Figure 232. Stacking two columns into one column



2. To save the current layout for a result file, choose **File > Save** from the menu bar.

Freeze table columns

In a result table, to more easily compare values in columns that are not next to each other, you can lock columns in place so that they are always visible as you scroll through the unlocked columns.

Note Except for the Input Files table, the Checked column is, by default, the first column in every result table—that is, Checked is the text in first column's heading row.

❖ **To lock table columns to the left of the first column**

1. Right-click the table and choose **Enable Column Fixing**.

   A pin icon, , appears to the right of each column heading.

2. Click the pin icons for the columns that you want to move to the left of the first column.

   The columns move to the left of the Checked column and their pins face down, .

Show or hide table columns

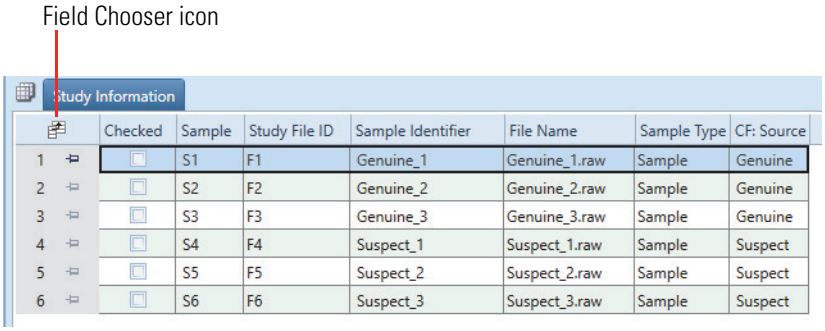
Use the Field Chooser dialog box to show or hide columns in any of the result tables or tables in the Lists & Libraries views. The changes to tables in any of the Lists & Libraries views are temporary. You can save the layout changes to a result table by choosing Window > Save Layout.

Note You can hide or show columns in these tables that are available from the Lists & Libraries menu—Expected Compounds, Transformations, Neutral Losses, Adducts, and Ion Definitions.

❖ To show or hide columns in a list view or result table

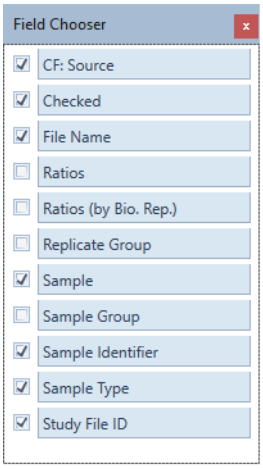
1. Click the **Field Chooser** icon, , in the upper-left corner of the table.

   Figure 233. Field chooser icon in the upper-left corner of the main Study Information table

   The Field Chooser dialog box opens with a list of all of the column headers for the current table in alphabetical order.

   Figure 234. Field Chooser dialog box for the Study Information table

2. In the Field Chooser dialog box, clear the check box for each column that you want to hide. To show those columns again, select their corresponding check boxes.

   The table updates and shows or hides your chosen columns immediately.

Copy table entries to the clipboard

You can copy a single table cell, a single table row, or multiple table rows to the Clipboard, and then paste the Clipboard contents into other documents, such as a Notepad text document or Microsoft Office documents.

Note The application does not copy the compound structure in the Structure column of the Expected Compounds library to the Clipboard.

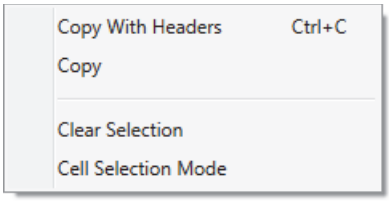
For details, see these topics:

- Copy the contents of a single table cell to the Clipboard
- Copy the contents of a single table row to the Clipboard
- Copy the contents of multiple rows to the Clipboard

Copy the contents of a single table cell to the Clipboard

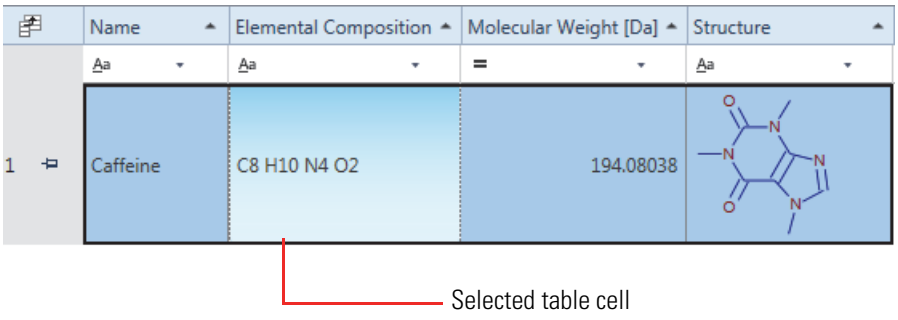
❖ To copy table cells to the Clipboard

1. Right-click anywhere in the table and choose **Cell Selection Mode**.



2. To select multiple table cells, use the CTRL key or the SHIFT key.

   The selected cells turn a lighter blue than the other cells in the row, as shown in the following figure.



3. Right-click and choose **Copy** from the shortcut menu.

Copy the contents of a single table row to the Clipboard

❖ **To copy a single table row to the Clipboard**

Do one of the following:

- To copy a single row to the Clipboard, right-click the row and choose **Copy**.
- To copy a single row and the table header, right-click the row and choose **Copy with Headers**.

Copy the contents of multiple rows to the Clipboard

❖ **To copy multiple rows to the Clipboard**

Do one of the following:

- To copy a range of contiguous rows to the Clipboard, while holding down the SHIFT key, click the first and last row in the range. Then, right-click the last row to open the shortcut menu and choose **Copy** to copy the row contents or choose **Copy with Headers** to copy the row contents and the table header.
- To copy noncontiguous rows to the Clipboard, while holding down the CTRL key, click each row that you want to copy. Then, right-click the last row to open the shortcut menu and choose **Copy** to copy the row contents or choose **Copy with Headers** to copy the row contents and the table header.

Filter the tables on a study page or a list or library view

For the tables on the study pages or in the Lists & Libraries views, use the filters in the filter row below the column headers to reduce the number of entries in the current display. The filtering effect is not permanent; closing a filtered list or study removes the filters.

Note For information about filtering the tables in the result files, see "Filter the data for data reduction."

To set up single-condition filters for the table columns, see these topics:

- Set up single-condition filters for the table columns
- Set up a single-condition wild card filter
- Set up a single-condition filter for numeric data

For information about setting up custom filters with the Custom Filter Selection dialog box, see "Set up a custom filter with multiple conditions."

Set up single-condition filters for the table columns

❖ **To set up filters for one or more table columns**

1. In the table's filter row, do the following for each column that you want to filter by:
   a. Click the operator symbol (**Aa** or **=**) and select an operator from the list.
   b. Set up the operand by selecting or typing a value in the operand box.

   After you set up a filter, the applied filter icon, , appears to the right of the operand box, and the table displays only those rows with entries that fulfill the filter condition.
2. To remove a single filter, click the filter icon, , to the right of the operand box.

Set up a single-condition wild card filter

❖ **To set up a wild card filter for a table column**

1. In the operator list in the filter row, select **Like (Wildcards)** or **Not Like (Wildcards)**.
2. In the operand box, select or type text and use an asterisk "*" to replace more than one character or use a question mark "?" to replace only one character.

Tip For example, to filter the entries in the transformations library by the presence of nitrogen in the arriving group, do the following in the Arriving Group column:

- Select * **Like (Wildcards)** in the operator list.
- Type ***N*** in the operand box.

Set up a single-condition filter for numeric data

❖ **To set up a filter for a table column with numeric data**

Do any of the following:

- To set up a filter that uses a specific table entry in the operand list, select any of these operators: Equals, Not Equals, Less Than, Less Than or Equal To, Greater Than, or Greater Than or Equal To.
- To set up a filter that uses any of these operands: (Blanks), (NonBlanks), Above Average, Below Average, Top 10, Top 10 percentile, Bottom 10, or Bottom 10 percentile, select either = **Equals** or ≠ **Not Equals** in the operator list.
- To display the top *n* number of entries, select ▲ **Top** in the operator list and type an integer value in the operand box.
- To display the bottom *n* number of entries, select ▼ **Bottom** in the operator list and type an integer value in the operand box.

- To display the top *n* percentile of entries, select **Top Percentile** in the operator list and type a numeric value in the operand box.
- To display the bottom *n* percentile of entries, select **Bottom Percentile** in the operator list and type a numeric value in the operand box.

Operators and operands for a single-condition table filter

The filter for each table column consists of an operator and an operand. In an unfiltered table, the filter row displays the default operator, which is represented by its symbol, and an empty operand box for each column. To set up a table filter, you select the operator from a fixed list, and you select the operand from a list or type a value in the operand box.

The selections in the operator list depend on whether the column contains text or numeric entries. After you select an operator, the operator symbol appears in the filter row to the left of the operand box. For more information about the operator lists, see Table 214 on page 748 and Table 215 on page 749.

For all columns, the operand list includes the following: Custom, Blanks, NonBlanks, and the column entries. For numerical-entry columns, the operand list also includes the following: Above Average, Below Average, Top 10, Top 10 Percentile, Bottom 10, and Bottom 10 Percentile. For more information, see Table 213.

After you set up a column filter, the applied filter icon, , appears to the right of the operand box. Figure 235 shows a filtered Ion Definitions list that reduces the number of displayed entries to 10 by using the total adduct mass. The filter row of the Adducts Total Mass column displays the equals symbol (=)for the mathematical operator, the selection of Top 10 for the operand, and the applied filter icon, .

Figure 235. Ion Definitions list that is filtered by the adduct mass

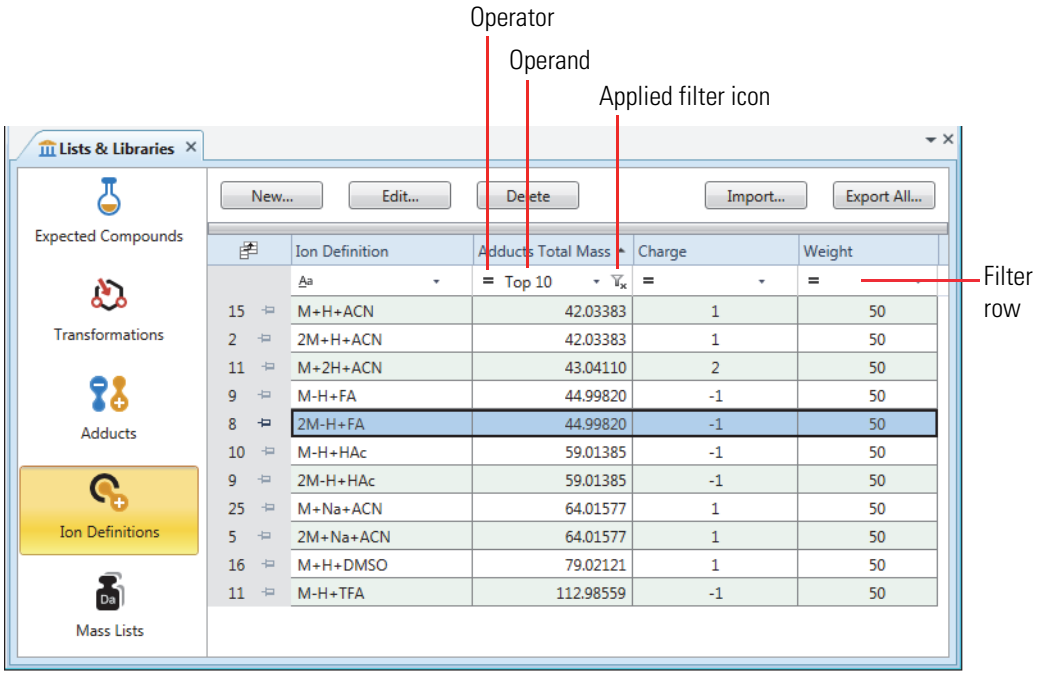


Table 213 describes the available operand selections and the valid typed operand entries for both text and numeric columns.

Table 213. Operands for the table columns on a study page or Lists & Libraries view (Sheet 1 of 3)

Operand	Description
All table columns	
(Custom)	Applies the custom filter that you set up by using the Custom Filter Selection dialog box. A custom filter contains more than one condition. If you set up a single-condition filter, the operand box lists the single condition rather than the (Custom) setting.
(Blanks)	Compatible operators: = Equals and ≠ Not Equals = (Blanks)—Displays the table rows that have blank entries in the filtered column. ≠ (Blanks)—Displays the table rows that have entries in the filtered column.

Table 213. Operands for the table columns on a study page or Lists & Libraries view (Sheet 2 of 3)

Operand	Description
(NonBlanks)	Compatible operators: = Equals and ≠ Not Equals = (NonBlanks)—Displays the table rows that have entries in the filtered column. ≠ (NonBlanks)—Displays the table rows that have blank entries in the filtered column.
Selected entry	Table 214 on page 748 describes the compatible operators for text entries. Table 215 on page 749 describes the compatible operators for numeric entries. Filters the table rows by using the selected entry and operator.
Typed alphanumeric text or numeric value	Table 214 describes the compatible operators for text entries. Table 215 describes the compatible operators for numeric entries. Filters the table rows by using the typed text entry and the selected operator.
Additional selections for numeric value columns	
Above Average	Compatible operators: = Equals and ≠ Not Equals = (Above Average)—Displays the table rows with numeric values in the filtered column that are greater than the calculated column average. ≠ (Above Average)—Displays the table rows with numeric values in the filtered column that are equal to or less than the calculated column average.
Below Average	Compatible operators: = Equals and ≠ Not Equals = (Below Average)—Displays the table rows with numeric values in the filtered column that are less than the calculated column average. ≠ (Below Average)—Displays the table rows with numeric values in the filtered column that are equal to or greater than the calculated column average.
Top 10	Compatible operators: = Equals and ≠ Not Equals = (Top 10)—Displays the top 10 table rows for the filter condition. ≠ (Top 10)—Displays the table rows with numeric values in the filtered column that are less than those of the top 10 table rows.

Table 213. Operands for the table columns on a study page or Lists & Libraries view (Sheet 3 of 3)

Operand	Description
Top 10 Percentile	Compatible operators: = Equals and ≠ Not Equals = (Top 10 Percentile)—Displays the top 10th percentile of table rows for the filter condition. ≠ (Top 10 Percentile)—Displays the table rows with numeric values in the filtered column that are less than those of the top 10th percentile.
Bottom 10	Compatible operators: = Equals and ≠ Not Equals = (Bottom 10)—Displays the bottom 10 table rows for the filter condition. ≠ (Bottom 10)—Displays the table rows with numeric values in the filtered column that are greater than those of the bottom 10 table rows.
Bottom 10 Percentile	Compatible operators: = Equals and ≠ Not Equals = (Bottom 10 Percentile)—Displays the bottom 10th percentile of table rows for the filter condition. ≠ (Bottom 10 Percentile)—Displays the table rows with numeric values in the filtered column that are greater than those of the bottom 10th percentile.

Table 214 describes the operators for columns with text entries.

Table 214. Operators for text columns

Symbol	Text selection	Effect
=	Equals	Displays the text entries that exactly match the selected or typed operand.
≠	Not equals	Displays the text entries that do not exactly match the selected or typed operand.
<	Less than	For alphabetic text entries, displays the text entries that begin with a letter in the alphabet that comes before the selected or typed operand.
≤	Less than or equal to	–
>	Greater than	–
≥	Greater than or equal to	–
▣	Contains	Displays the text entries that contain the text in the selected or typed operand.
▣	Does not contain	Displays the text entries that do not contain the text in the selected or typed operand.
*	Like (wildcards)	Displays the text entries that contain the selected or typed text and any additional text represented by an asterisk.
*	Not like (wildcards)	Hides the text entries that contain the selected or typed text and any additional text represented by an asterisk.
.*	Match (regular expression)	Displays the text entries that contain the same text as the selected or typed operand.
.*	Does not match (regular expression)	Displays the text entries that do not contain the same text as the selected or typed operand.
Aa	Starts with	Displays the text entries that start with the selected or typed operand.
Aa	Does not start with	Displays the text entries that do not start with the selected or typed operand.
aA	Ends with	Displays the text entries that end with the selected or typed operand.
aA	Does not end with	Displays the text entries that do not end with the selected or typed operand.

Table 215 describes the operators for columns with numeric entries.

Table 215. Operators for numeric columns

Symbol	Text selection	Effect
=	Equals	Displays the numerical entries that equal the selected operand.
≠	Not equals	Displays the numerical entries that are not equal to the selected operand.
<	Less than	Displays the numerical entries that are less than the selected operand.
≤	Less than or equal to	Displays the numerical entries that are less than or equal to the selected operand.
>	Greater than	Displays the numerical entries that are greater than the selected operand.
≥	Greater than or equal to	Displays the numerical entries that are greater than or equal to the selected operand.
▲	Top	Displays the *n* highest entries in the table, where *n* equals the integer typed in the operand box.
▼	Bottom	Displays the *n* lowest entries in the table, where *n* equals the integer typed in the operand box.
% ▲	Top percentile	Displays the entries in the top n^{th} percentile, where *n* equals the percentage typed in the operand box.
% ▼	Bottom percentile	Displays the entries in the bottom n^{th} percentile, where *n* equals the percentage typed in the operand box.

Set up a custom filter with multiple conditions

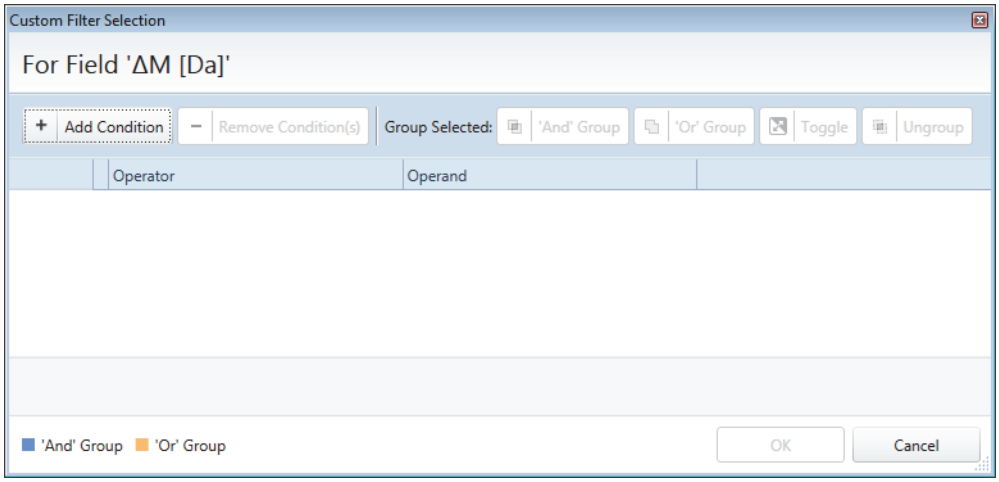
Use the Custom Filter Selection dialog box to set up a custom filter with multiple conditions for a library or list table or a table on a study page.

❖ To set up a custom filter

1. Select **(Custom)** from the operand list for a table column.

   The Custom Filter Selection dialog box opens.

Figure 236. Custom Filter Selection dialog box with no conditions



2. Do the following for each condition that you want to add to a group:
   a. Click **Add Condition**.

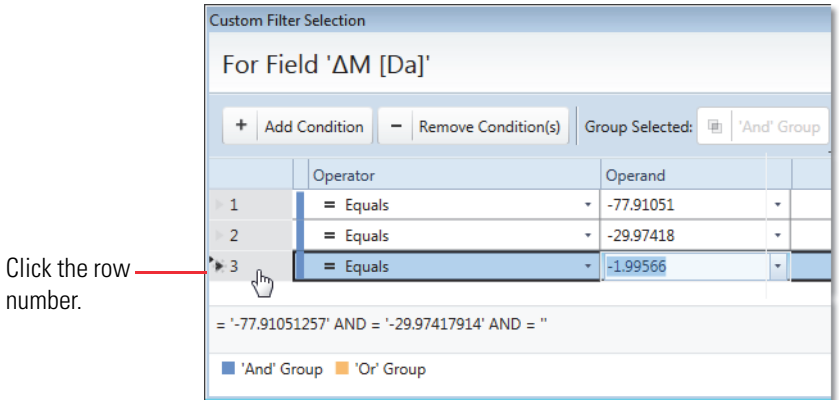
      A new table row appears.

   b. Select an operator from the Operator list and an operand from the Operand list.

      As you add conditions to the group, the application updates the group filter in the gray area below the table.

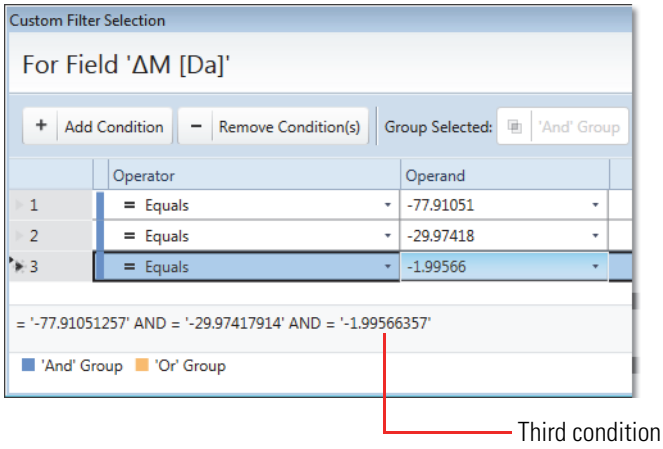
3. To add the last condition to the group, click its row number.

Figure 237. Clicking the row number in the last row to add the row to the group



The last condition appears in the group filter area. By default, the application applies the AND operator to all of the conditions in the group (Figure 238). A vertical blue bar to the left of the condition rows indicates an AND group.

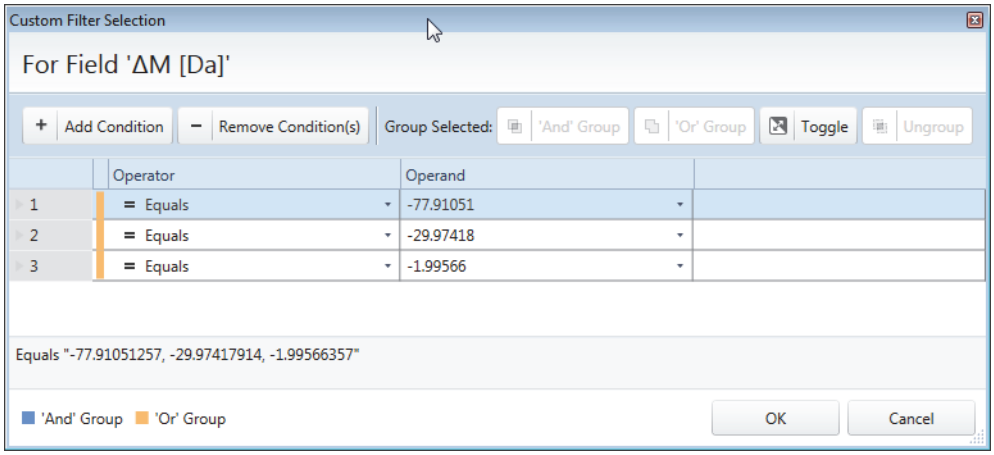
Figure 238. Group filter with three conditions and the AND group operator



4. To change the group operator from AND to OR or from OR to AND, click **Toggle**.

   An orange bar to the left of the condition rows indicates an OR group.

   Figure 239. Group filter with three conditions and the OR group operator

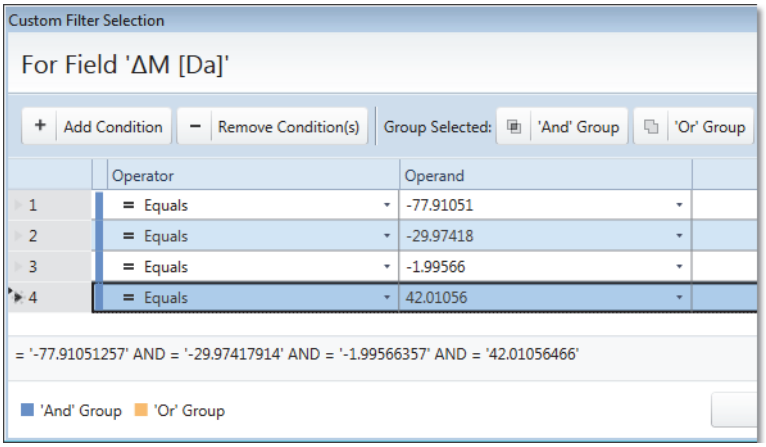


5. To add an overlapping group to the filter, do the following:

   a. Select the rows that you want to group, using the SHIFT key for contiguous rows or the CTRL key for noncontiguous rows.

      The selected rows are highlighted in blue and the 'And' Group and 'Or' Group buttons become available.

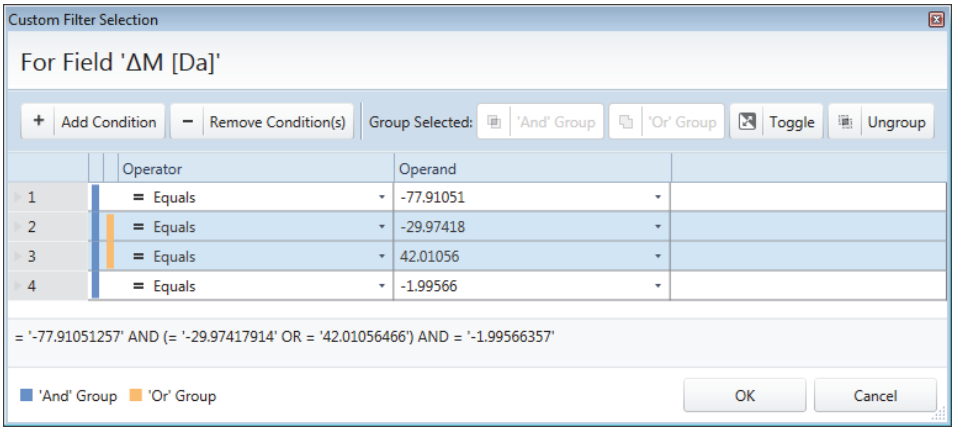
Figure 240. Selection of two noncontiguous rows



b. Specify the group type by clicking **'And' Group** or **'Or' Group**.

The application applies the second group definition and the Ungroup button becomes available.

Figure 241. A set of filter conditions with two groups



6. To remove conditions from a group, select the conditions and click **Ungroup**.
7. To apply the filter, click **OK**.

The Custom Filter Selection dialog box closes, the text (Custom) appears in the operand box, and the application applies the custom filter to the entries in the selected filter column.

Custom Filter Selection dialog box

Table 216 describes the features of the Custom Filter Selection dialog box.

Table 216. Custom Filter Selection dialog box features

Feature	Description
Buttons or icons	
+ Add Condition	Adds a blank condition row to the condition table.
– Remove Condition(s)	Removes the selected conditions. Selected conditions are highlighted in blue.
'And' Group	When the filter contains more than one group, applies the AND group type to a set of selected conditions.
'Or' Group	When the filter contains more than one group, applies the OR group type to a set of selected conditions.
Toggle	Changes the selected AND group to an OR group or the reverse.
Ungroup	As you create groups, group label columns appear to the left of the Operator column. When conditions belong to more than one group, removes the second group condition for the selected conditions.
OK	Closes the dialog box and applies the filter conditions.
Cancel	Closes the dialog box without applying the filter conditions.
Table	
Operator column	Use to select an operator for the filter condition. See Table 214 on page 748 for a list of the operators for the text entry columns. See Table 215 on page 749 for a list of the operators for the numerical entry columns.
Operand column	Use to select or type an operand for the filter condition. See Table 213 on page 745 for a list of the operands for the library columns.
Third column	Displays comments about the filter condition. For example, this box displays "Condition is empty" until you define the operator and the operand for a condition.
Filter description area	
This area, which is highlighted in gray, displays the group filter conditions.	

16

Explore compound relations with the molecular networks viewer

To use the molecular networks feature to investigate possible relations between compounds in the Compounds table, see the following topics:

Overview of using the molecular networks feature

To use the molecular networks feature, follow this process:

1. Process your raw data files with a processing workflow that includes the Generate Molecular Networks node, which is a node under Compound Scoring.
2. To review the processed results, open the result file. See "Open, close, and update result files."
3. (Optional) Using the Result Filters view, apply a filter to display only the compounds of interest.

Note For an LC study, the compounds must have MS2 scans.

4. Do one or both of the following:

   - To view a table of similar compounds, select a compound of interest in the Compounds table. Then, open the related Similar Compounds Related table for the selected compound.
   - To view the molecular networks, follow the instructions in "Send compounds to the molecular networks viewer."

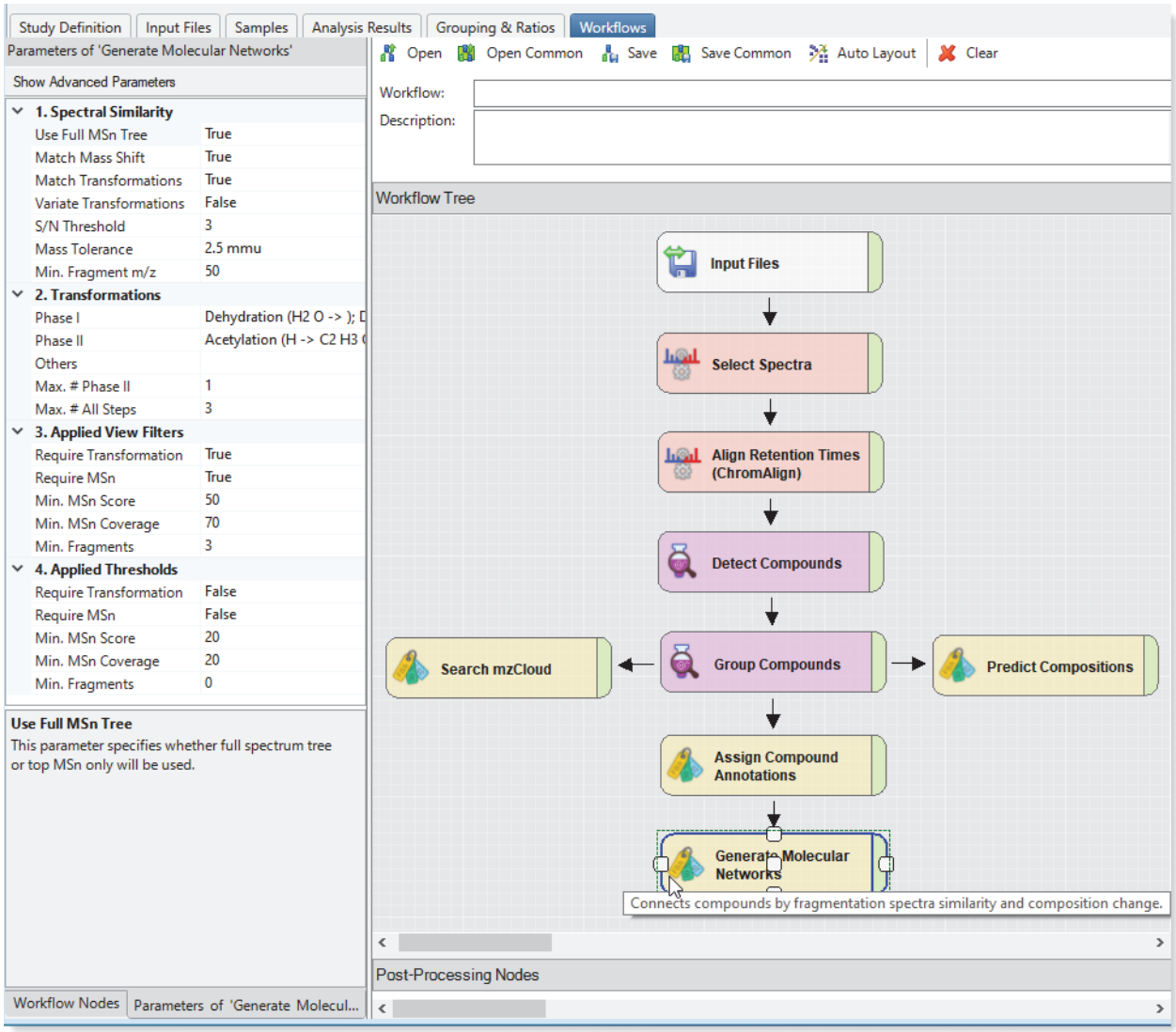
     The viewer opens in a local browser window—that is, the viewer retrieves the data from the current result file. The viewer does not connect to the Internet.

How the Generate Molecular Networks node works

To express the similarity between pairs of compounds, the Generate Molecular Networks node uses the assigned elemental compositions and fragmentation data.

For an LC study, a minimum processing workflow that includes the Generate Molecular Networks node consists of untargeted compound detection, grouping, and annotation assignment. To validate the elemental composition differences, the workflow must contain at least one search node or the Predict Compositions node.

Figure 242. Example processing workflow with the Generate Molecular Networks node



The input to the Generate Molecular Networks node is a list of annotated compounds, and the output from the node is a table of similar compounds for each detected compound.

Note If you do not select any transformations for the Generate Molecular Networks node, the node does not consider the elemental compositions of the detected compounds for scoring.

The node processes the data as follows:

1. Generates possible transformation pathways according to the user-specified settings.
    - If there are multiple pathways to the same elemental composition, the node selects the shorter pathway.

- If there are compounds with the same elemental composition (isomers with different retention times), the node adds a pathway of length 0.

2. For each pair of compounds that have assigned elemental compositions, the node finds a matching pathway that explains the elemental composition difference between the two compounds.
3. For each pair of compounds that have fragmentation data, the node calculates the spectral similarity by FISh Scoring as follows:
   a. Matches the fragments for both compounds by directly comparing their masses.
   b. For the remaining unmatched fragments, the node does the following to match the fragments:
      - Uses the mass shift of the assigned pathway to match "shifted" fragments (if enabled). In addition, it uses all possible permutations of the individual pathway steps (if enabled).
      - Uses the mass shift between the two compounds to match "shifted" fragments (if enabled).
   c. Calculates the similarity scores.
4. Applies specified rules and thresholds to the connections (matched pairs).
5. Stores valid connections to the results file.
6. Applies specified view filters on the results table.

Information displayed in the Similar Compounds table

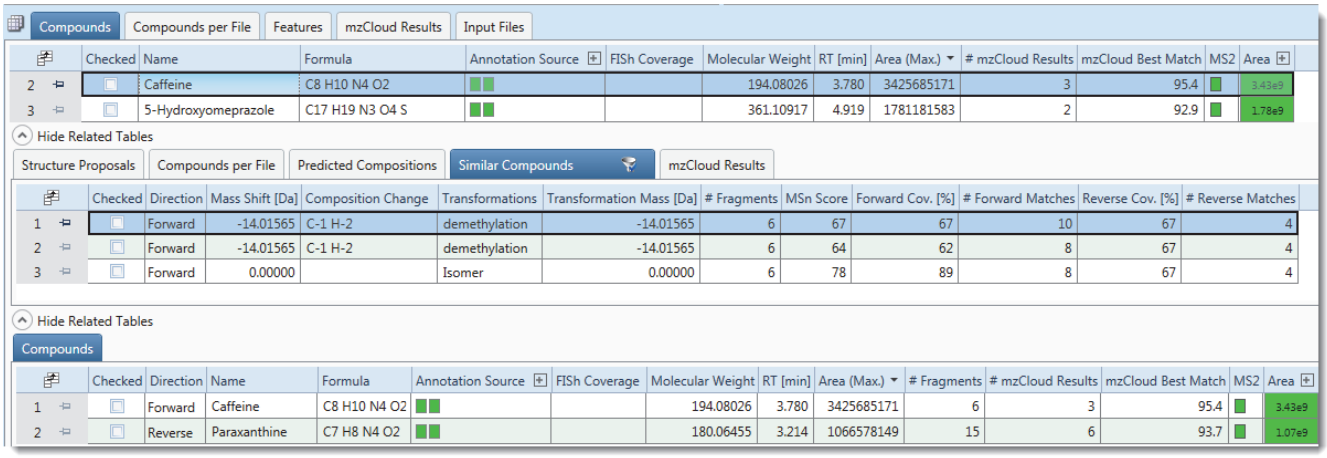
The Generate Molecular Networks node stores all the valid connections between each pair of compounds and creates a related table of Similar Compounds. The table shows all the connections between the selected compound and its related compounds, with additional information about the similarity between them.

You can consider each stored connection as a reaction, where one compound is a substrate that is converted into a product through a specific transformation pathway. The Direction column indicates the direction of the reaction between the selected compound in the main compounds table and the similar compound in the related Similar Compounds table.

A Forward connection indicates that the selected compound is a substrate, to which the transformation has been applied to generate the similar compound. A Reverse connection indicates that the selected compound is a product of applying the transformation to the similar compound.

In Figure 243, paraxanthine is listed as a demethylation product of caffeine (substrate).

Figure 243. Caffeine and one of its demethylation products (the Tags column is hidden)



	Checked	Name	Formula	Annotation Source	FISh Coverage	Molecular Weight	RT [min]	Area (Max.)	# mzCloud Results	mzCloud Best Match	MS2	Area
2	☐	Caffeine	C8 H10 N4 O2			194.08026	3.780	3425685171	3	95.4		3.43e9
3	☐	5-Hydroxyomeprazole	C17 H19 N3 O4 S			361.10917	4.919	1781181583	2	92.9		1.78e9

	Checked	Direction	Mass Shift [Da]	Composition Change	Transformations	Transformation Mass [Da]	# Fragments	MSn Score	Forward Cov. [%]	# Forward Matches	Reverse Cov. [%]	# Reverse Matches
1	☐	Forward	-14.01565	C-1 H-2	demethylation	-14.01565	6	67	67	10	67	4
2	☐	Forward	-14.01565	C-1 H-2	demethylation	-14.01565	6	64	62	8	67	4
3	☐	Forward	0.00000		Isomer	0.00000	6	78	89	8	67	4

	Checked	Direction	Name	Formula	Annotation Source	FISh Coverage	Molecular Weight	RT [min]	Area (Max.)	# Fragments	# mzCloud Results	mzCloud Best Match	MS2	Area
1	☐	Forward	Caffeine	C8 H10 N4 O2			194.08026	3.780	3425685171	6	3	95.4		3.43e9
2	☐	Reverse	Paraxanthine	C7 H8 N4 O2			180.06455	3.214	1066578149	15	6	93.7		1.07e9

Send compounds to the molecular networks viewer

After you process a set of input files with a processing workflow that includes the Generate Molecular Networks node, you can export the molecular networks for a specified number of compounds to the molecular networks viewer. The viewer takes on the appearance of your default browser, but it is not connected to the Internet.

Note For an LC study, you can export compounds to the molecular networks viewer from the Compounds table.

❖ To send the molecular networks to the viewer

1. (Optional) To display only the compounds of interest, filter the compounds table.
2. (Optional) Sort the compounds table by the columns of interest.

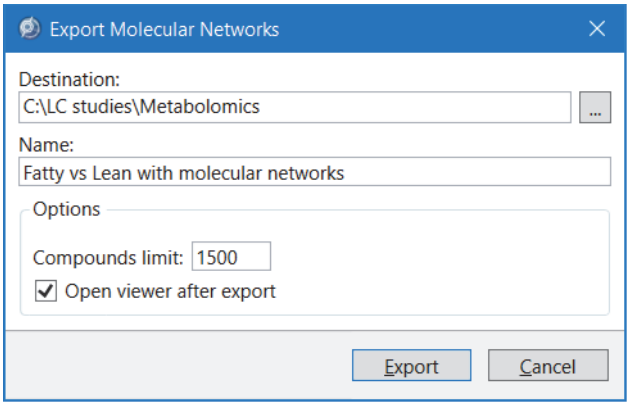
   Note The application only exports compounds that appear in the table in the order that they appear in the table, beginning with row 1. It does not export compounds that are hidden by applied result filters or compounds in row numbers greater than the Compounds Limit value.

3. Right-click the compounds table and choose **Molecular Networks > Send to Viewer**.

   The Export Molecular Networks dialog box opens with the following default settings:

   - Destination: Study folder where the current result file resides
   - Name: Name of the current result file
   - Compounds Limit: 3000
   - Open Viewer After Export: Selected

Figure 244. Export Molecular Networks dialog box



4. Do any of the following:

   - To change the destination folder, click the browse icon and select another folder.
   - To change the name of the final folder where the application stores the web page components, type a different name in the Name box.
   - To change the maximum number of compounds to export, type a number from **1** to **3000** in the Compounds Limit box.

     Note Increasing the number of compounds increases the processing time.

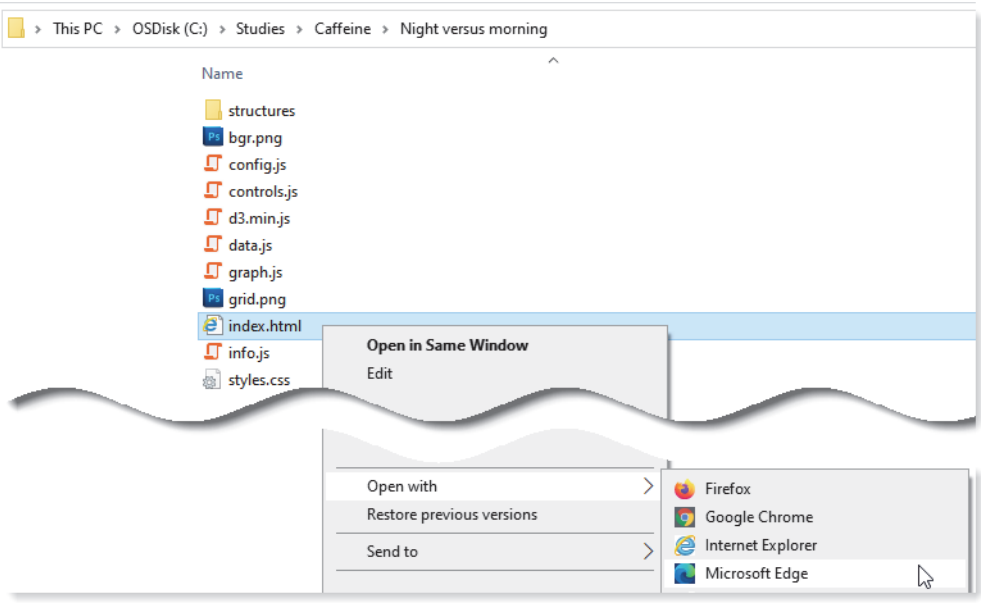
   - To set the viewer to NOT automatically open in the default browser after you click Export, clear the **Open Viewer After Export** check box.

5. Click **Export**.

   If you selected the Open Viewer After Export check box and Internet Explorer is not the default browser, the viewer opens in the Move mode ( ) in the default browser.

6. If you did not select the Open Viewer After Export check box, browse to the destination folder. Then, right-click the index.html file and choose a browser.

Figure 245. Choosing a browser for the molecular networks viewer



Note For the Internet Explorer browser, click **Allow Blocked Content**.

The viewer opens in the Move mode ( ) in the browser that you selected.

The browser does not connect to the Internet. The application derives the information that it plots in the browser from the current result file.

Mark selected compounds in the main compounds table

You can copy the information for selected nodes in the molecular networks viewer to the Clipboard, and then use this information to mark compounds in the Compounds table of a result file for an LC study.

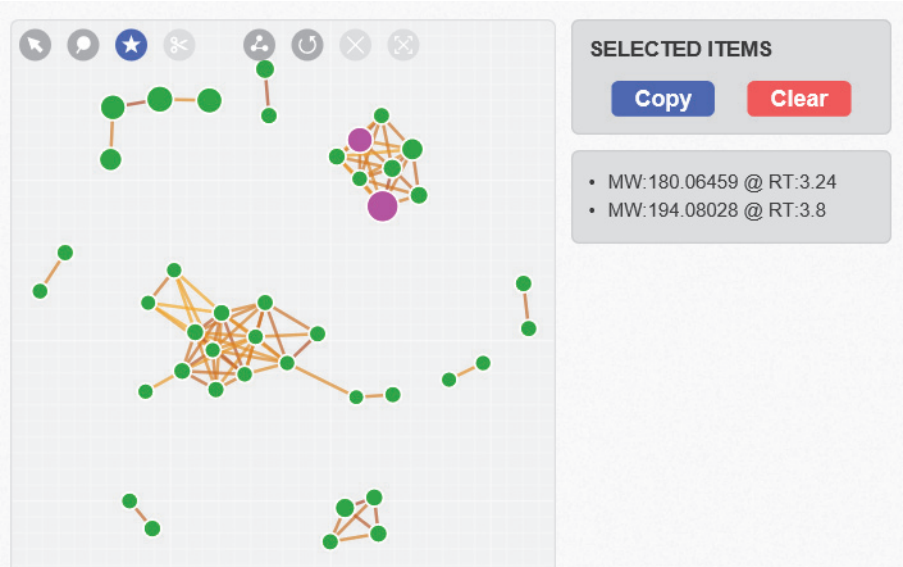
❖ To mark selected compounds in a compounds table

1. Send compounds to the molecular networks viewer as described in "Send compounds to the molecular networks viewer."
2. Keep the compounds table open.
3. In the molecular networks viewer, do the following:
   a. Turn on the selection mode by clicking the **Selection Tool** icon, . Then, click the nodes that you want to select, one-by-one. Or, hold down the **SHIFT** key and drag mouse cursor across the nodes that you want to select.

   Note To deselect a single node, click it. To deselect multiple nodes, hold down the **CTRL+SHIFT** keys and drag the mouse cursor across all the selected nodes.

When you select a node it turns pink, and its molecular weight and retention time appear in the Selected Items pane.

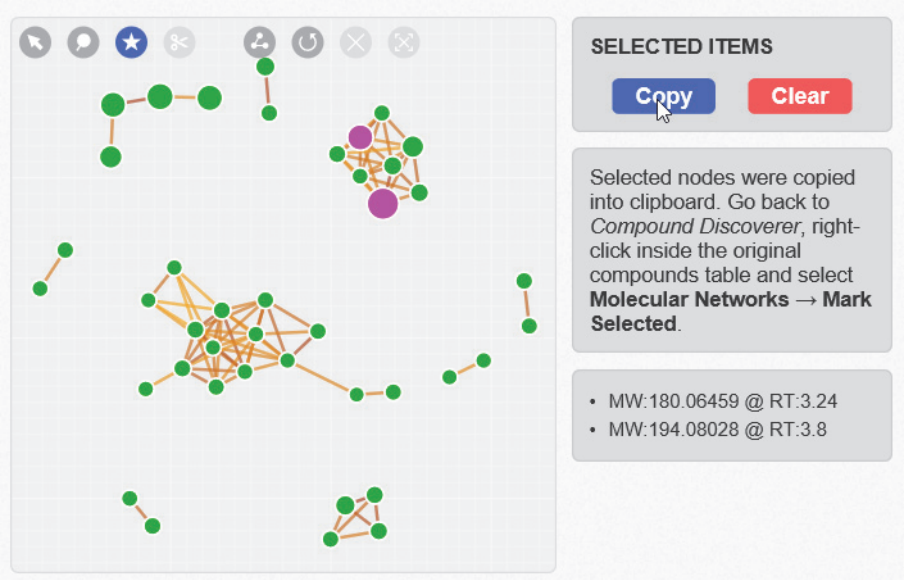
Figure 246. Molecular networks viewer with information about selected nodes in the Selected Items pane



b. Click **Copy**.

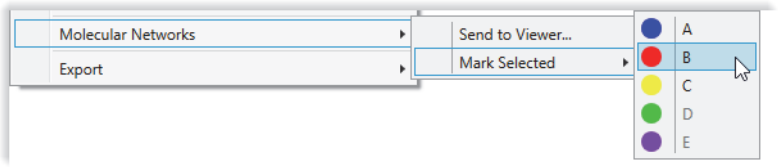
The viewer copies the list of selected compounds to the Clipboard and displays instructions about how to mark the selected compounds.

Figure 247. Instructions in the right pane about marking the compounds



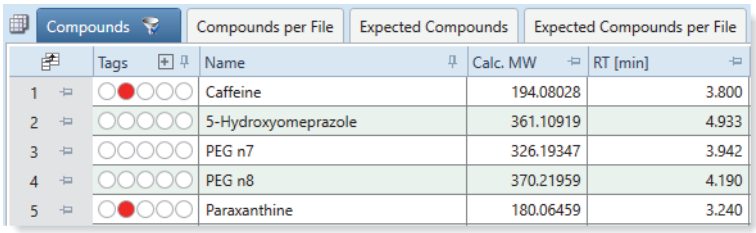
4. Right-click the Compounds table for LC studies and choose **Molecular Networks > Mark Selected > *one of the tags***.

Figure 248. Molecular Networks shortcut menu commands



The Compound Discoverer application marks the compounds in the result table that match the selected items list from the Clipboard with the selected tag.

Figure 249. Marked compounds in the Compounds table



	Tags	Name	Calc. MW	RT [min]
1		Caffeine	194.08028	3.800
2		5-Hydroxyomeprazole	361.10919	4.933
3		PEG n7	326.19347	3.942
4		PEG n8	370.21959	4.190
5		Paraxanthine	180.06459	3.240

Modify the simulation in the molecular networks viewer

Use the molecular networks viewer to visualize the similarity between compounds of interest and to tag compounds of interest in the compounds table.

Note For an LC study, you can visualize the similarity between the compounds in the Compounds table for an untargeted workflow.

When you send compounds from a Compounds table to the molecular networks viewer, the following occur:

1. The Compound Discoverer application sends the user-specified number of compounds to the viewer. The application sends only compounds that are visible in the table, it does not send compounds that are currently filtered out (with any of the result filters). In addition, it sends the compounds in order of their row numbers, which can vary depending on how you sort the table.
2. The viewer opens in a local browser window and displays the data in the current result file; it does not connect to the Internet. The viewer processes the data and displays an initial molecular network simulation using filter and threshold settings that you specified in the Generate Molecular Networks workflow node.

In the left pane of the viewer, you can change the settings for the filters and the thresholds, the node style, and the link style. In addition, you can search for a named compound or transformation and isolate the display to a specific cluster.

In the right pane of the viewer, you can view information for each node or link that you point to in the graph area.

The viewer has three independent modes—Move, Seek, or Selection. When the viewer is in one of the basic modes, you can turn the fourth mode—Isolation—on or off by double-clicking a node. By default, the viewer opens in the Move mode ( ) where you can move and rearrange the nodes.

For details, see these topics:

- Move, Seek, and Selection modes
- Use the Isolation mode to display specific clusters
- Use the Toggle Backbone tool to display the backbone of a cluster
- Color-coded nodes
- Change the node style to display a pie chart or a structure
- Size the nodes by peak area or MW of a compound
- Colorize a link by its score, coverage, or number of fragments
- Add directional arrows to the links
- Interactive functions performed by using the mouse pointer

Move, Seek, and Selection modes

The molecular networks viewer has three independent modes—Move, Seek, and Selection.

- Use the Move mode to move and rearrange the nodes.
- Use the Seek mode to reveal information about filtered links.
- Use the Selection mode to select individual nodes and add them to the export list where you can them to the Clipboard.

The functions in the left pane are available in all three modes.

Move mode

The molecular networks viewer opens to the Move mode ( ) for moving and rearranging the nodes.

Seek mode

When you turn on the Seek mode ( ), you can mark nodes as parent compounds. Then, view connection details in the right pane. A parent compound is the starting compound that undergoes chemical transformations.

❖ To view the connections for a parent node

1. Click the **Seek** icon,  , in the toolbar at the top left of the graph pane to turn on the Seek mode.

   The right pane changes to the Seek Links pane.

2. Click a node of interest in the graph pane.

   A red outline indicates the selected node. Information about the selected node appears in the Seek Links pane.

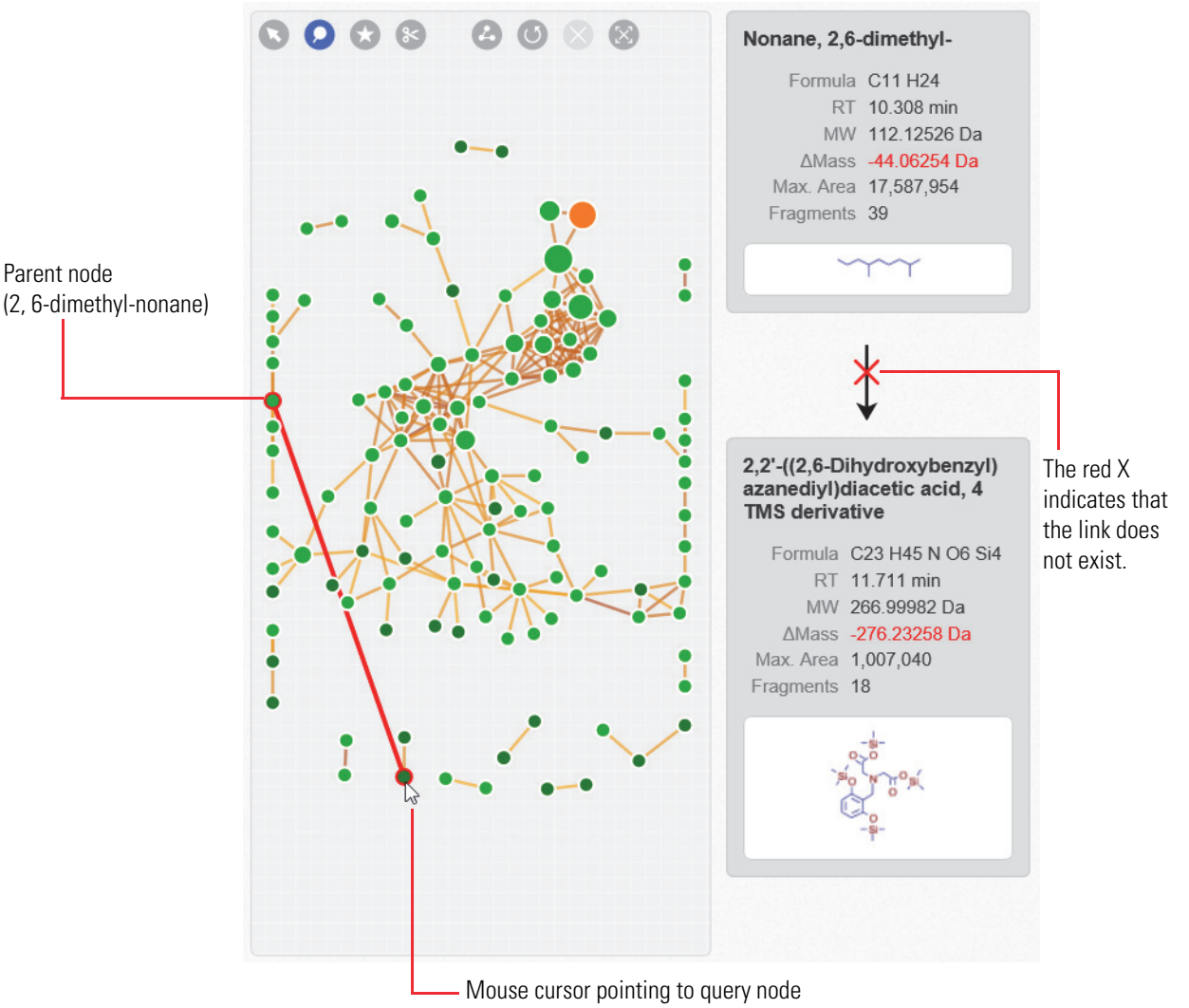
3. Point to another node in the graph pane.

   In the graph pane, a link appears between the parent node and the query node. If the two nodes are linked, the link is black. If the nodes are not linked, the link is red.

   A description of the query link appears in the Seek Links pane at the right.

   - If the compounds are related through a transformation reaction, the Seek Links pane describes the transformation with a black arrow showing the direction of the transformation.
   - If the compounds are not related through a transformation reaction, the Seek Links pane describes the nonexistent link between the two compounds with a red X over the black arrow.

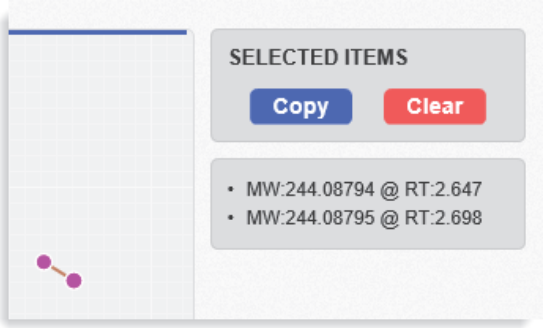
Figure 250. Seek mode showing a nonexistent link



Selection mode

When you turn on the Selection mode ( ), you can select individual nodes (compounds) and add them to the export list in the right pane of the view.

Table 217. Selection mode tasks

Task	Procedure
Turn on the Selection mode.	Click the **Selection** icon, , in the upper-left corner of the plot area.
Select nodes.	Turn on the Selection mode. Then, click the nodes, one by one. Or, hold down the SHIFT key and drag the mouse cursor across the nodes that you want to select. When you click a node, it turns pink, and its molecular weight and retention time appear in the Selected Items list. 
Copy selected nodes to the Clipboard.	In the Selected Items pane, click **Copy**.
Clear the export list.	In the Select Items pane, click **Clear**.
Deselect nodes.	Click each selected node one-by-one. Or, hold down the CTRL+SHIFT keys and drag the mouse cursor across the selected nodes. When you click a selected node, its color turns from pink to its original color and its molecular weight and retention time disappear from the selected items pane.

Use the Isolation mode to display specific clusters

Use the Isolation mode to display only the cluster of interest. The graph displays the connections to the selected node up to the maximum reaction depth that you specify under Isolation. See "Isolation pane."

❖ **To turn on the isolation mode to isolate a specific cluster**

1. Double-click the node of interest.
2. To exit the Isolation mode, double-click the orange node—that is, double-click the node that you clicked to enter the isolation mode.

Use the Toggle Backbone tool to display the backbone of a cluster

The backbone of a node cluster includes only the links with the highest confidence.

❖ **To view the backbones of the clusters in the molecular networks graph area**

Click the **Toggle Backbone** icon, , in the molecular networks toolbar.

Figure 251. Graph area with five clusters with more than two nodes

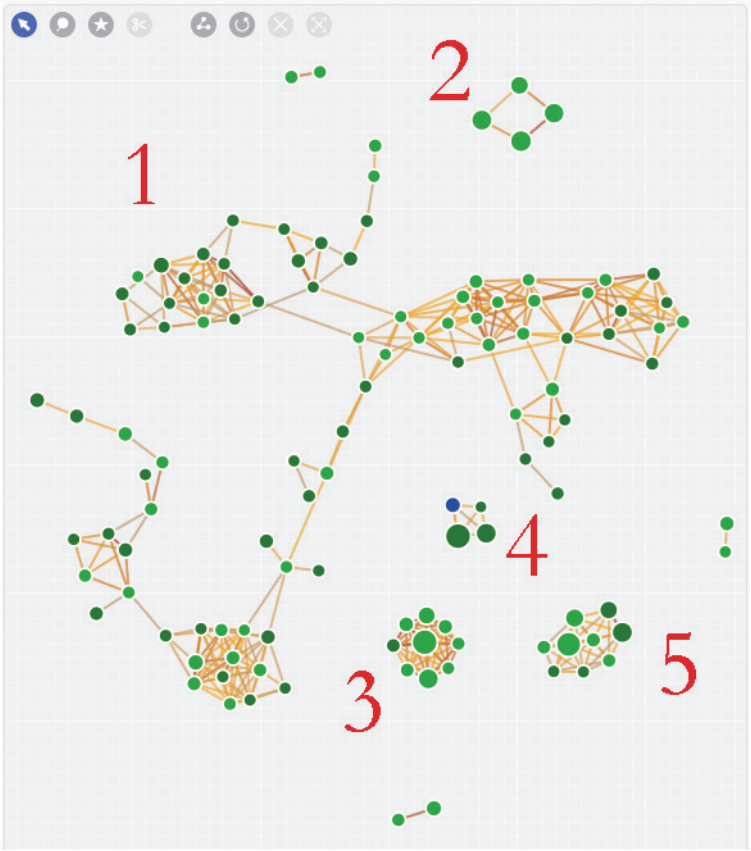
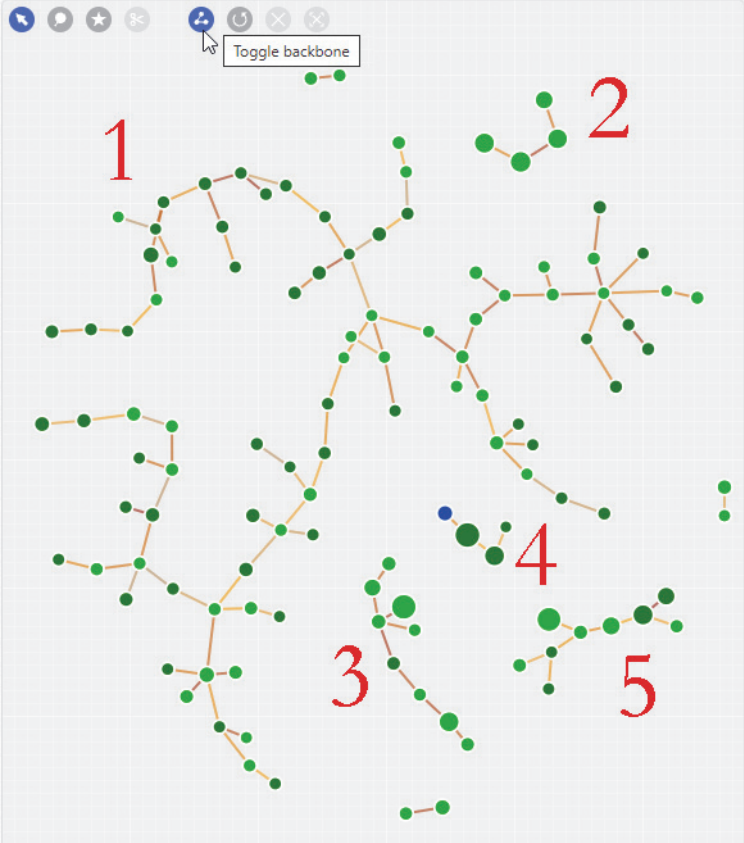


Figure 252. Backbone view



Color-coded nodes

In the molecular networks viewer, the identification status for a compound is indicated by the color of its node.

Table 218. Node colors for compounds in the Compounds table

Color	Meaning
Light green	The processing workflow identified the compound by its fragmentation spectra during an mzCloud or mzVault library search.
Dark green	The processing workflow identified the compound by its formula and a database match (but not an mzCloud match). The database match is from a mass list search or a ChemSpider search.
Blue	For LC/MS/MS data, the processing workflow determined only the formula of the compound.
Gray	The processing workflow determined only the mass of the compound or the mass of the compound does not match the formula annotation—that is, the difference between the formula annotation and the observed mass is greater than 5 ppm. This difference is highlighted by an orange background in the Annot. ΔMass column.

Figure 253 shows the molecular networks display for the 13 compounds in the Compounds table shown in Figure 254. Pointing to one of the gray nodes displays the information for the unknown compound.

Figure 253. Pointing to one of the gray nodes shows the information for the unknown compound without a formula

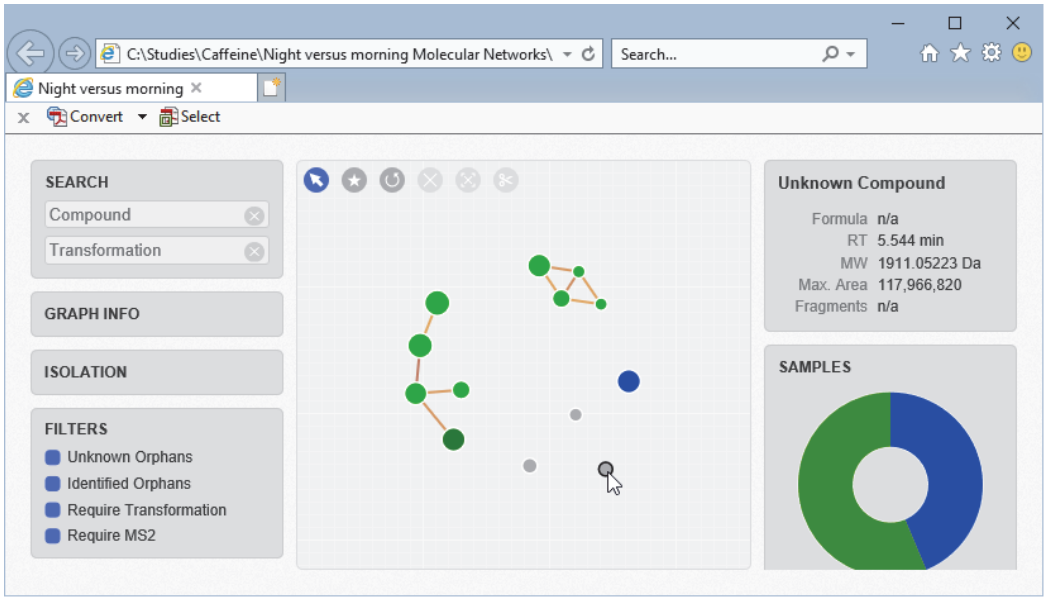
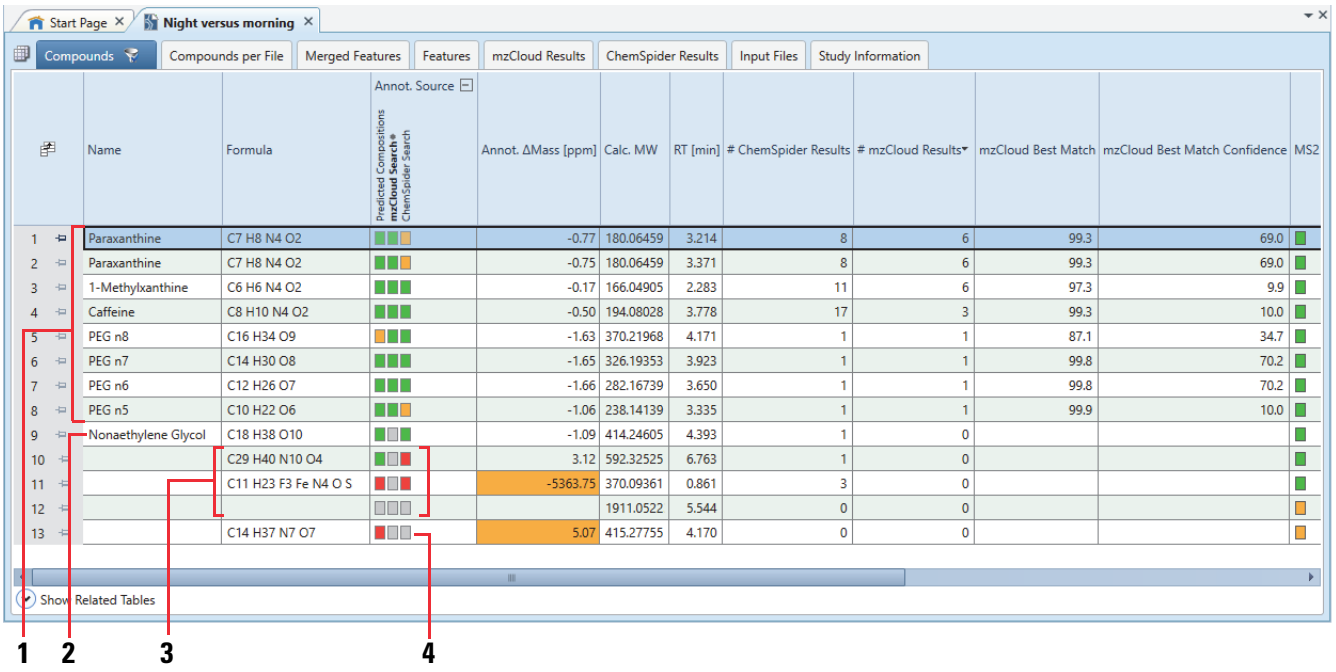


Figure 254 shows the Compounds table for the 13 compounds that were sent to the molecular networks viewer.

No.	Description
1	Light green nodes represent the eight compounds that are identified by name and formula and have mzCloud matches.
2	A dark green node represents the compound that is identified by formula and a ChemSpider database match but does not have any mzCloud matches.
3	A blue node represents the unknown compound that has a formula annotation but no database matches.
4	Gray nodes represent one compound that is identified only by its molecular weight and two compounds that are identified by formula and molecular weight, but the mass annotation for each of these compounds does not match the formula annotation (Annot. ΔMass > 5 ppm).

Figure 254. Compounds table with identified and unidentified compounds



Change the node style to display a pie chart or a structure

By default, the nodes appear as circles of different sizes depending on the confidence of the match. You can also select to display the nodes as pie charts or to show the structure of the compound they represent.

❖ To display each node as a pie chart

1. In the left pane of the molecular networks viewer, click **Node Style**.
2. Do one of the following:
   - Select the **Show Confidence** option.

     Each node appears as a solid circle. The color of the node reflects the confidence of the match.
   - Select the **Show Pie Charts** option.

     Each node appears as a pie chart of the relative areas of the compound in the study groups. The color of the node's border reflects the confidence of the match.
   - Select the **Show Structures** option.

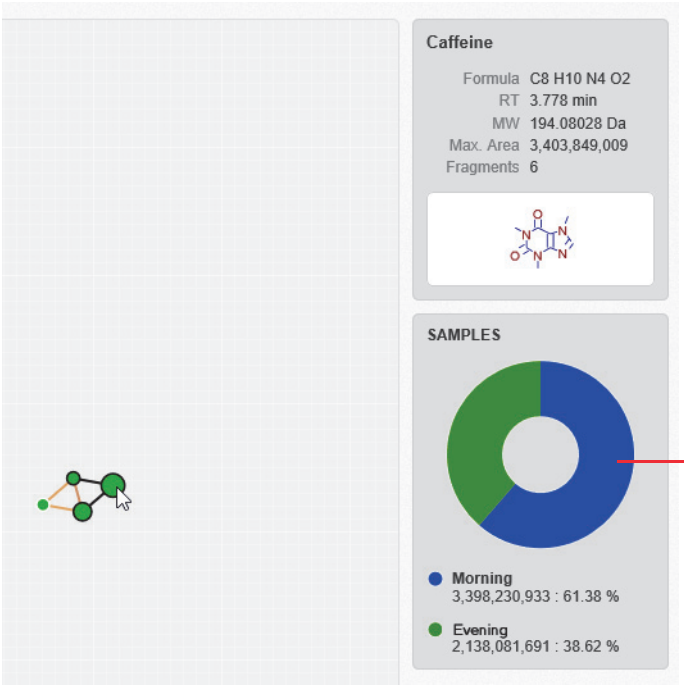
     Each node appears as a circle with a molecular weight, formula, or structure. The color of the node's border reflects the confidence of the match.

Regardless of the node style, pointing to a node displays the following information about the compound at the top of the right pane: name, formula, RT, maximum area (across the input files), and number of fragments in the fragmentation spectrum.

The bottom of the right pane displays a pie chart for the relative areas of the compound in the study groups or the separate input files when the analysis does not include study groups.

Figure 255 shows a pie chart for the relative areas for caffeine in samples collected from a human subject in the morning versus the evening.

Figure 255. Information displayed when you point to a node



Size the nodes by peak area or MW of a compound

In the molecular networks viewer, the node size is proportional to the Max. Area or MW of a compound, depending on the option that you select.

❖ **To select whether the node size is proportional to the compound's peak area or MW**

1. In the left pane of the molecular networks viewer, click **Node Style**.
2. Select one of these options: **By Area** or **By Mass**.

Colorize a link by its score, coverage, or number of fragments

The molecular networks viewer displays links in the following colors: gray > orange > dark-red. The link color is proportional to the MSn Score, the Forward or Reverse Coverage (max), or the number of Forward or Reverse Matches (max), depending on the option that you select. If a connection has no fragmentation data, the link appears as a dashed gray line.

❖ **To select a different option to colorize a link by**

1. In the left pane of the molecular networks viewer, click **Link Style**.
2. Select one of these options: **By Score**, **By Coverage**, or **By Fragments**.

Tip By default, the link color is a function of the MSn score. The length of each link has no meaning. To investigate the clusters, try colorizing the links by the other options.

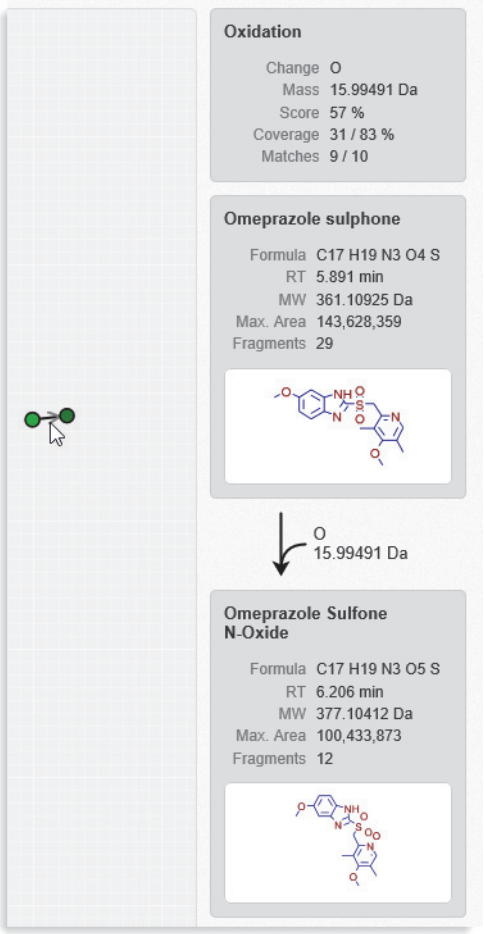
Add directional arrows to the links

By default, the connections between the nodes do not show the transformation direction.

❖ To add directional arrows to the links

1. In the left pane of the molecular networks viewer, click **Link Style**.
2. Click the **Show Arrows** check box.
3. To display the transformation in the right pane, point to the arrow.

Figure 256. Pointing to a directional arrow for a link



Interactive functions performed by using the mouse pointer

Table 219 describes the interactive tasks that you can perform with the mouse pointer in the molecular networks viewer.

Table 219. Interactive functions in the molecular networks viewer

Task	Procedure
Show information about a compound. (graph node)	Point to the compound. Information about the compound appears in the right pane, and all the compound's relations are highlighted in the graph area.
Show information about a graph link (relation).	Point to the link (connecting line). Information about the connection between the two compounds appears.

Molecular networks viewer toolbar

The toolbar at the top left of the graph pane includes eight tools.

Table 220. Molecular network viewer toolbar icons

Toolbar icon	Tooltip	Use
	Move Tool	Move and rearrange nodes.
	Seek Tool	Reveal missing connections between nodes.
	Selection Tool	Add nodes to the export list.
	Toggle Isolation	Isolate a node.
	Toggle Backbone	Display the backbone node connections in a cluster. The backbone node connections in a cluster are the connections with the highest confidence.
	Restart Simulation	Restart the simulation in the graph area of the molecular network viewer.
	Stop Simulation	Stop the simulation while it is processing.
	Reset Pan and Zoom	Reset, pan, and zoom in the graph area.

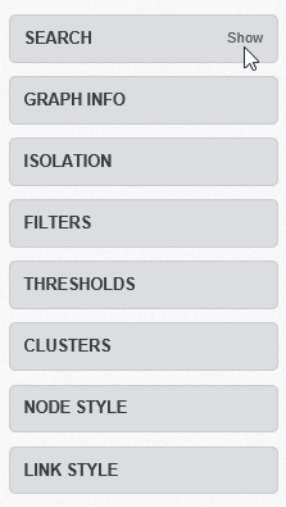
Panes at the left of the molecular networks viewer

The molecular networks viewer has the following panes to the left of the graphical display:

- Search pane
- Graph Info pane
- Isolation pane
- Filters pane
- Thresholds pane
- Clusters pane
- Node Style pane
- Link Style pane

Tip To open or close a pane, point to the upper-right corner of the pane to display the Hide text or the Show text. When text appears, click it.

Figure 257. Dropdown panes to the left of the graphical display



Search pane

Use the Search pane of the molecular networks viewer to highlight nodes or links in the graph area by searching for the name of a compound or the name of a transformation, respectively.

Task	Procedure
Highlight nodes, in red, for compounds with a specified text string in their names.	In the Search pane, type the compound's name in the Compound box. The viewer highlights all compounds with the specified text string in the graph area.
Highlight links, in red, for the same named transformation.	In the Search pane, type the transformation's name in the Transformation box.

Graph Info pane

The Graph Info pane of the molecular networks viewer provides a visual summary about the compounds that you exported from the compounds table of a result file.

The two bar colors and the background color behind the bars represent the following:

- Blue bar—represents the relative portion of the currently visible items.
- Dark gray bar—represents the relative portion of all items of a particular type.
- Light-gray background—represents the total number of items.

Figure 258. Graph Info pane of the molecular networks viewer

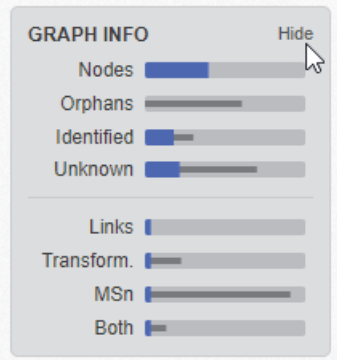


Table 221. Graph Info pane of the molecular networks viewer (Sheet 1 of 2)

Parameter	Description
Nodes	Indicates the number of nodes in the graph area.
Orphans	Indicates the number of nodes without any connection (according to the current filters and thresholds).
Identified	Indicates the number of compounds with an assigned name.

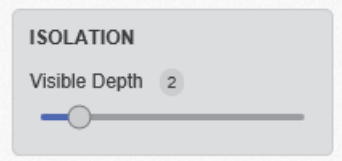
Table 221. Graph Info pane of the molecular networks viewer (Sheet 2 of 2)

Parameter	Description
Unknown	Indicates the number of compounds without an assigned name.
Links	Indicates the number of all connections.
Transform.	Indicates the number of connections with assigned transformations.
MSn	Indicates the number of connections with fragmentation data.
Both	Indicates the number of connections with assigned transformations and fragmentation data.

Isolation pane

If the main graph is in the Isolation mode, the Isolation pane of the molecular networks viewer provides dynamic control over the maximum depth of the graph.

Figure 259. Isolation pane of the molecular networks viewer



For information about turning on the Isolation mode, see "Use the Isolation mode to display specific clusters."

Filters pane

Use the filters in the Filters pane of the molecular networks viewer to limit the amount of visible data.

Figure 260. Filters pane of the molecular networks viewer (default settings)

Table 222. Filters pane of the molecular networks viewer

Filter	Description
Unknown Orphans	Select to display compounds without a name or connection. Default: Not enabled
Identified Orphans	Select to display named compounds without a connection. Default: Not enabled
Require Transformation	Clear to display links without assigned transformations. Default: Enabled
Require MSn	Clear to display links without fragmentation data. Default: Enabled

Thresholds pane

To show or hide low confidence relationships between compounds in the molecular networks viewer, adjust the settings in the Thresholds pane. By default, the thresholds are set to those specified in the processing workflow.

Figure 261. Thresholds pane of the molecular networks viewer

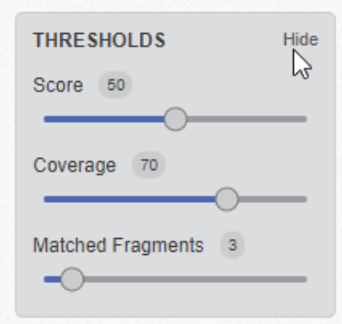


Table 223. Thresholds pane in the molecular networks viewer

Threshold	Description
Score	Specifies the minimum MSn Score for a connection to be visible. Range: 0 to 100
Coverage	Specifies the minimum Forward or Reverse Coverage for a connection to be visible. Range: 0 to 100
Matched Fragments	Specifies the minimum number of matched fragments for a Forward or Reverse search for a connection to be visible. Minimum: 0

Clusters pane

Use the Clusters pane to limit the number of nodes per cluster. The viewer applies the Node Links limit first and then applies the Cluster size limit. By default, the thresholds are set to those specified in the processing workflow.

Figure 262. Clusters pane of the molecular networks viewer

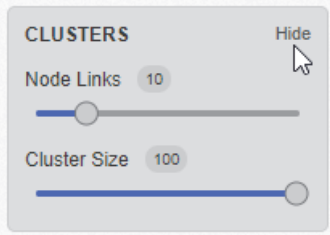


Table 224. Clusters pane in the molecular networks viewer

Threshold	Description
Node Links	Specifies the maximum number of connections for a single node, which limits the number of direct neighbors for each node. Range: 1 to 50
Cluster Size	Specifies the maximum number of nodes within a single cluster. As you reduce the cluster size, the algorithm excludes nodes connected by links with lower scores. Reducing the cluster size to 2 reduces the number of nodes per cluster to two nodes with one shared link. Range: 2 to 100

Node Style pane

Use the Node Style pane to specify what determines the size of the node and whether to display each node as a pie chart or a single color.

You can select either Show Confidence or Show Pie Charts and either Size by Area or Size by Mass.

Figure 263. Node Style pane of the molecular networks viewer

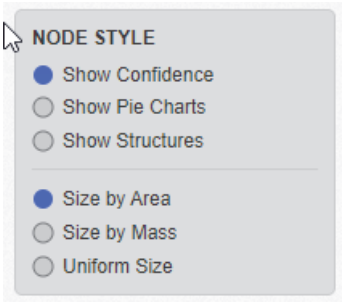


Table 225. Node Style pane in the molecular networks viewer

Option	Description
Show Confidence	Displays each node as a solid color according to the confidence of the identification. A matching spectrum in the mzCloud mass spectral database provides the most confidence.
Show Pie Charts	Displays each node as a pie chart of the relative areas of the compound in each input file or each study group.
Show Structures	Displays a structure when available on the node.
Size by Area	Sizes each node according to the maximum area of the compound relative to the other compounds.
Size by Mass	Sizes each node according to the molecular weight of the compound relative to the other compounds.
Uniform Size	Displays all the nodes at a uniform size.

Link Style pane

Use the Link Style pane to specify whether the connectors between the nodes display the transformation direction and what determines the color of each connector.

Figure 264. Link Style pane of the molecular networks viewer

Table 226. Node Style pane in the molecular networks viewer

Option	Description
Show Arrows	Selecting this option turns on directional arrows for the connectors.
Select the option that determines the color of each link. The molecular networks viewer displays links in the following colors: gray > orange > dark-red. If a connection has no fragmentation data, the link appears as a gray-dashed line.	
Color by Score	The link color is proportional to the MSn Score.
Color by Coverage	The link color is proportional to the Forward or Reverse Coverage (max).
Color by Fragments	The link color is proportional to the number of Forward or Reverse Matches (max).

Pane at the right of the molecular networks viewer

When you point to a link or node in the molecular networks viewer, information appears on the right side of the viewer. For a link, the information pane displays the assigned pathway name, elemental composition, mass difference, and fragmentation scores, followed by the reaction from one compound to the other. For each compound, it shows the assigned name, elemental composition, retention time, molecular weight, maximum area, and number of used fragments.

The information automatically disappears from the right pane when you move the pointer away from the node or link.

Tip To prevent the information about the selected node or link from disappearing or changing when you move the mouse pointer, hold the SHIFT key while you move the pointer.

When the molecular networks view is in the Selection mode and you are not pointing to a node or connector, the Selected Items pane appears to the right of the graphical display. For details about creating a list of compounds to mark, see "Mark selected compounds in the main compounds table."

Test communication to the online databases

A typical Compound Discoverer analysis that identifies unknown compounds searches mass spectrum databases on the Internet. To run these searches, the application must have unblocked access to the mass spectral databases on the Internet.

The following topics describe how to test and troubleshoot the application's access to the online mass spectrum databases:

- Troubleshoot access to the online databases
- Run the communication tests
- Check the URLs for the online databases in your browser
- Specify the IP address of the proxy server
- Set the correct time and time zone on the processing computer

Troubleshoot access to the online databases

❖ **To test and troubleshoot the application's access to the online databases**

1. Run the communication tests. See "Run the communication tests."

   If the communication tests succeed, the application has access to the online databases.

2. If a communication test fails, do the following:

   - If only the mzCloud communication test fails, check the Date and Time settings on the processing computer. See "Set the correct time and time zone on the processing computer."
   - If the Check BioCyc user credentials test for the BioCyc database fails, check the subscription information in the BioCyc User Login view of the Configuration page.

     IMPORTANT If you do not have an organization subscription for the BioCyc database, you must create a BioCyc user account or obtain an individual subscription, and then enter, test, and save your account credentials in the BioCyc User Login view. See "Set up a BioCyc account and optionally purchase a subscription."

- If any of the other communication tests also fail, check the access to the URLs for the online databases. See "Check the URLs for the online databases in your browser."

  If you can access the URLs for the online databases through your browser, but the communication tests still fail, the firewall or proxy setting for your company network is blocking the application's access to the online databases.

3. If the communication tests fail, but you can access the URLs for the online databases, do the following as applicable:

   - If a firewall is blocking the application's access to the online databases, ask your IT department to make sure that the company firewall is not blocking "Thermo Compound Discoverer" or "Thermo Compound Discoverer Server" from accessing the URLs. The application uses the following protocol: http port 80.
   - If a proxy setting is blocking access, see "Specify the IP address of the proxy server."

Run the communication tests

Use the Communication Tests dialog box to test your processing computer's access to the online databases.

❖ **To verify that your computer has access to the external databases**

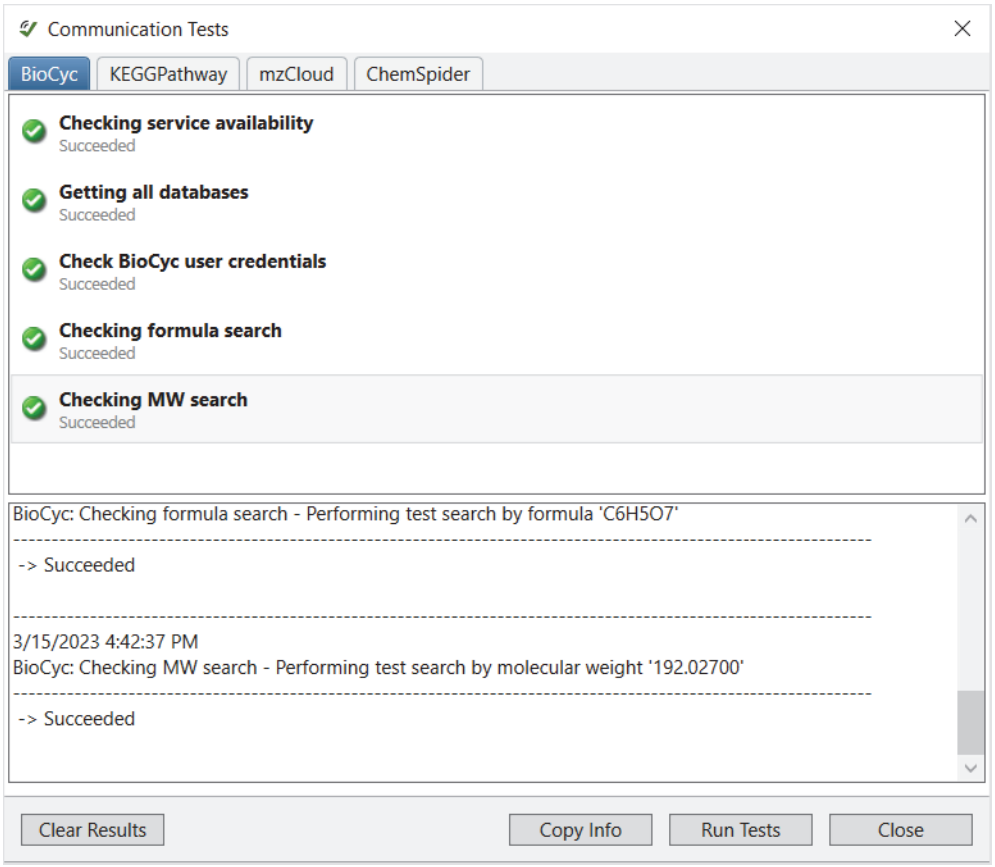
1. From the menu bar, choose **Help > Communication Tests**.

   The Communication Tests dialog box opens.

2. To open the page for the database that you want to access, click its tab.
3. Click **Run Tests**.

   Figure 265 shows the communication tests in progress.

Figure 265. BioCyc communication tests



4. Depending on whether the communication tests are successful, do the following:

   - If the tests are successful, your computer has access to the required databases on the Internet and you can run analyses that require access to these databases.
   - If only the mzCloud test fails, check the Date and Time settings for the processing computer. See "Set the correct time and time zone on the processing computer."
   - If any of the other tests also fail, check the access to the URLs in your browser. See "Check the URLs for the online databases in your browser."

Check the URLs for the online databases in your browser

Table 227 lists the URLs for the online mass spectrum databases. If a communication test fails, test the URL for the affected database.

Table 227. URLs of online mass spectrum databases

Database	URL
mzCloud Identity	https://www.mzcloud.org/
	https://identity.mzcloud.org/
	https://www.mzcloud.org/Services/MzCloudApiV1.svc
	https://www.mzcloud.org/Services/MzCloudApiLightService.svc
ChemSpider	http://www.chemspider.com
	http://api.rsc.org/
KEGG: Kyoto Encyclopedia of Genes and Genomes	http://www.kegg.jp/
	http://rest.kegg.jp
	https://proxy.online-licensing.net
BioCyc	https://biocyc.org/
	https://biocyc.org/web-services.shtml
	https://tf.biocy.org

Specify the IP address of the proxy server

If the communication tests fail but you can access the online databases through your browser, follow this procedure to specify the IP address of the proxy server.

❖ **To configure the IP address of the proxy server**

1. Go to *drive*:\Program Files\Thermo\Compound Discoverer 3.3\bin\Config.
2. Open the **Proxy.config** file in Notepad.
3. Remove the text that is highlighted in yellow in Figure 266—that is, remove the XML comment delimiters: <!-- and -->.

Figure 266. Proxy configuration setting with XML comment delimiters

4. Replace the text that is highlighted in yellow in Figure 267 with your company proxy address.

Figure 267. Default proxy address highlighted in yellow

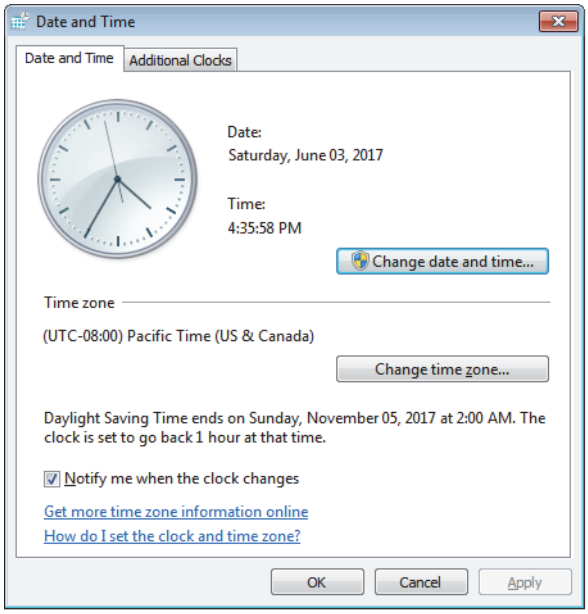
```
1  <?xml version="1.0" encoding="utf-8" ?>
2  <defaultProxy enabled="true">
3    <proxy bypassonlocal="true" proxyaddress=
     "http://127.0.0.1:8118/" />
4  </defaultProxy>
```

Set the correct time and time zone on the processing computer

The mzCloud communication test includes a validation of the date and time settings on the processing computer. If the mzCloud communication test fails, but the other communication tests succeed, check the date and time settings for the processing computer.

❖ To check the time and time zone settings

1. Open the **Date and Time** dialog box or view by typing **Date** in the Windows search box.



2. Make sure that both the date and time and time zone settings are correct.

> **Tip** If your computer is not part of a network domain that synchronizes the computer's clock to the network server, you can use an Internet server to synchronize the computer's clock.

3. If the Internet Time tab is available, click it and synchronize the computer's clock with an Internet server.

A

Experiment design for comparison statistics

To understand how and when to use the biological replicate study factor, see these topics:

- Biological versus technical replicates
- Non-Nested versus nested experiment designs

Biological versus technical replicates

Biological replicates are samples from biological individuals (or non-biological entities) of the same type under the same conditions and provide a measure of the variability associated with these conditions.

Technical replicates are replicate samples from the same entity under the same conditions. Technical replicates from the same entity under the same conditions provide a measure of the sampling error, and replicate injections from the same sample solution provide a measure of the instrument error.

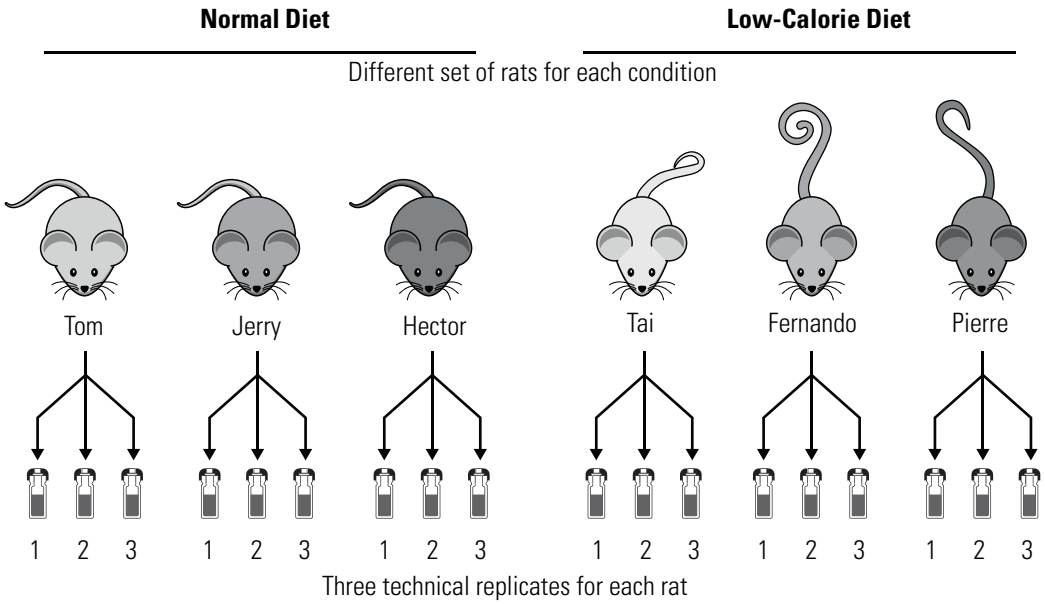
You can add only one biological replicate factor to a study. The application treats study factors nested under a biological replicate factor as technical replicates.

Non-Nested versus nested experiment designs

When you add a biological replicate factor to study, you can set up two different experiment designs—nested and non-nested. In non-nested experiments, the biological replicates are independent of each other—that is, you do not reuse individual entities to study multiple condition states (study factor items).

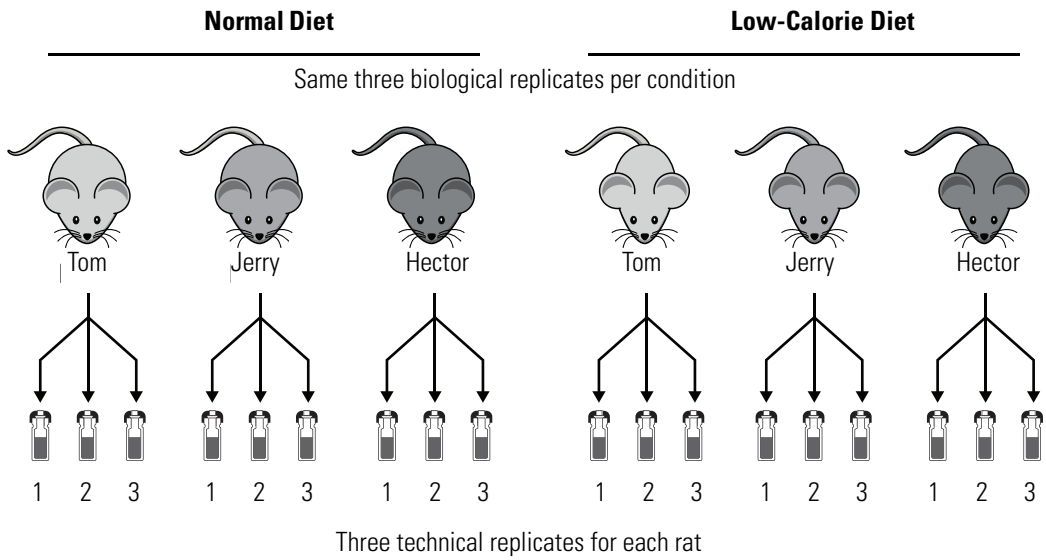
In non-nested experiments, different sets of biological replicates are used for each condition. Figure 268 shows a non-nested experiment where replicate samples are taken from two sets of rats under two conditions. Tom, Jerry, and Hector are fed a normal diet; and Tai, Fernando, and Pierre are fed a low-calorie diet.

Figure 268. Non-nested design with independent sets of rats for the two dietary conditions



In nested experiments, the same set of biological replicates are used for each condition. Figure 269 shows a nested experiment where replicate samples are taken from the same three rats under two conditions—a normal diet and a low-calorie diet. Tom, Jerry, and Pierre are the biological replicates.

Figure 269. Nested design with the same three rats under two dietary conditions



To set up the comparison ratios for a nested design with technical replicates, add the following study factors:

- A factor for the variable being studied with an itemized list of the variable states
- A biological replicate factor with an itemized list of the entities being studied
- (Optional) A factor for the technical replicates

Figure 270 shows the study factors for the experiment shown in Figure 269.

Figure 270. Study factors for the nested design experiment

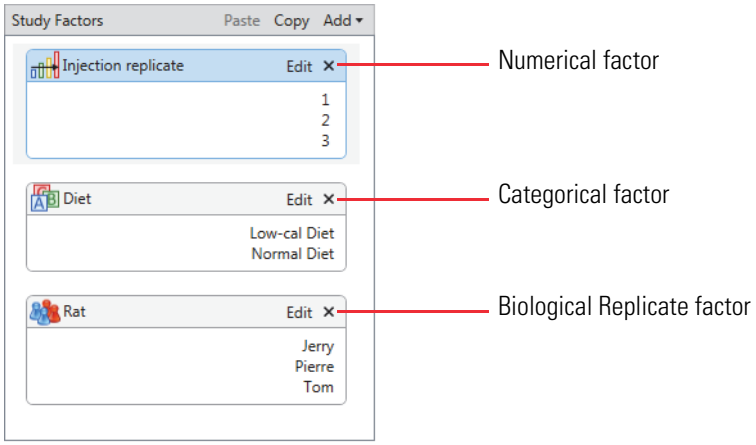
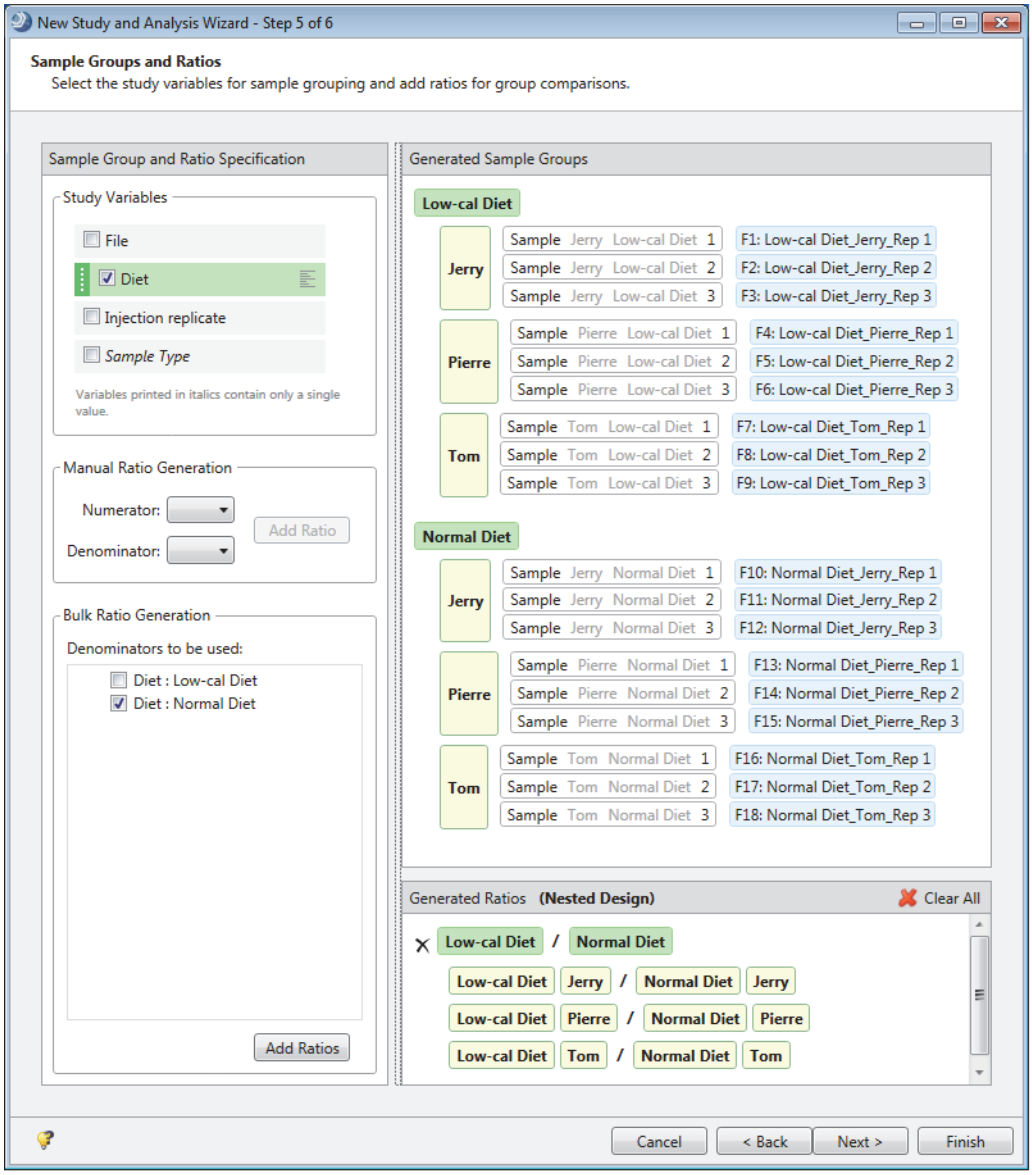


Figure 271 shows the generated sample groups and ratios for the nested design. The sample groups—Low-cal Diet and Normal Diet—are highlighted in green. The two sample groups contain the same values for the Rat Biological Replicate factor—Tom, Jerry, and Pierre. The technical replicates for each biological replicate are grouped together and the biological replicates are highlighted in yellow. As shown in the Generated Ratios area, for each selected denominator, the Differential Analysis node calculates one group ratio and individual ratios for each biological replicate. In the result file, the Compounds table includes a Ratio column for the group ratio and Bio. Rep. Ratio columns for the biological replicate ratios.

Note The application calculates p-values as follows:

- Uses the t-test when comparing two sample groups.
- Uses ANOVA when comparing more than two sample groups.

Figure 271. Nested design example



Index

A

B

C

D

E

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

T

U

V

W

X

Y

Z